Entering Gaussian System, Link 0=/opt/gaussian/g09/g09
Initial command:
/opt/gaussian/g09/l1.exe "/tmp/Gau-7246.inp" -scrdir="/tmp/"
Entering Link 1 = /opt/gaussian/g09/l1.exe PID= 7247.

assistance to any competitor of Gaussian, Inc. The licensee
of this program is prohibited from giving any competitor of
Gaussian, Inc. access to this program. By using this program,
the user acknowledges that Gaussian, Inc. is engaged in the
business of creating and licensing software in the field of
computational chemistry and represents and warrants to the
licensee that it is not a competitor of Gaussian, Inc. and that
it will not use this program in any manner prohibited above.

Cite this work as:
Gaussian 09, Revision D.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci,
G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian,
A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada,
M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima,
Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr.,
J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers,
K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand,
K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi,
M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross,
V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,
O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,
R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth,
P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels,
O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski,
and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

****
Gaussian 09: EM64L-G09RevD.01 24-Apr-2013
25-Jul-2024
****
%chk=/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk
%mem=1000MB
%nprocl=1
Will use up to 1 processors via Linda.
%nprocs=8
Will use up to 8 processors via shared memory.
---
opt b3lyp/6-311++g(d,p)

1/14=-1,18=20,19=15,26=3,38=1/1,3;

2/9=110,12=2,17=6,18=5,40=1/2;
3/5=4,6=6,7=1111,11=2,16=1,25=1,30=1,71=1,74=-5/1,2,3;
4//1;
5/5=2,38=5/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(2);
2/9=110/2;
99//99;
2/9=110/2;
3/5=4,6=6,7=1111,11=2,16=1,25=1,30=1,71=1,74=-5/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;
--
oh
--
Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-2.91419	2.12334	-0.2483
C	-3.85466	1.19291	0.05692
N	-3.20378	-0.03601	0.10333
C	-1.8988	0.15629	-0.16611
N	-1.70404	1.46193	-0.38739
C	-0.39101	2.08624	-0.67358
C	0.29263	2.65867	0.572
H	-3.00293	3.18709	-0.38792
H	-4.90946	1.30057	0.2336
H	0.23352	1.30737	-1.11469
H	-0.54793	2.8712	-1.4148
H	-0.31528	3.47456	0.97603
H	0.3334	1.86621	1.33419
Br	0.40516	-2.15891	-0.25456
H	-1.11029	-0.63607	-0.19638
C	-3.73494	-1.32414	0.39304
C	-5.00632	-1.55933	0.68646
H	-2.97118	-2.09322	0.35453
H	-5.31826	-2.57213	0.89926
H	-5.76501	-0.78758	0.72962
N	1.59467	3.18771	0.17116

H	1.97543	3.79681	0.88553
H	2.25701	2.42642	0.0289
C	3.87516	-0.19996	-1.05837
C	3.86857	-0.40772	0.39187
O	3.59583	0.90215	-0.16751
H	4.82215	-0.11736	-1.58739
H	3.02604	-0.55433	-1.63527
H	2.98013	-0.89124	0.7922
C	5.13104	-0.53056	1.19865
H	4.99796	-0.09798	2.19481
H	5.39202	-1.58587	1.32476
H	5.96245	-0.0197	0.70765

Add virtual bond connecting atoms O26 and H23 Dist= 3.85D+00.
Add virtual bond connecting atoms H15 and Br14 Dist= 4.06D+00.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.

! Initial Parameters !
! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.	!
! R1	R(1,2)	1.3577	estimate D2E/DX2	!
! R2	R(1,5)	1.3861	estimate D2E/DX2	!
! R3	R(1,8)	1.0765	estimate D2E/DX2	!
! R4	R(2,3)	1.3914	estimate D2E/DX2	!
! R5	R(2,9)	1.0749	estimate D2E/DX2	!
! R6	R(3,4)	1.3463	estimate D2E/DX2	!
! R7	R(3,16)	1.4231	estimate D2E/DX2	!
! R8	R(4,5)	1.3385	estimate D2E/DX2	!
! R9	R(4,15)	1.1183	estimate D2E/DX2	!
! R10	R(5,6)	1.4818	estimate D2E/DX2	!
! R11	R(6,7)	1.5318	estimate D2E/DX2	!
! R12	R(6,10)	1.0915	estimate D2E/DX2	!
! R13	R(6,11)	1.091	estimate D2E/DX2	!
! R14	R(7,12)	1.0947	estimate D2E/DX2	!
! R15	R(7,13)	1.1003	estimate D2E/DX2	!
! R16	R(7,21)	1.4615	estimate D2E/DX2	!
! R17	R(14,15)	2.1492	estimate D2E/DX2	!
! R18	R(16,17)	1.3258	estimate D2E/DX2	!
! R19	R(16,18)	1.0846	estimate D2E/DX2	!

! R20	R(17,19)	1.0809	estimate D2E/DX2	!
! R21	R(17,20)	1.0831	estimate D2E/DX2	!
! R22	R(21,22)	1.0131	estimate D2E/DX2	!
! R23	R(21,23)	1.0191	estimate D2E/DX2	!
! R24	R(23,26)	2.0382	estimate D2E/DX2	!
! R25	R(24,25)	1.4651	estimate D2E/DX2	!
! R26	R(24,26)	1.4444	estimate D2E/DX2	!
! R27	R(24,27)	1.0879	estimate D2E/DX2	!
! R28	R(24,28)	1.086	estimate D2E/DX2	!
! R29	R(25,26)	1.4502	estimate D2E/DX2	!
! R30	R(25,29)	1.0878	estimate D2E/DX2	!
! R31	R(25,30)	1.5033	estimate D2E/DX2	!
! R32	R(30,31)	1.0942	estimate D2E/DX2	!
! R33	R(30,32)	1.0944	estimate D2E/DX2	!
! R34	R(30,33)	1.0924	estimate D2E/DX2	!
! A1	A(2,1,5)	107.4764	estimate D2E/DX2	!
! A2	A(2,1,8)	130.4828	estimate D2E/DX2	!
! A3	A(5,1,8)	122.0364	estimate D2E/DX2	!
! A4	A(1,2,3)	106.7822	estimate D2E/DX2	!
! A5	A(1,2,9)	130.3946	estimate D2E/DX2	!
! A6	A(3,2,9)	122.8214	estimate D2E/DX2	!
! A7	A(2,3,4)	108.6988	estimate D2E/DX2	!
! A8	A(2,3,16)	129.1699	estimate D2E/DX2	!
! A9	A(4,3,16)	122.127	estimate D2E/DX2	!
! A10	A(3,4,5)	108.2678	estimate D2E/DX2	!
! A11	A(3,4,15)	125.993	estimate D2E/DX2	!
! A12	A(5,4,15)	125.7388	estimate D2E/DX2	!
! A13	A(1,5,4)	108.7737	estimate D2E/DX2	!
! A14	A(1,5,6)	126.296	estimate D2E/DX2	!
! A15	A(4,5,6)	124.8792	estimate D2E/DX2	!
! A16	A(5,6,7)	113.3195	estimate D2E/DX2	!
! A17	A(5,6,10)	106.5243	estimate D2E/DX2	!
! A18	A(5,6,11)	107.8737	estimate D2E/DX2	!
! A19	A(7,6,10)	109.8726	estimate D2E/DX2	!
! A20	A(7,6,11)	110.3514	estimate D2E/DX2	!
! A21	A(10,6,11)	108.7338	estimate D2E/DX2	!
! A22	A(6,7,12)	109.3158	estimate D2E/DX2	!
! A23	A(6,7,13)	108.0997	estimate D2E/DX2	!
! A24	A(6,7,21)	108.0509	estimate D2E/DX2	!
! A25	A(12,7,13)	107.5591	estimate D2E/DX2	!
! A26	A(12,7,21)	109.0362	estimate D2E/DX2	!
! A27	A(13,7,21)	114.6902	estimate D2E/DX2	!
! A28	A(3,16,17)	124.2993	estimate D2E/DX2	!
! A29	A(3,16,18)	111.8256	estimate D2E/DX2	!

! A30	A(17,16,18)	123.8726	estimate D2E/DX2	!
! A31	A(16,17,19)	119.1122	estimate D2E/DX2	!
! A32	A(16,17,20)	123.6512	estimate D2E/DX2	!
! A33	A(19,17,20)	117.2365	estimate D2E/DX2	!
! A34	A(7,21,22)	111.0438	estimate D2E/DX2	!
! A35	A(7,21,23)	110.2983	estimate D2E/DX2	!
! A36	A(22,21,23)	107.6569	estimate D2E/DX2	!
! A37	A(25,24,27)	119.7389	estimate D2E/DX2	!
! A38	A(25,24,28)	118.4277	estimate D2E/DX2	!
! A39	A(26,24,27)	114.2259	estimate D2E/DX2	!
! A40	A(26,24,28)	115.1767	estimate D2E/DX2	!
! A41	A(27,24,28)	116.556	estimate D2E/DX2	!
! A42	A(24,25,29)	115.5303	estimate D2E/DX2	!
! A43	A(24,25,30)	122.6202	estimate D2E/DX2	!
! A44	A(26,25,29)	112.9435	estimate D2E/DX2	!
! A45	A(26,25,30)	116.0254	estimate D2E/DX2	!
! A46	A(29,25,30)	116.8758	estimate D2E/DX2	!
! A47	A(23,26,24)	139.2071	estimate D2E/DX2	!
! A48	A(23,26,25)	139.6265	estimate D2E/DX2	!
! A49	A(25,30,31)	110.7426	estimate D2E/DX2	!
! A50	A(25,30,32)	109.9324	estimate D2E/DX2	!
! A51	A(25,30,33)	111.0846	estimate D2E/DX2	!
! A52	A(31,30,32)	107.7776	estimate D2E/DX2	!
! A53	A(31,30,33)	108.4757	estimate D2E/DX2	!
! A54	A(32,30,33)	108.7384	estimate D2E/DX2	!
! A55	L(4,15,14,7,-1)	180.0	estimate D2E/DX2	!
! A56	L(21,23,26,3,-1)	180.3258	estimate D2E/DX2	!
! A57	L(4,15,14,7,-2)	180.0	estimate D2E/DX2	!
! A58	L(21,23,26,3,-2)	182.599	estimate D2E/DX2	!
! D1	D(5,1,2,3)	0.086	estimate D2E/DX2	!
! D2	D(5,1,2,9)	-179.4183	estimate D2E/DX2	!
! D3	D(8,1,2,3)	179.3187	estimate D2E/DX2	!
! D4	D(8,1,2,9)	-0.1856	estimate D2E/DX2	!
! D5	D(2,1,5,4)	-0.2719	estimate D2E/DX2	!
! D6	D(2,1,5,6)	-177.7639	estimate D2E/DX2	!
! D7	D(8,1,5,4)	-179.5834	estimate D2E/DX2	!
! D8	D(8,1,5,6)	2.9246	estimate D2E/DX2	!
! D9	D(1,2,3,4)	0.1276	estimate D2E/DX2	!
! D10	D(1,2,3,16)	179.3723	estimate D2E/DX2	!
! D11	D(9,2,3,4)	179.6784	estimate D2E/DX2	!
! D12	D(9,2,3,16)	-1.0769	estimate D2E/DX2	!
! D13	D(2,3,4,5)	-0.2983	estimate D2E/DX2	!
! D14	D(2,3,4,15)	179.4728	estimate D2E/DX2	!
! D15	D(16,3,4,5)	-179.6069	estimate D2E/DX2	!

! D16	D(16,3,4,15)	0.1642	estimate D2E/DX2	!
! D17	D(2,3,16,17)	-0.3663	estimate D2E/DX2	!
! D18	D(2,3,16,18)	-179.8204	estimate D2E/DX2	!
! D19	D(4,3,16,17)	178.789	estimate D2E/DX2	!
! D20	D(4,3,16,18)	-0.6651	estimate D2E/DX2	!
! D21	D(3,4,5,1)	0.3523	estimate D2E/DX2	!
! D22	D(3,4,5,6)	177.8884	estimate D2E/DX2	!
! D23	D(15,4,5,1)	-179.4195	estimate D2E/DX2	!
! D24	D(15,4,5,6)	-1.8835	estimate D2E/DX2	!
! D25	D(1,5,6,7)	81.8758	estimate D2E/DX2	!
! D26	D(1,5,6,10)	-157.1934	estimate D2E/DX2	!
! D27	D(1,5,6,11)	-40.5992	estimate D2E/DX2	!
! D28	D(4,5,6,7)	-95.2293	estimate D2E/DX2	!
! D29	D(4,5,6,10)	25.7014	estimate D2E/DX2	!
! D30	D(4,5,6,11)	142.2957	estimate D2E/DX2	!
! D31	D(5,6,7,12)	-63.9732	estimate D2E/DX2	!
! D32	D(5,6,7,13)	52.8274	estimate D2E/DX2	!
! D33	D(5,6,7,21)	177.4888	estimate D2E/DX2	!
! D34	D(10,6,7,12)	177.0048	estimate D2E/DX2	!
! D35	D(10,6,7,13)	-66.1945	estimate D2E/DX2	!
! D36	D(10,6,7,21)	58.4669	estimate D2E/DX2	!
! D37	D(11,6,7,12)	57.116	estimate D2E/DX2	!
! D38	D(11,6,7,13)	173.9166	estimate D2E/DX2	!
! D39	D(11,6,7,21)	-61.422	estimate D2E/DX2	!
! D40	D(6,7,21,22)	164.3645	estimate D2E/DX2	!
! D41	D(6,7,21,23)	-76.3727	estimate D2E/DX2	!
! D42	D(12,7,21,22)	45.6484	estimate D2E/DX2	!
! D43	D(12,7,21,23)	164.9112	estimate D2E/DX2	!
! D44	D(13,7,21,22)	-75.0074	estimate D2E/DX2	!
! D45	D(13,7,21,23)	44.2554	estimate D2E/DX2	!
! D46	D(3,16,17,19)	-179.6078	estimate D2E/DX2	!
! D47	D(3,16,17,20)	0.2359	estimate D2E/DX2	!
! D48	D(18,16,17,19)	-0.2182	estimate D2E/DX2	!
! D49	D(18,16,17,20)	179.6255	estimate D2E/DX2	!
! D50	D(7,21,26,24)	70.9474	estimate D2E/DX2	!
! D51	D(7,21,26,25)	-31.507	estimate D2E/DX2	!
! D52	D(22,21,26,24)	-168.6831	estimate D2E/DX2	!
! D53	D(22,21,26,25)	88.8624	estimate D2E/DX2	!
! D54	D(27,24,25,29)	-154.9563	estimate D2E/DX2	!
! D55	D(27,24,25,30)	-0.7341	estimate D2E/DX2	!
! D56	D(28,24,25,29)	-1.4815	estimate D2E/DX2	!
! D57	D(28,24,25,30)	152.7407	estimate D2E/DX2	!
! D58	D(27,24,26,23)	114.9389	estimate D2E/DX2	!
! D59	D(28,24,26,23)	-23.9313	estimate D2E/DX2	!

! D60	D(29,25,26,23)	25.9221	estimate D2E/DX2 !
! D61	D(30,25,26,23)	-112.9272	estimate D2E/DX2 !
! D62	D(24,25,30,31)	146.233	estimate D2E/DX2 !
! D63	D(24,25,30,32)	-94.779	estimate D2E/DX2 !
! D64	D(24,25,30,33)	25.6225	estimate D2E/DX2 !
! D65	D(26,25,30,31)	77.3392	estimate D2E/DX2 !
! D66	D(26,25,30,32)	-163.6728	estimate D2E/DX2 !
! D67	D(26,25,30,33)	-43.2713	estimate D2E/DX2 !
! D68	D(29,25,30,31)	-59.8669	estimate D2E/DX2 !
! D69	D(29,25,30,32)	59.1211	estimate D2E/DX2 !
! D70	D(29,25,30,33)	179.5225	estimate D2E/DX2 !

Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-06

Number of steps in this run= 172 maximum allowed number of steps= 198.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.914191	2.123340	-0.248301
2	6	0	-3.854662	1.192906	0.056918
3	7	0	-3.203779	-0.036010	0.103331
4	6	0	-1.898802	0.156293	-0.166113
5	7	0	-1.704037	1.461926	-0.387385
6	6	0	-0.391013	2.086245	-0.673582
7	6	0	0.292634	2.658673	0.571997
8	1	0	-3.002927	3.187087	-0.387918
9	1	0	-4.909460	1.300573	0.233596
10	1	0	0.233516	1.307365	-1.114695
11	1	0	-0.547932	2.871199	-1.414796
12	1	0	-0.315275	3.474564	0.976030
13	1	0	0.333399	1.866212	1.334193
14	35	0	0.405161	-2.158911	-0.254560
15	1	0	-1.110291	-0.636065	-0.196383
16	6	0	-3.734936	-1.324139	0.393040
17	6	0	-5.006323	-1.559332	0.686458
18	1	0	-2.971180	-2.093223	0.354528
19	1	0	-5.318257	-2.572131	0.899258
20	1	0	-5.765007	-0.787576	0.729615
21	7	0	1.594674	3.187707	0.171156
22	1	0	1.975430	3.796807	0.885534
23	1	0	2.257006	2.426415	0.028904

24	6	0	3.875163	-0.199956	-1.058367
25	6	0	3.868574	-0.407715	0.391865
26	8	0	3.595834	0.902151	-0.167513
27	1	0	4.822154	-0.117360	-1.587387
28	1	0	3.026036	-0.554333	-1.635271
29	1	0	2.980132	-0.891236	0.792195
30	6	0	5.131040	-0.530555	1.198646
31	1	0	4.997960	-0.097979	2.194812
32	1	0	5.392020	-1.585874	1.324758
33	1	0	5.962453	-0.019700	0.707652

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357701	0.000000			
3	N	2.206875	1.391416	0.000000		
4	C	2.215185	2.224792	1.346308	0.000000	
5	N	1.386104	2.212457	2.175739	1.338496	0.000000
6	C	2.559036	3.650829	3.608215	2.501133	1.481795
7	C	3.353088	4.428752	4.439129	3.407213	2.517799
8	H	1.076534	2.213615	3.266500	3.233265	2.159467
9	H	2.211395	1.074898	2.170892	3.245490	3.269004
10	H	3.365191	4.254289	3.886289	2.602221	2.075327
11	H	2.742113	3.989621	4.220201	3.279447	2.092415
12	H	3.174769	4.310219	4.629167	3.850061	2.799691
13	H	3.621773	4.429969	4.200607	3.187077	2.697855
14	Br	5.418100	5.429345	4.202290	3.267451	4.192472
15	H	3.297130	3.307698	2.198314	1.118256	2.188740
16	C	3.601396	2.542209	1.423143	2.423988	3.534936
17	C	4.337380	3.049173	2.430990	3.650607	4.602850
18	H	4.259819	3.415810	2.085504	2.545856	3.846449
19	H	5.398507	4.126397	3.396532	4.502442	5.567015
20	H	4.190096	2.832710	2.741710	4.079309	4.774874
21	N	4.651740	5.804097	5.781185	4.637628	3.764543
22	H	5.290980	6.438702	6.490496	5.419315	4.539875
23	H	5.187483	6.234967	5.990764	4.739433	4.097975
24	C	7.221443	7.933103	7.175503	5.853350	5.859995
25	C	7.267871	7.894463	7.087989	5.821690	5.929315
26	O	6.624066	7.459544	6.869370	5.545028	5.333885
27	H	8.164859	8.927915	8.202484	6.875039	6.820947
28	H	6.661825	7.297969	6.488605	5.188202	5.291135
29	H	6.701742	7.183223	6.280661	5.081306	5.373101
30	C	8.594333	9.220450	8.421015	7.193956	7.294090
31	H	8.573517	9.198146	8.464435	7.294104	7.349681

32	H	9.231789	9.738078	8.819395	7.642900	7.910407
33	H	9.181573	9.913103	9.186146	7.911622	7.884757

		6	7	8	9	10
6	C	0.000000				
7	C	1.531834	0.000000			
8	H	2.848781	3.472950	0.000000		
9	H	4.675106	5.387089	2.753195	0.000000	
10	H	1.091454	2.162050	3.812627	5.316779	0.000000
11	H	1.090951	2.167733	2.679788	4.920060	1.773781
12	H	2.157403	1.094748	3.027618	5.136534	3.060891
13	H	2.145774	1.100272	3.980132	5.386913	2.513830
14	Br	4.339449	4.889271	6.341336	6.360151	3.575523
15	H	2.855880	3.662500	4.270275	4.285923	2.534962
16	C	4.893896	5.667110	4.636474	2.879938	4.994666
17	C	6.036640	6.773744	5.262734	2.897158	6.238431
18	H	5.018189	5.768907	5.332345	3.910167	4.898234
19	H	6.960749	7.677923	6.339256	3.950703	7.066023
20	H	6.253609	6.971118	4.967485	2.310490	6.616082
21	N	2.422757	1.461458	4.631468	6.772661	2.653648
22	H	3.310123	2.055592	5.174696	7.352409	3.637651
23	H	2.760653	2.051256	5.330972	7.257248	2.579652
24	C	4.855413	4.864603	7.696082	9.005018	3.941673
25	C	5.049663	4.714078	7.794112	8.944114	4.292420
26	O	4.189646	3.813578	6.986641	8.524063	3.516608
27	H	5.733064	5.734619	8.578461	10.001541	4.827927
28	H	4.424220	4.760980	7.204340	8.360947	3.396334
29	H	4.730593	4.457913	7.336374	8.207419	4.001747
30	C	6.391084	5.828725	9.082922	10.251634	5.719724
31	H	6.483791	5.689706	9.026425	10.196043	5.968899
32	H	7.135916	6.677317	9.807627	10.753730	6.397806
33	H	6.834423	6.272076	9.584456	10.962041	6.156522

		11	12	13	14	15
11	H	0.000000				
12	H	2.476737	0.000000			
13	H	3.056744	1.770835	0.000000		
14	Br	5.249432	5.811146	4.327921	0.000000	
15	H	3.755220	4.347858	3.269296	2.149195	0.000000
16	C	5.570110	5.921276	5.255041	4.272778	2.776621
17	C	6.627377	6.886936	6.377032	5.525321	4.100109
18	H	5.800700	6.200028	5.249487	3.431469	2.426875
19	H	7.598729	7.848455	7.199255	5.853167	4.759807
20	H	6.723318	6.922871	6.678223	6.396885	4.748348
21	N	2.684433	2.092370	2.165599	5.493860	4.698207
22	H	3.537743	2.315029	2.573860	6.263875	5.508409

23	H	3.185872	2.934671	2.391207	4.953271	4.557217
24	C	5.396555	5.933013	4.747366	4.065037	5.078185
25	C	5.789717	5.737415	4.307689	3.934435	5.018693
26	O	4.754331	4.818897	3.718604	4.422451	4.951217
27	H	6.148097	6.772459	5.711314	5.045214	6.115378
28	H	4.955414	5.849381	4.682633	3.368979	4.380215
29	H	5.610166	5.472998	3.860373	3.055024	4.215917
30	C	7.117073	6.764088	5.364720	5.205505	6.396206
31	H	7.252738	6.517588	5.133891	5.598274	6.581647
32	H	7.915408	7.635631	6.124266	5.262260	6.745076
33	H	7.432846	7.189699	5.969545	6.032045	7.156877

		16	17	18	19	20
16	C	0.000000				
17	C	1.325834	0.000000			
18	H	1.084572	2.130029	0.000000		
19	H	2.078616	1.080902	2.456594	0.000000	
20	H	2.126587	1.083084	3.106586	1.847431	0.000000
21	N	6.986468	8.146967	6.983471	9.027429	8.383296
22	H	7.686021	8.801860	7.709953	9.683049	8.997513
23	H	7.078320	8.311107	6.918604	9.117433	8.670261
24	C	7.828408	9.152765	7.242454	9.694250	9.822172
25	C	7.658538	8.954150	7.044471	9.451984	9.646982
26	O	7.681847	8.988063	7.236744	9.626508	9.554337
27	H	8.865788	10.190614	8.271102	10.725541	10.858438
28	H	7.100520	8.421356	6.503390	8.951121	9.106565
29	H	6.740836	8.015048	6.087236	8.467593	8.745977
30	C	8.937802	10.202296	8.294603	10.651079	10.909165
31	H	9.000740	10.222346	8.418719	10.687573	10.884108
32	H	9.178122	10.417949	8.434564	10.764004	11.201372
33	H	9.789785	11.076324	9.177908	11.567456	11.752593

		21	22	23	24	25
21	N	0.000000				
22	H	1.013072	0.000000			
23	H	1.019061	1.640449	0.000000		
24	C	4.264812	4.833410	3.270843	0.000000	
25	C	4.259858	4.637425	3.280425	1.465053	0.000000
26	O	3.056649	3.480467	2.038240	1.444398	1.450186
27	H	4.942931	5.435060	3.957673	1.087877	2.216091
28	H	4.394865	5.137183	3.499392	1.086010	2.200147
29	H	4.352351	4.795403	3.480278	2.168762	1.087835
30	C	5.233268	5.364884	4.286262	2.603964	1.503265
31	H	5.145218	5.100907	4.310052	3.443000	2.149899
32	H	6.207875	6.390560	5.254142	3.146571	2.139915
33	H	5.445437	5.522112	4.491605	2.740090	2.152814

		26	27	28	29	30
26	O	0.000000				
27	H	2.135253	0.000000			
28	H	2.144838	1.849129	0.000000		
29	H	2.125174	3.107143	2.451163	0.000000	
30	C	2.505174	2.833394	3.530254	2.218490	0.000000
31	H	2.923491	3.786332	4.332006	2.582290	1.094157
32	H	3.412246	3.310871	3.927306	2.565804	1.094401
33	H	2.686375	2.564571	3.794426	3.108209	1.092381

		31	32	33
31	H	0.000000		
32	H	1.768081	0.000000	
33	H	1.774266	1.777390	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.914191	2.123340	-0.248301
2	6	0	-3.854662	1.192906	0.056918
3	7	0	-3.203779	-0.036010	0.103331
4	6	0	-1.898802	0.156293	-0.166113
5	7	0	-1.704037	1.461926	-0.387385
6	6	0	-0.391013	2.086245	-0.673582
7	6	0	0.292634	2.658673	0.571997
8	1	0	-3.002927	3.187087	-0.387918
9	1	0	-4.909460	1.300573	0.233596
10	1	0	0.233516	1.307365	-1.114695
11	1	0	-0.547932	2.871199	-1.414796
12	1	0	-0.315275	3.474564	0.976030
13	1	0	0.333399	1.866212	1.334193
14	35	0	0.405161	-2.158911	-0.254560
15	1	0	-1.110291	-0.636065	-0.196383
16	6	0	-3.734936	-1.324139	0.393040
17	6	0	-5.006323	-1.559332	0.686458
18	1	0	-2.971180	-2.093223	0.354528
19	1	0	-5.318257	-2.572131	0.899258
20	1	0	-5.765007	-0.787576	0.729615

21	7	0	1.594674	3.187707	0.171156
22	1	0	1.975430	3.796807	0.885534
23	1	0	2.257006	2.426415	0.028904
24	6	0	3.875163	-0.199956	-1.058367
25	6	0	3.868574	-0.407715	0.391865
26	8	0	3.595834	0.902151	-0.167513
27	1	0	4.822154	-0.117360	-1.587387
28	1	0	3.026036	-0.554333	-1.635271
29	1	0	2.980132	-0.891236	0.792195
30	6	0	5.131040	-0.530555	1.198646
31	1	0	4.997960	-0.097979	2.194812
32	1	0	5.392020	-1.585874	1.324758
33	1	0	5.962453	-0.019700	0.707652

Rotational constants (GHZ): 0.5219570 0.2258947 0.1659502

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1285.9057588528 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 3.82D-06 NBF= 482

NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

```
No special actions if energy rises.
SCF Done:  E(RB3LYP) =  -3205.64622891     A.U. after   15 cycles
           NFock= 15  Conv=0.43D-08     -V/T= 2.0018

**********************************************************************

           Population analysis using the SCF density.

**********************************************************************

Orbital symmetries:
      Occupied  (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
      Virtual   (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A)

The electronic state is 1-A.

Alpha occ. eigenvalues -- -482.69405 -62.34740 -56.16520 -56.16509 -56.16505
Alpha occ. eigenvalues -- -19.12272 -14.44894 -14.43948 -14.29523 -10.29101
Alpha occ. eigenvalues -- -10.27027 -10.26951 -10.26186 -10.24549 -10.21869
Alpha occ. eigenvalues -- -10.21464 -10.20913 -10.20320 -10.15674 -8.55648
Alpha occ. eigenvalues -- -6.37982 -6.37916 -6.37898 -2.49222 -2.49202
Alpha occ. eigenvalues -- -2.49187 -2.49135 -2.49134 -1.11202 -1.05554
Alpha occ. eigenvalues -- -0.99845 -0.89509 -0.84876 -0.82022 -0.77488
Alpha occ. eigenvalues -- -0.73572 -0.70884 -0.68069 -0.65124 -0.64918
Alpha occ. eigenvalues -- -0.63079 -0.62878 -0.58133 -0.58072 -0.54029
Alpha occ. eigenvalues -- -0.53136 -0.51933 -0.50799 -0.50163 -0.49200
Alpha occ. eigenvalues -- -0.48838 -0.47792 -0.45965 -0.45183 -0.44202
Alpha occ. eigenvalues -- -0.43104 -0.42931 -0.41563 -0.39579 -0.38395
Alpha occ. eigenvalues -- -0.37524 -0.36316 -0.35398 -0.31406 -0.29828
Alpha occ. eigenvalues -- -0.29508 -0.26654 -0.25099 -0.19819 -0.19326
Alpha occ. eigenvalues -- -0.19095
Alpha virt. eigenvalues -- -0.07862 -0.04458 -0.02992 -0.01592 -0.00371
Alpha virt. eigenvalues -- -0.00208 0.00258 0.00936 0.01015 0.01507
Alpha virt. eigenvalues -- 0.02294 0.02659 0.03464 0.03943 0.04336
Alpha virt. eigenvalues -- 0.04730 0.05133 0.05370 0.05884 0.06204
Alpha virt. eigenvalues -- 0.06316 0.07068 0.07395 0.07510 0.08244
Alpha virt. eigenvalues -- 0.08337 0.08704 0.08893 0.09104 0.09300
Alpha virt. eigenvalues -- 0.09518 0.09829 0.10510 0.10665 0.11102
Alpha virt. eigenvalues -- 0.11646 0.11785 0.12058 0.12422 0.12534
Alpha virt. eigenvalues -- 0.12725 0.13104 0.13200 0.13740 0.13836
Alpha virt. eigenvalues -- 0.14292 0.14456 0.14779 0.14813 0.15128
Alpha virt. eigenvalues -- 0.15774 0.15922 0.16152 0.16328 0.16805
Alpha virt. eigenvalues -- 0.17310 0.17468 0.17729 0.18027 0.18247
Alpha virt. eigenvalues -- 0.18586 0.18917 0.19493 0.19599 0.19774
Alpha virt. eigenvalues -- 0.20145 0.20301 0.21194 0.21407 0.21628
Alpha virt. eigenvalues -- 0.21791 0.22321 0.22751 0.23231 0.23409
Alpha virt. eigenvalues -- 0.23667 0.24075 0.24467 0.24976 0.25085
Alpha virt. eigenvalues -- 0.25782 0.26022 0.26341 0.26560 0.27264
Alpha virt. eigenvalues -- 0.27740 0.27964 0.28374 0.28640 0.28966
Alpha virt. eigenvalues -- 0.30063 0.30336 0.30961 0.31502 0.32181
Alpha virt. eigenvalues -- 0.32429 0.33006 0.33443 0.34101 0.34366

Alpha virt. eigenvalues --	0.34756	0.35715	0.36059	0.37447	0.38151
Alpha virt. eigenvalues --	0.38745	0.38937	0.39821	0.40895	0.41446
Alpha virt. eigenvalues --	0.42276	0.44118	0.46257	0.47288	0.48285
Alpha virt. eigenvalues --	0.49097	0.50157	0.50662	0.51059	0.51832
Alpha virt. eigenvalues --	0.52498	0.53355	0.53884	0.54726	0.55493
Alpha virt. eigenvalues --	0.55949	0.56033	0.57130	0.58128	0.58872
Alpha virt. eigenvalues --	0.59131	0.60014	0.60465	0.61793	0.62009
Alpha virt. eigenvalues --	0.63078	0.63465	0.63896	0.64697	0.65443
Alpha virt. eigenvalues --	0.65909	0.66246	0.66553	0.67664	0.68302
Alpha virt. eigenvalues --	0.68997	0.69429	0.69507	0.70127	0.70725
Alpha virt. eigenvalues --	0.71383	0.71758	0.72273	0.73530	0.73831
Alpha virt. eigenvalues --	0.75046	0.75418	0.75860	0.76350	0.76560
Alpha virt. eigenvalues --	0.76981	0.78305	0.78439	0.79402	0.79981
Alpha virt. eigenvalues --	0.81004	0.81504	0.82871	0.84378	0.85362
Alpha virt. eigenvalues --	0.85423	0.88044	0.89306	0.89996	0.90400
Alpha virt. eigenvalues --	0.90621	0.93168	0.93900	0.95544	0.96527
Alpha virt. eigenvalues --	0.97163	0.98827	0.99624	1.00523	1.01389
Alpha virt. eigenvalues --	1.02473	1.03824	1.04214	1.05595	1.08830
Alpha virt. eigenvalues --	1.09318	1.10868	1.11481	1.12299	1.12840
Alpha virt. eigenvalues --	1.15756	1.16806	1.19322	1.21474	1.21918
Alpha virt. eigenvalues --	1.22425	1.26796	1.27766	1.27976	1.30492
Alpha virt. eigenvalues --	1.32039	1.33701	1.36373	1.38933	1.40916
Alpha virt. eigenvalues --	1.42215	1.43486	1.45527	1.46681	1.47883
Alpha virt. eigenvalues --	1.49297	1.49536	1.50471	1.51251	1.53111
Alpha virt. eigenvalues --	1.54097	1.55223	1.55641	1.56999	1.58625
Alpha virt. eigenvalues --	1.58831	1.59450	1.59855	1.60442	1.61284
Alpha virt. eigenvalues --	1.61390	1.62346	1.65549	1.66751	1.67248
Alpha virt. eigenvalues --	1.67617	1.68336	1.69117	1.70538	1.71307
Alpha virt. eigenvalues --	1.71608	1.72602	1.73511	1.73818	1.74257
Alpha virt. eigenvalues --	1.74864	1.77421	1.78834	1.79854	1.80860
Alpha virt. eigenvalues --	1.82526	1.83204	1.86103	1.86863	1.87667
Alpha virt. eigenvalues --	1.89405	1.91100	1.91351	1.92424	1.94801
Alpha virt. eigenvalues --	1.97473	1.99681	2.01169	2.03149	2.04145
Alpha virt. eigenvalues --	2.05400	2.05847	2.07737	2.08213	2.09451
Alpha virt. eigenvalues --	2.10947	2.11680	2.12932	2.13476	2.15530
Alpha virt. eigenvalues --	2.16708	2.18009	2.18908	2.20483	2.20866
Alpha virt. eigenvalues --	2.24070	2.25124	2.27430	2.28379	2.30800
Alpha virt. eigenvalues --	2.33620	2.36023	2.38854	2.41960	2.42202
Alpha virt. eigenvalues --	2.43409	2.45961	2.46398	2.46688	2.48294
Alpha virt. eigenvalues --	2.50779	2.50870	2.52999	2.54297	2.54731
Alpha virt. eigenvalues --	2.55118	2.55985	2.56596	2.57717	2.57912
Alpha virt. eigenvalues --	2.60814	2.61349	2.62086	2.62429	2.65398
Alpha virt. eigenvalues --	2.65732	2.67013	2.69009	2.70579	2.71400
Alpha virt. eigenvalues --	2.71872	2.72613	2.73384	2.75838	2.76153

Alpha virt. eigenvalues -- 2.76945 2.77455 2.79216 2.80482 2.81706
Alpha virt. eigenvalues -- 2.82262 2.82428 2.83094 2.83699 2.86532
Alpha virt. eigenvalues -- 2.87259 2.87994 2.88937 2.91915 2.93043
Alpha virt. eigenvalues -- 2.94284 2.96006 2.96887 3.03395 3.10235
Alpha virt. eigenvalues -- 3.10811 3.15009 3.15756 3.19875 3.21981
Alpha virt. eigenvalues -- 3.23339 3.26781 3.27908 3.37375 3.38129
Alpha virt. eigenvalues -- 3.50260 3.53923 3.57002 3.58795 3.64286
Alpha virt. eigenvalues -- 3.66864 3.71404 3.72987 3.75666 3.76433
Alpha virt. eigenvalues -- 3.78832 3.81488 3.82204 3.82354 3.84812
Alpha virt. eigenvalues -- 3.85917 3.87897 3.97025 4.05751 4.07874
Alpha virt. eigenvalues -- 4.08904 4.13101 4.25393 4.27440 4.28465
Alpha virt. eigenvalues -- 4.30145 4.32487 4.49713 4.52233 4.70048
Alpha virt. eigenvalues -- 4.77129 4.83195 4.93895 5.02848 5.14547
Alpha virt. eigenvalues -- 5.22433 5.50636 5.61917 6.77461 7.68843
Alpha virt. eigenvalues -- 7.74683 7.81410 23.70364 23.75330 23.83680
Alpha virt. eigenvalues -- 23.86655 23.87461 23.88208 23.91322 23.98852
Alpha virt. eigenvalues -- 24.13691 24.23292 35.43774 35.56628 35.62018
Alpha virt. eigenvalues -- 48.06131 49.92485 289.89608 289.95286 290.01078
Alpha virt. eigenvalues -- 1020.85099

Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	6.985341	-1.030300	0.281865	-0.008115	-0.086890	-0.052381
2	C	-1.030300	6.548356	-0.063346	0.089568	0.343199	-0.272575
3	N	0.281865	-0.063346	6.750720	0.174471	-0.419126	-0.106615
4	C	-0.008115	0.089568	0.174471	7.762401	0.405960	-0.440255
5	N	-0.086890	0.343199	-0.419126	0.405960	7.023750	0.040340
6	C	-0.052381	-0.272575	-0.106615	-0.440255	0.040340	6.983149
7	C	-0.002788	0.138376	-0.045321	-0.057770	0.144089	-0.722483
8	H	0.502331	-0.101320	0.035049	0.018549	-0.061732	-0.058040
9	H	-0.123034	0.511779	-0.079767	0.006334	0.029274	0.001797
10	H	0.014544	-0.030803	-0.013164	0.046912	-0.029633	0.393977
11	H	-0.054663	0.031270	-0.011617	-0.036385	-0.048844	0.555347
12	H	0.026925	-0.052642	0.011369	-0.009093	-0.044968	0.010764
13	H	-0.021956	0.039029	-0.013233	-0.001453	0.060983	-0.087333
14	Br	-0.022378	0.003369	-0.014260	-0.090977	-0.026462	0.049968
15	H	-0.248005	0.002606	0.048274	-1.106165	-0.122512	0.237790
16	C	0.284528	-0.295496	0.371830	-0.267627	-0.294988	-0.163326
17	C	-0.178759	0.114541	-0.019569	-0.386384	-0.053700	-0.043766
18	H	-0.002424	0.017148	-0.108817	0.215050	0.043638	-0.004050
19	H	-0.002710	0.005428	0.023664	-0.015340	-0.000792	0.000172
20	H	0.001267	0.007295	-0.036639	0.005989	-0.001045	-0.003470
21	N	-0.019348	-0.000011	0.006918	0.058922	-0.015538	-0.070530
22	H	0.000038	0.000724	0.000088	-0.003928	-0.001055	-0.001318
23	H	0.006604	-0.001606	-0.000185	-0.001371	0.004900	-0.017587

24	C	-0.004143	0.000095	-0.000208	-0.037713	-0.005787	0.025466
25	C	0.002346	0.001271	-0.000388	0.031635	0.007823	-0.018516
26	O	-0.003115	0.000887	-0.000072	-0.006717	-0.003055	0.010771
27	H	-0.000190	0.000029	-0.000042	-0.001403	-0.000079	0.004221
28	H	0.001719	0.000058	0.001584	0.016677	-0.000923	-0.015372
29	H	-0.000840	-0.000145	-0.000808	-0.004024	-0.000100	0.003000
30	C	-0.000308	0.000558	-0.000056	0.005724	0.001075	-0.013183
31	H	-0.000105	0.000027	0.000010	0.000024	-0.000161	-0.000039
32	H	0.000046	-0.000013	0.000007	0.000403	0.000038	-0.000673
33	H	0.000048	-0.000013	-0.000003	0.000013	0.000049	0.000151

		7	8	9	10	11	12
1	C	-0.002788	0.502331	-0.123034	0.014544	-0.054663	0.026925
2	C	0.138376	-0.101320	0.511779	-0.030803	0.031270	-0.052642
3	N	-0.045321	0.035049	-0.079767	-0.013164	-0.011617	0.011369
4	C	-0.057770	0.018549	0.006334	0.046912	-0.036385	-0.009093
5	N	0.144089	-0.061732	0.029274	-0.029633	-0.048844	-0.044968
6	C	-0.722483	-0.058040	0.001797	0.393977	0.555347	0.010764
7	C	6.588580	0.022531	0.001883	-0.061478	-0.214198	0.425723
8	H	0.022531	0.493124	-0.010075	0.003577	-0.014359	-0.004369
9	H	0.001883	-0.010075	0.498287	-0.000440	0.001708	-0.000026
10	H	-0.061478	0.003577	-0.000440	0.549232	-0.044606	0.005463
11	H	-0.214198	-0.014359	0.001708	-0.044606	0.603684	-0.016516
12	H	0.425723	-0.004369	-0.000026	0.005463	-0.016516	0.651377
13	H	0.325762	0.001850	0.000037	-0.002853	0.020537	-0.103235
14	Br	-0.046746	-0.000919	-0.000734	-0.012288	0.005295	0.002205
15	H	-0.126307	-0.011261	-0.002547	-0.073493	0.019443	0.016527
16	C	-0.041716	0.003510	-0.003044	-0.014870	-0.005711	0.001908
17	C	-0.007713	-0.000887	-0.007663	-0.001292	-0.001849	-0.000094
18	H	0.012558	0.001071	0.001043	0.005977	-0.002326	-0.000749
19	H	-0.000315	-0.000157	-0.000801	-0.000266	0.000088	0.000029
20	H	0.000007	0.000660	0.005310	0.000147	-0.000314	-0.000154
21	N	0.028238	-0.001651	-0.000061	0.024889	0.024241	-0.060451
22	H	-0.015126	-0.000326	0.000053	-0.001543	0.000667	-0.014826
23	H	-0.033322	0.000863	-0.000070	-0.006920	-0.001641	0.008715
24	C	0.072781	-0.000306	0.000115	-0.021299	0.004909	0.003365
25	C	-0.061720	0.000255	-0.000090	0.024671	-0.002458	-0.003757
26	O	-0.010774	-0.000219	0.000009	0.002177	0.005195	-0.000752
27	H	-0.004385	-0.000011	0.000002	0.003253	0.001169	-0.000036
28	H	-0.001955	0.000057	-0.000014	-0.012892	-0.003392	-0.000171
29	H	-0.005282	0.000048	-0.000045	0.004127	-0.000213	-0.000917
30	C	-0.003592	-0.000014	0.000006	-0.001429	-0.000932	-0.001183
31	H	0.001207	-0.000011	0.000001	0.000123	0.000083	0.000240
32	H	0.000125	0.000003	0.000000	-0.000026	-0.000092	-0.000034
33	H	0.000013	0.000003	0.000000	-0.000383	-0.000029	-0.000019

		13	14	15	16	17	18
1	C	-0.021956	-0.022378	-0.248005	0.284528	-0.178759	-0.002424
2	C	0.039029	0.003369	0.002606	-0.295496	0.114541	0.017148
3	N	-0.013233	-0.014260	0.048274	0.371830	-0.019569	-0.108817
4	C	-0.001453	-0.090977	-1.106165	-0.267627	-0.386384	0.215050
5	N	0.060983	-0.026462	-0.122512	-0.294988	-0.053700	0.043638
6	C	-0.087333	0.049968	0.237790	-0.163326	-0.043766	-0.004050
7	C	0.325762	-0.046746	-0.126307	-0.041716	-0.007713	0.012558
8	H	0.001850	-0.000919	-0.011261	0.003510	-0.000887	0.001071
9	H	0.000037	-0.000734	-0.002547	-0.003044	-0.007663	0.001043
10	H	-0.002853	-0.012288	-0.073493	-0.014870	-0.001292	0.005977
11	H	0.020537	0.005295	0.019443	-0.005711	-0.001849	-0.002326
12	H	-0.103235	0.002205	0.016527	0.001908	-0.000094	-0.000749
13	H	0.720372	-0.009079	-0.064857	-0.000402	-0.001562	0.001566
14	Br	-0.009079	35.637186	0.254848	-0.042657	0.022578	0.034984
15	H	-0.064857	0.254848	2.064541	-0.102996	0.200313	-0.091777
16	C	-0.000402	-0.042657	-0.102996	6.584977	-0.354335	0.244811
17	C	-0.001562	0.022578	0.200313	-0.354335	6.449425	-0.030688
18	H	0.001566	0.034984	-0.091777	0.244811	-0.030688	0.479922
19	H	-0.000023	-0.001673	0.007192	-0.087374	0.446401	-0.009700
20	H	0.000198	0.000437	-0.001322	0.100350	0.284848	-0.000350
21	N	-0.063716	-0.003264	-0.021946	0.006099	0.000347	-0.000204
22	H	0.001173	-0.001333	-0.003600	-0.000206	-0.000042	0.000106
23	H	0.012736	0.004497	0.007413	0.000385	0.000059	-0.000181
24	C	-0.013159	-0.015101	0.024291	-0.005738	-0.001126	-0.000811
25	C	0.011965	0.003149	-0.031467	0.004206	0.000735	0.001250
26	O	0.002950	-0.000140	-0.000182	-0.000367	-0.000017	-0.000172
27	H	0.000800	0.003053	-0.000903	-0.000221	-0.000036	-0.000049
28	H	0.000416	0.009669	0.000058	0.003742	0.000265	-0.000186
29	H	-0.001012	-0.004247	0.009811	0.000111	0.000742	-0.000018
30	C	0.003208	-0.015110	-0.007962	-0.000209	-0.000074	-0.000080
31	H	-0.001125	0.001253	-0.000096	-0.000003	-0.000002	-0.000017
32	H	0.000069	0.000519	-0.000451	0.000038	0.000001	0.000025
33	H	0.000189	0.000080	0.000097	0.000008	0.000003	0.000011

		19	20	21	22	23	24
1	C	-0.002710	0.001267	-0.019348	0.000038	0.006604	-0.004143
2	C	0.005428	0.007295	-0.000011	0.000724	-0.001606	0.000095
3	N	0.023664	-0.036639	0.006918	0.000088	-0.000185	-0.000208
4	C	-0.015340	0.005989	0.058922	-0.003928	-0.001371	-0.037713
5	N	-0.000792	-0.001045	-0.015538	-0.001055	0.004900	-0.005787
6	C	0.000172	-0.003470	-0.070530	-0.001318	-0.017587	0.025466
7	C	-0.000315	0.000007	0.028238	-0.015126	-0.033322	0.072781
8	H	-0.000157	0.000660	-0.001651	-0.000326	0.000863	-0.000306
9	H	-0.000801	0.005310	-0.000061	0.000053	-0.000070	0.000115

10	H	-0.000266	0.000147	0.024889	-0.001543	-0.006920	-0.021299
11	H	0.000088	-0.000314	0.024241	0.000667	-0.001641	0.004909
12	H	0.000029	-0.000154	-0.060451	-0.014826	0.008715	0.003365
13	H	-0.000023	0.000198	-0.063716	0.001173	0.012736	-0.013159
14	Br	-0.001673	0.000437	-0.003264	-0.001333	0.004497	-0.015101
15	H	0.007192	-0.001322	-0.021946	-0.003600	0.007413	0.024291
16	C	-0.087374	0.100350	0.006099	-0.000206	0.000385	-0.005738
17	C	0.446401	0.284848	0.000347	-0.000042	0.000059	-0.001126
18	H	-0.009700	-0.000350	-0.000204	0.000106	-0.000181	-0.000811
19	H	0.458770	-0.019122	-0.000001	-0.000002	0.000004	0.000012
20	H	-0.019122	0.535345	0.000013	-0.000003	0.000010	-0.000037
21	N	-0.000001	0.000013	6.812545	0.379869	0.321696	-0.002122
22	H	-0.000002	-0.000003	0.379869	0.483858	-0.054847	0.004887
23	H	0.000004	0.000010	0.321696	-0.054847	0.425002	0.000832
24	C	0.000012	-0.000037	-0.002122	0.004887	0.000832	6.830382
25	C	-0.000012	0.000035	-0.002092	-0.007109	-0.008563	-1.263900
26	O	0.000001	-0.000002	0.018397	0.002598	-0.018292	0.046100
27	H	0.000001	-0.000001	0.001099	-0.000381	-0.003671	0.251276
28	H	0.000004	0.000014	0.001559	0.000182	0.006873	0.396674
29	H	-0.000006	0.000009	-0.002680	-0.000884	0.006025	-0.028701
30	C	0.000003	-0.000001	0.013180	0.002783	-0.012063	-0.036568
31	H	0.000000	0.000000	0.001396	0.000346	-0.002697	-0.001477
32	H	0.000000	0.000000	0.000097	0.000014	0.000764	0.012027
33	H	0.000000	0.000000	-0.000409	-0.000248	0.001213	0.015269

		25	26	27	28	29	30
1	C	0.002346	-0.003115	-0.000190	0.001719	-0.000840	-0.000308
2	C	0.001271	0.000887	0.000029	0.000058	-0.000145	0.000558
3	N	-0.000388	-0.000072	-0.000042	0.001584	-0.000808	-0.000056
4	C	0.031635	-0.006717	-0.001403	0.016677	-0.004024	0.005724
5	N	0.007823	-0.003055	-0.000079	-0.000923	-0.000100	0.001075
6	C	-0.018516	0.010771	0.004221	-0.015372	0.003000	-0.013183
7	C	-0.061720	-0.010774	-0.004385	-0.001955	-0.005282	-0.003592
8	H	0.000255	-0.000219	-0.000011	0.000057	0.000048	-0.000014
9	H	-0.000090	0.000009	0.000002	-0.000014	-0.000045	0.000006
10	H	0.024671	0.002177	0.003253	-0.012892	0.004127	-0.001429
11	H	-0.002458	0.005195	0.001169	-0.003392	-0.000213	-0.000932
12	H	-0.003757	-0.000752	-0.000036	-0.000171	-0.000917	-0.001183
13	H	0.011965	0.002950	0.000800	0.000416	-0.001012	0.003208
14	Br	0.003149	-0.000140	0.003053	0.009669	-0.004247	-0.015110
15	H	-0.031467	-0.000182	-0.000903	0.000058	0.009811	-0.007962
16	C	0.004206	-0.000367	-0.000221	0.003742	0.000111	-0.000209
17	C	0.000735	-0.000017	-0.000036	0.000265	0.000742	-0.000074
18	H	0.001250	-0.000172	-0.000049	-0.000186	-0.000018	-0.000080
19	H	-0.000012	0.000001	0.000001	0.000004	-0.000006	0.000003

20	H	0.000035	-0.000002	-0.000001	0.000014	0.000009	-0.000001
21	N	-0.002092	0.018397	0.001099	0.001559	-0.002680	0.013180
22	H	-0.007109	0.002598	-0.000381	0.000182	-0.000884	0.002783
23	H	-0.008563	-0.018292	-0.003671	0.006873	0.006025	-0.012063
24	C	-1.263900	0.046100	0.251276	0.396674	-0.028701	-0.036568
25	C	6.748001	0.197634	0.076551	-0.024008	0.379517	-0.122728
26	O	0.197634	8.177929	-0.053327	-0.045010	-0.006606	-0.108456
27	H	0.076551	-0.053327	0.614053	-0.056170	0.001029	0.028157
28	H	-0.024008	-0.045010	-0.056170	0.552735	-0.001474	0.003873
29	H	0.379517	-0.006606	0.001029	-0.001474	0.467938	-0.017278
30	C	-0.122728	-0.108456	0.028157	0.003873	-0.017278	5.793314
31	H	0.003223	-0.016496	0.000204	-0.002633	0.000001	0.367639
32	H	-0.073723	0.014704	-0.006284	0.001854	0.001496	0.406783
33	H	-0.049616	0.006866	0.003004	0.003676	-0.005775	0.382833

		31	32	33
1	C	-0.000105	0.000046	0.000048
2	C	0.000027	-0.000013	-0.000013
3	N	0.000010	0.000007	-0.000003
4	C	0.000024	0.000403	0.000013
5	N	-0.000161	0.000038	0.000049
6	C	-0.000039	-0.000673	0.000151
7	C	0.001207	0.000125	0.000013
8	H	-0.000011	0.000003	0.000003
9	H	0.000001	0.000000	0.000000
10	H	0.000123	-0.000026	-0.000383
11	H	0.000083	-0.000092	-0.000029
12	H	0.000240	-0.000034	-0.000019
13	H	-0.001125	0.000069	0.000189
14	Br	0.001253	0.000519	0.000080
15	H	-0.000096	-0.000451	0.000097
16	C	-0.000003	0.000038	0.000008
17	C	-0.000002	0.000001	0.000003
18	H	-0.000017	0.000025	0.000011
19	H	0.000000	0.000000	0.000000
20	H	0.000000	0.000000	0.000000
21	N	0.001396	0.000097	-0.000409
22	H	0.000346	0.000014	-0.000248
23	H	-0.002697	0.000764	0.001213
24	C	-0.001477	0.012027	0.015269
25	C	0.003223	-0.073723	-0.049616
26	O	-0.016496	0.014704	0.006866
27	H	0.000204	-0.006284	0.003004
28	H	-0.002633	0.001854	0.003676
29	H	0.000001	0.001496	-0.005775

30	C	0.367639	0.406783	0.382833
31	H	0.581207	-0.041749	-0.036230
32	H	-0.041749	0.566857	-0.024379
33	H	-0.036230	-0.024379	0.566624

Mulliken charges:

		1
1	C	-0.245149
2	C	-0.007343
3	N	0.227389
4	C	-0.363913
5	N	0.112271
6	C	-0.225404
7	C	-0.298882
8	H	0.182176
9	H	0.170773
10	H	0.250608
11	H	0.186507
12	H	0.149380
13	H	0.181159
14	Br	-0.725723
15	H	0.124646
16	C	0.074781
17	C	-0.430701
18	H	0.193440
19	H	0.196526
20	H	0.120525
21	N	-0.435482
22	H	0.229392
23	H	0.354425
24	C	-0.250284
25	C	0.175880
26	O	-0.212450
27	H	0.139287
28	H	0.162509
29	H	0.207200
30	C	-0.667908
31	H	0.145856
32	H	0.141554
33	H	0.136956

Sum of Mulliken charges = 0.00000

Mulliken charges with hydrogens summed into heavy atoms:

		1
1	C	-0.062974
2	C	0.163430

3 N 0.227389
4 C -0.239267
5 N 0.112271
6 C 0.211711
7 C 0.031657
14 Br -0.725723
16 C 0.268220
17 C -0.113650
21 N 0.148335
24 C 0.051512
25 C 0.383080
26 O -0.212450
30 C -0.243542

Electronic spatial extent (au): <R**2>= 6328.0072

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= -8.1116 Y= 6.8852 Z= 1.5298 Tot= 10.7491

Quadrupole moment (field-independent basis, Debye-Ang):

XX= -69.2255 YY= -115.2295 ZZ= -107.5025

XY= -6.5340 XZ= -0.4153 YZ= -0.1977

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

XX= 28.0937 YY= -17.9103 ZZ= -10.1833

XY= -6.5340 XZ= -0.4153 YZ= -0.1977

Octapole moment (field-independent basis, Debye-Ang**2):

XXX= -92.4505 YYY= 1.7368 ZZZ= -9.7030 XYY= -45.7128

XXY= -36.3692 XXZ= 15.9241 XZZ= 24.0764 YZZ= -8.2962

YYZ= 21.0358 XYZ= 16.3388

Hexadecapole moment (field-independent basis, Debye-Ang**3):

XXXX= -4988.9611 YYYY= -2159.3864 ZZZZ= -373.3109 XXXY= -83.6550

XXXZ= -126.4542 YYYX= -37.6636 YYYZ= 55.2548 ZZZX= 4.2138

ZZZY= 18.4140 XXYY= -1225.7377 XXZZ= -1055.9766 YYZZ= -417.9380

XXYZ= -15.7205 YYXZ= 34.3250 ZZXY= -0.3541

N-N= 1.285905758853D+03 E-N=-1.019628611447D+04 KE= 3.199791014147D+03

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Atomic Forces (Hartrees/Bohr)

Number	Number	X	Y	Z
1	6	-0.000587707	0.000055784	0.000066059
2	6	-0.000559395	0.000273170	-0.000149321
3	7	0.001962007	0.002019520	0.000047253
4	6	0.003074858	0.004556492	-0.000913392
5	7	0.000074727	-0.002357739	0.001857963
6	6	-0.000674640	-0.002399798	-0.002997924
7	6	0.000507255	0.000426351	0.001487299
8	1	-0.000214802	-0.000005270	0.000157441
9	1	0.000125306	0.000028709	-0.000153381
10	1	-0.000380137	0.000316730	-0.000005002
11	1	0.000064139	-0.000613079	-0.000213023
12	1	-0.000008393	0.000067937	0.000442074
13	1	0.000574632	0.000293418	0.000457683
14	35	0.000376837	-0.000075329	0.000085210
15	1	-0.000764419	0.000020415	-0.000127384
16	6	0.000818959	-0.000091995	0.000221936
17	6	-0.000690649	-0.000177086	0.000137986
18	1	-0.000196502	0.000094812	-0.000218886
19	1	-0.000109128	-0.000179676	-0.000083696
20	1	0.000104057	-0.000199469	-0.000053359
21	7	-0.004467821	-0.001308588	0.000254890
22	1	-0.000316673	0.000048565	0.000064089
23	1	0.001809951	-0.000385056	-0.000402204
24	6	0.000146283	-0.000345690	-0.000176241
25	6	0.000121191	0.000137409	-0.000323606
26	8	-0.000847817	0.000096871	-0.000065934
27	1	-0.000140240	-0.000095394	0.000326553
28	1	-0.000032763	0.000212063	-0.000080247
29	1	-0.000072988	-0.000030618	0.000143338
30	6	0.000022950	-0.000505971	0.000293215
31	1	0.000046951	0.000028978	-0.000053339
32	1	0.000095146	0.000033489	0.000021839
33	1	0.000138825	0.000060044	-0.000047889

Cartesian Forces: Max 0.004556492 RMS 0.000992421

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.006211821 RMS 0.001033142
Search for a local minimum.

Step number 1 out of a maximum of 172

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Second derivative matrix not updated -- first step.

ITU= 0

Eigenvalues ---	0.00230	0.00230	0.00230	0.00230	0.00230
Eigenvalues ---	0.00345	0.00610	0.00723	0.00879	0.01386
Eigenvalues ---	0.01472	0.01855	0.01987	0.02083	0.02150
Eigenvalues ---	0.02267	0.02322	0.02357	0.02395	0.02455
Eigenvalues ---	0.03046	0.03070	0.03070	0.03192	0.03932
Eigenvalues ---	0.04045	0.04084	0.04617	0.04629	0.04653
Eigenvalues ---	0.05323	0.05690	0.05766	0.05905	0.08612
Eigenvalues ---	0.09523	0.11501	0.11968	0.12350	0.12513
Eigenvalues ---	0.12724	0.12870	0.15478	0.15998	0.15999
Eigenvalues ---	0.16000	0.16000	0.16000	0.16000	0.16000
Eigenvalues ---	0.16000	0.16000	0.16000	0.17091	0.21862
Eigenvalues ---	0.22000	0.22034	0.22817	0.23549	0.24962
Eigenvalues ---	0.24997	0.29255	0.29543	0.31741	0.32037
Eigenvalues ---	0.32534	0.33652	0.34270	0.34309	0.34337
Eigenvalues ---	0.34365	0.34539	0.34645	0.34703	0.35059
Eigenvalues ---	0.35064	0.35278	0.35448	0.35624	0.35886
Eigenvalues ---	0.36416	0.36618	0.36782	0.37950	0.41991
Eigenvalues ---	0.42640	0.44488	0.45462	0.45764	0.49182
Eigenvalues ---	0.54584	0.55852	0.60501		

RFO step: Lambda=-2.45661923D-03 EMin= 2.30000000D-03

Linear search not attempted -- first point.

Maximum step size (0.300) exceeded in Quadratic search.

-- Step size scaled by 0.553

Iteration 1 RMS(Cart)= 0.26287808 RMS(Int)= 0.01154711

Iteration 2 RMS(Cart)= 0.14717316 RMS(Int)= 0.00231215

Iteration 3 RMS(Cart)= 0.00445979 RMS(Int)= 0.00114520

Iteration 4 RMS(Cart)= 0.00002865 RMS(Int)= 0.00114520

Iteration 5 RMS(Cart)= 0.00000021 RMS(Int)= 0.00114520

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56568	-0.00078	0.00000	-0.00046	-0.00046	2.56522
R2	2.61936	0.00063	0.00000	0.00067	0.00068	2.62003
R3	2.03435	-0.00001	0.00000	-0.00001	-0.00001	2.03434
R4	2.62939	0.00013	0.00000	0.00044	0.00044	2.62983
R5	2.03126	-0.00015	0.00000	-0.00022	-0.00022	2.03105
R6	2.54415	-0.00115	0.00000	-0.00132	-0.00133	2.54283
R7	2.68935	0.00053	0.00000	0.00070	0.00070	2.69005
R8	2.52939	-0.00621	0.00000	-0.00629	-0.00630	2.52309
R9	2.11320	-0.00023	0.00000	-0.00040	-0.00040	2.11280

R10	2.80019	-0.00453	0.00000	-0.00723	-0.00725	2.79294
R11	2.89475	0.00036	0.00000	0.00068	0.00073	2.89548
R12	2.06255	-0.00044	0.00000	-0.00070	-0.00070	2.06185
R13	2.06160	-0.00031	0.00000	-0.00048	-0.00048	2.06111
R14	2.06877	0.00022	0.00000	0.00035	0.00035	2.06913
R15	2.07921	0.00013	0.00000	0.00021	0.00021	2.07942
R16	2.76175	-0.00385	0.00000	-0.00575	-0.00576	2.75599
R17	4.06139	0.00032	0.00000	0.00361	0.00361	4.06500
R18	2.50546	0.00077	0.00000	0.00070	0.00070	2.50616
R19	2.04954	-0.00020	0.00000	-0.00031	-0.00031	2.04924
R20	2.04261	0.00018	0.00000	0.00028	0.00028	2.04289
R21	2.04673	-0.00022	0.00000	-0.00034	-0.00034	2.04640
R22	1.91443	-0.00004	0.00000	-0.00005	-0.00005	1.91437
R23	1.92575	0.00148	0.00000	0.00183	0.00222	1.92796
R24	3.85171	-0.00005	0.00000	-0.00061	-0.00081	3.85091
R25	2.76855	0.00020	0.00000	0.00095	-0.00108	2.76747
R26	2.72952	-0.00006	0.00000	-0.00031	0.00050	2.73002
R27	2.05579	-0.00029	0.00000	-0.00045	-0.00045	2.05534
R28	2.05226	0.00000	0.00000	0.00000	0.00000	2.05226
R29	2.74045	0.00030	0.00000	0.00005	0.00129	2.74175
R30	2.05571	0.00013	0.00000	0.00020	0.00020	2.05591
R31	2.84076	0.00040	0.00000	0.00069	0.00069	2.84145
R32	2.06766	-0.00004	0.00000	-0.00007	-0.00007	2.06759
R33	2.06812	-0.00001	0.00000	-0.00001	-0.00001	2.06811
R34	2.06430	0.00016	0.00000	0.00025	0.00025	2.06455
A1	1.87582	-0.00113	0.00000	-0.00199	-0.00199	1.87383
A2	2.27735	0.00032	0.00000	0.00015	0.00015	2.27750
A3	2.12994	0.00081	0.00000	0.00182	0.00182	2.13175
A4	1.86370	-0.00122	0.00000	-0.00155	-0.00156	1.86214
A5	2.27582	0.00055	0.00000	0.00057	0.00057	2.27639
A6	2.14364	0.00067	0.00000	0.00099	0.00099	2.14463
A7	1.89715	0.00076	0.00000	0.00193	0.00193	1.89908
A8	2.25444	0.00034	0.00000	0.00065	0.00064	2.25508
A9	2.13152	-0.00110	0.00000	-0.00252	-0.00252	2.12899
A10	1.88963	-0.00033	0.00000	-0.00191	-0.00191	1.88771
A11	2.19899	0.00024	0.00000	0.00120	0.00120	2.20019
A12	2.19456	0.00009	0.00000	0.00071	0.00071	2.19527
A13	1.89846	0.00192	0.00000	0.00351	0.00351	1.90197
A14	2.20428	0.00279	0.00000	0.00644	0.00642	2.21070
A15	2.17955	-0.00472	0.00000	-0.01005	-0.01004	2.16952
A16	1.97780	-0.00383	0.00000	-0.01005	-0.00973	1.96807
A17	1.85920	0.00086	0.00000	-0.00170	-0.00182	1.85738
A18	1.88275	0.00130	0.00000	0.00489	0.00480	1.88755
A19	1.91764	0.00086	0.00000	0.00002	-0.00008	1.91756

A20	1.92599	0.00157	0.00000	0.00697	0.00688	1.93287
A21	1.89776	-0.00071	0.00000	-0.00010	-0.00006	1.89770
A22	1.90792	0.00105	0.00000	0.00492	0.00500	1.91292
A23	1.88670	0.00135	0.00000	0.00276	0.00289	1.88958
A24	1.88584	-0.00287	0.00000	-0.00761	-0.00801	1.87784
A25	1.87726	-0.00057	0.00000	0.00012	0.00005	1.87731
A26	1.90304	0.00108	0.00000	0.00425	0.00437	1.90741
A27	2.00172	0.00006	0.00000	-0.00393	-0.00381	1.99791
A28	2.16943	0.00070	0.00000	0.00174	0.00174	2.17117
A29	1.95173	-0.00033	0.00000	-0.00079	-0.00079	1.95093
A30	2.16199	-0.00036	0.00000	-0.00090	-0.00091	2.16108
A31	2.07890	0.00001	0.00000	0.00002	0.00002	2.07892
A32	2.15812	0.00005	0.00000	0.00018	0.00018	2.15830
A33	2.04616	-0.00006	0.00000	-0.00020	-0.00020	2.04596
A34	1.93808	0.00015	0.00000	-0.00020	0.00650	1.94458
A35	1.92507	-0.00164	0.00000	-0.00579	-0.00388	1.92119
A36	1.87897	0.00082	0.00000	0.00280	0.00074	1.87970
A37	2.08984	-0.00051	0.00000	-0.00194	-0.00004	2.08980
A38	2.06695	0.00045	0.00000	0.00199	-0.00008	2.06687
A39	1.99362	0.00026	0.00000	0.00072	-0.00026	1.99336
A40	2.01021	-0.00039	0.00000	-0.00135	-0.00076	2.00945
A41	2.03429	0.00007	0.00000	0.00029	0.00034	2.03463
A42	2.01638	0.00032	0.00000	0.00109	-0.00071	2.01568
A43	2.14013	-0.00025	0.00000	-0.00094	0.00077	2.14090
A44	1.97124	-0.00031	0.00000	-0.00082	-0.00017	1.97107
A45	2.02503	0.00053	0.00000	0.00179	0.00069	2.02571
A46	2.03987	-0.00013	0.00000	-0.00047	-0.00035	2.03951
A47	2.42962	0.00027	0.00000	0.00336	0.00201	2.43163
A48	2.43694	0.00037	0.00000	0.00343	0.00182	2.43876
A49	1.93282	0.00001	0.00000	0.00004	0.00004	1.93286
A50	1.91868	0.00014	0.00000	0.00056	0.00056	1.91924
A51	1.93879	0.00000	0.00000	-0.00008	-0.00008	1.93871
A52	1.88107	-0.00004	0.00000	0.00005	0.00005	1.88112
A53	1.89326	-0.00004	0.00000	-0.00030	-0.00030	1.89296
A54	1.89784	-0.00008	0.00000	-0.00028	-0.00028	1.89756
A55	3.14159	-0.00093	0.00000	-0.10841	-0.10841	3.03318
A56	3.14728	-0.00278	0.00000	-0.27722	-0.27898	2.86830
A57	3.14159	-0.00017	0.00000	-0.01960	-0.01960	3.12199
A58	3.18695	-0.00008	0.00000	0.00296	0.00029	3.18724
D1	0.00150	0.00016	0.00000	0.00380	0.00379	0.00529
D2	-3.13144	0.00013	0.00000	0.00311	0.00311	-3.12833
D3	3.12970	0.00011	0.00000	0.00177	0.00175	3.13146
D4	-0.00324	0.00007	0.00000	0.00108	0.00107	-0.00217
D5	-0.00475	-0.00016	0.00000	-0.00350	-0.00352	-0.00826

D6	-3.10257	0.00006	0.00000	-0.00085	-0.00088	-3.10345
D7	-3.13432	-0.00011	0.00000	-0.00167	-0.00167	-3.13600
D8	0.05104	0.00011	0.00000	0.00098	0.00096	0.05200
D9	0.00223	-0.00013	0.00000	-0.00283	-0.00282	-0.00060
D10	3.13064	0.00008	0.00000	0.00236	0.00237	3.13301
D11	3.13598	-0.00010	0.00000	-0.00221	-0.00221	3.13377
D12	-0.01879	0.00011	0.00000	0.00299	0.00299	-0.01580
D13	-0.00521	0.00003	0.00000	0.00068	0.00066	-0.00454
D14	3.13239	0.00004	0.00000	0.00055	0.00056	3.13295
D15	-3.13473	-0.00017	0.00000	-0.00410	-0.00411	-3.13884
D16	0.00287	-0.00016	0.00000	-0.00423	-0.00421	-0.00135
D17	-0.00639	0.00003	0.00000	0.00049	0.00050	-0.00590
D18	-3.13846	-0.00023	0.00000	-0.00494	-0.00494	3.13979
D19	3.12046	0.00027	0.00000	0.00634	0.00633	3.12679
D20	-0.01161	0.00002	0.00000	0.00090	0.00090	-0.01071
D21	0.00615	0.00008	0.00000	0.00172	0.00174	0.00789
D22	3.10474	0.00010	0.00000	-0.00038	-0.00032	3.10442
D23	-3.13146	0.00006	0.00000	0.00185	0.00184	-3.12962
D24	-0.03287	0.00008	0.00000	-0.00026	-0.00022	-0.03309
D25	1.42900	0.00047	0.00000	0.01175	0.01173	1.44073
D26	-2.74354	-0.00020	0.00000	0.00455	0.00460	-2.73894
D27	-0.70859	0.00005	0.00000	0.00599	0.00597	-0.70261
D28	-1.66207	0.00052	0.00000	0.01440	0.01434	-1.64773
D29	0.44857	-0.00015	0.00000	0.00720	0.00721	0.45578
D30	2.48353	0.00011	0.00000	0.00864	0.00858	2.49211
D31	-1.11654	-0.00063	0.00000	-0.02034	-0.02036	-1.13690
D32	0.92201	0.00001	0.00000	-0.01599	-0.01593	0.90608
D33	3.09776	-0.00087	0.00000	-0.02382	-0.02376	3.07400
D34	3.08932	0.00019	0.00000	-0.01164	-0.01172	3.07759
D35	-1.15531	0.00083	0.00000	-0.00729	-0.00730	-1.16261
D36	1.02044	-0.00005	0.00000	-0.01512	-0.01513	1.00531
D37	0.99686	-0.00046	0.00000	-0.01593	-0.01596	0.98091
D38	3.03542	0.00018	0.00000	-0.01157	-0.01153	3.02389
D39	-1.07202	-0.00070	0.00000	-0.01941	-0.01936	-1.09137
D40	2.86870	0.00026	0.00000	0.00855	0.00700	2.87570
D41	-1.33295	0.00033	0.00000	0.00816	0.00955	-1.32340
D42	0.79671	0.00004	0.00000	0.00462	0.00318	0.79989
D43	2.87824	0.00010	0.00000	0.00423	0.00573	2.88397
D44	-1.30913	-0.00006	0.00000	0.00398	0.00246	-1.30667
D45	0.77240	0.00000	0.00000	0.00359	0.00501	0.77741
D46	-3.13475	-0.00026	0.00000	-0.00496	-0.00496	-3.13971
D47	0.00412	-0.00009	0.00000	-0.00219	-0.00219	0.00193
D48	-0.00381	0.00003	0.00000	0.00111	0.00111	-0.00269
D49	3.13506	0.00019	0.00000	0.00389	0.00389	3.13894

D50	1.23827	-0.00007	0.00000	-0.06000	-0.05313	1.18514
D51	-0.54990	0.00059	0.00000	0.09629	0.09681	-0.45309
D52	-2.94408	-0.00048	0.00000	-0.08250	-0.08313	-3.02721
D53	1.55094	0.00018	0.00000	0.07379	0.06680	1.61774
D54	-2.70450	0.00002	0.00000	0.00009	0.00021	-2.70429
D55	-0.01281	-0.00012	0.00000	-0.00077	-0.00061	-0.01342
D56	-0.02586	0.00007	0.00000	0.00097	0.00083	-0.02502
D57	2.66583	-0.00007	0.00000	0.00010	0.00002	2.66584
D58	2.00606	-0.00002	0.00000	-0.00432	-0.00285	2.00321
D59	-0.41768	0.00002	0.00000	-0.00402	-0.00217	-0.41985
D60	0.45243	0.00008	0.00000	0.00534	0.00358	0.45601
D61	-1.97095	0.00003	0.00000	0.00497	0.00354	-1.96741
D62	2.55225	-0.00001	0.00000	-0.00038	-0.00007	2.55218
D63	-1.65421	0.00004	0.00000	0.00006	0.00038	-1.65383
D64	0.44720	0.00003	0.00000	0.00002	0.00034	0.44754
D65	1.34982	-0.00005	0.00000	-0.00060	-0.00083	1.34899
D66	-2.85663	0.00000	0.00000	-0.00016	-0.00039	-2.85702
D67	-0.75523	-0.00001	0.00000	-0.00019	-0.00043	-0.75565
D68	-1.04487	-0.00005	0.00000	-0.00089	-0.00097	-1.04585
D69	1.03186	0.00000	0.00000	-0.00045	-0.00053	1.03133
D70	3.13326	0.00000	0.00000	-0.00048	-0.00057	3.13269

Item	Value	Threshold	Converged?
Maximum Force	0.006212	0.000450	NO
RMS Force	0.001033	0.000300	NO
Maximum Displacement	1.721010	0.001800	NO
RMS Displacement	0.406857	0.001200	NO

Predicted change in Energy=-1.125349D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.765904	2.070912	-0.269591
2	6	0	-3.621789	1.068366	0.054519
3	7	0	-2.864730	-0.097392	0.121944
4	6	0	-1.582615	0.201191	-0.156773
5	7	0	-1.504508	1.511125	-0.402991
6	6	0	-0.248045	2.228488	-0.704740
7	6	0	0.389590	2.856228	0.539072
8	1	0	-2.946325	3.120423	-0.427342
9	1	0	-4.681690	1.086811	0.231798
10	1	0	0.430883	1.492489	-1.138125

11	1	0	-0.463595	2.990494	-1.454740
12	1	0	-0.266408	3.639666	0.932482
13	1	0	0.477451	2.077734	1.311774
14	35	0	1.048560	-1.731187	-0.123782
15	1	0	-0.728101	-0.519555	-0.175496
16	6	0	-3.279580	-1.422960	0.433645
17	6	0	-4.525158	-1.767820	0.730998
18	1	0	-2.450795	-2.121620	0.403077
19	1	0	-4.745061	-2.802012	0.956296
20	1	0	-5.350491	-1.067475	0.763078
21	7	0	1.658221	3.449554	0.132263
22	1	0	2.010705	4.087510	0.835843
23	1	0	2.358402	2.720071	-0.003670
24	6	0	3.346493	-0.212708	-1.065515
25	6	0	3.276232	-0.406680	0.384362
26	8	0	3.314082	0.929000	-0.180925
27	1	0	4.293409	-0.349405	-1.582835
28	1	0	2.445670	-0.367513	-1.652005
29	1	0	2.296391	-0.674523	0.773957
30	6	0	4.468008	-0.809555	1.207928
31	1	0	4.424707	-0.353208	2.201392
32	1	0	4.481301	-1.895933	1.339480
33	1	0	5.399807	-0.503147	0.726838

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357455	0.000000			
3	N	2.205586	1.391646	0.000000		
4	C	2.215572	2.225953	1.345605	0.000000	
5	N	1.386462	2.210934	2.170965	1.335160	0.000000
6	C	2.560039	3.647534	3.597244	2.488228	1.477959
7	C	3.350792	4.418417	4.414575	3.379796	2.506870
8	H	1.076527	2.213454	3.265380	3.233393	2.160849
9	H	2.211353	1.074783	2.171578	3.246471	3.267642
10	H	3.362793	4.245755	3.869956	2.585475	2.070389
11	H	2.747878	3.993323	4.217395	3.273704	2.092417
12	H	3.186448	4.317520	4.623187	3.839530	2.801262
13	H	3.608340	4.404916	4.161375	3.149907	2.681348
14	Br	5.387704	5.448069	4.247765	3.264698	4.136267
15	H	3.297275	3.308751	2.198153	1.118043	2.185915
16	C	3.600770	2.543137	1.423512	2.422013	3.529829
17	C	4.339587	3.052483	2.432755	3.650164	4.600189
18	H	4.257828	3.415953	2.085156	2.542168	3.839536

19	H	5.400487	4.129743	3.398052	4.501024	5.563452
20	H	4.194754	2.837654	2.744288	4.080750	4.774984
21	N	4.651347	5.792634	5.747871	4.597654	3.747914
22	H	5.301381	6.438220	6.464744	5.385230	4.530915
23	H	5.172101	6.204369	5.935906	4.679723	4.067319
24	C	6.573417	7.173045	6.324764	5.029238	5.190641
25	C	6.563042	7.061675	6.154343	4.926533	5.210890
26	O	6.186927	6.941265	6.270800	4.950549	4.858703
27	H	7.577365	8.206179	7.362658	6.071612	6.202375
28	H	5.917558	6.464367	5.605373	4.334308	4.548981
29	H	5.852627	6.211289	5.234059	4.084094	4.539724
30	C	7.925253	8.384614	7.446850	6.284429	6.606933
31	H	7.980413	8.448433	7.584552	6.477362	6.739001
32	H	8.417063	8.723432	7.660373	6.588458	7.104517
33	H	8.619599	9.182094	8.296572	7.073265	7.280342

		6	7	8	9	10
6	C	0.000000				
7	C	1.532222	0.000000			
8	H	2.855383	3.483115	0.000000		
9	H	4.673086	5.379883	2.753459	0.000000	
10	H	1.091083	2.162055	3.815877	5.308453	0.000000
11	H	1.090695	2.172841	2.690051	4.925520	1.773234
12	H	2.161540	1.094934	3.049703	5.148081	3.063332
13	H	2.148348	1.100382	3.979192	5.363303	2.519263
14	Br	4.206866	4.681666	6.292009	6.395570	3.435477
15	H	2.839418	3.627086	4.270057	4.286860	2.513607
16	C	4.880491	5.637852	4.636236	2.881944	4.973714
17	C	6.027065	6.750808	5.265870	2.902175	6.219773
18	H	5.000280	5.732822	5.330494	3.911555	4.872489
19	H	6.948966	7.652085	6.342330	3.956243	7.044128
20	H	6.249225	6.956591	4.973490	2.317434	6.602444
21	N	2.413592	1.458408	4.650090	6.766604	2.636351
22	H	3.306253	2.057216	5.206058	7.359158	3.623054
23	H	2.743486	2.046784	5.336657	7.230897	2.551328
24	C	4.360080	4.553717	7.149586	8.235502	3.378424
25	C	4.533297	4.359267	7.198579	8.098291	3.744438
26	O	3.827767	3.575647	6.637451	8.007972	3.089755
27	H	5.295412	5.478903	8.111019	9.268658	4.302261
28	H	3.859098	4.406902	6.537516	7.514189	2.789811
29	H	4.133784	4.019610	6.582614	7.217330	3.439784
30	C	5.926985	5.524384	8.549337	9.394999	5.205934
31	H	6.078269	5.417190	8.562036	9.427588	5.523549
32	H	6.599727	6.321849	9.135377	9.699697	5.833165
33	H	6.435019	6.035141	9.171713	10.218102	5.670172

		11	12	13	14	15
11	H	0.000000				
12	H	2.481760	0.000000			
13	H	3.061421	1.771108	0.000000		
14	Br	5.133453	5.629467	4.110336	0.000000	
15	H	3.745247	4.328960	3.226645	2.151104	0.000000
16	C	5.565460	5.912548	5.209726	4.374760	2.774390
17	C	6.626862	6.886106	6.336536	5.639000	4.098480
18	H	5.790869	6.184192	5.199512	3.560267	2.422609
19	H	7.595866	7.845644	7.156321	5.989932	4.756736
20	H	6.728118	6.930640	6.645172	6.494219	4.748434
21	N	2.689130	2.093010	2.160406	5.222769	4.641452
22	H	3.545754	2.322745	2.572270	5.975269	5.454256
23	H	3.184713	2.934563	2.383477	4.641531	4.477856
24	C	4.992872	5.646754	4.373674	2.910865	4.181937
25	C	5.376746	5.405891	3.855590	2.641032	4.044856
26	O	4.488119	4.626802	3.405027	3.494632	4.293901
27	H	5.813814	6.559836	5.369478	3.816701	5.217769
28	H	4.447353	5.485656	4.317071	2.479312	3.503715
29	H	5.100682	5.020488	3.342559	1.865357	3.173803
30	C	6.771328	6.502779	4.926638	3.783580	5.384933
31	H	6.960110	6.289653	4.720352	4.324769	5.677032
32	H	7.492452	7.304057	5.641064	3.735236	5.597091
33	H	7.165493	7.022192	5.588620	4.600542	6.194007

		16	17	18	19	20
16	C	0.000000				
17	C	1.326202	0.000000			
18	H	1.084411	2.129716	0.000000		
19	H	2.079083	1.081051	2.456144	0.000000	
20	H	2.126868	1.082906	3.106293	1.847295	0.000000
21	N	6.943637	8.112561	6.927866	8.986831	8.362028
22	H	7.649454	8.775726	7.658038	9.649891	8.987010
23	H	7.010191	8.250109	6.836357	9.048432	8.623249
24	C	6.900509	8.222452	6.277679	8.733010	8.928152
25	C	6.634299	7.926824	5.978311	8.390820	8.660278
26	O	7.027502	8.340152	6.548370	8.953408	8.941581
27	H	7.910049	9.226747	7.250440	9.703423	9.951067
28	H	6.184043	7.498801	5.592461	8.027244	8.191624
29	H	5.636259	6.908739	4.976687	7.358091	7.656979
30	C	7.810307	9.056642	7.087956	9.429414	9.831954
31	H	7.976549	9.179502	7.323505	9.572437	9.906231
32	H	7.827868	9.027899	6.998695	9.278662	9.883456
33	H	8.732913	10.005216	8.022233	10.404604	10.765160

		21	22	23	24	25

21	N	0.000000				
22	H	1.013043	0.000000			
23	H	1.020233	1.641817	0.000000		
24	C	4.206791	4.887879	3.271854	0.000000	
25	C	4.189517	4.690750	3.281700	1.464481	0.000000
26	O	3.032021	3.564939	2.037812	1.444662	1.450870
27	H	4.931315	5.544994	3.957234	1.087638	2.215354
28	H	4.286454	5.121114	3.501113	1.086009	2.199581
29	H	4.222208	4.770996	3.483075	2.167866	1.087939
30	C	5.214591	5.491633	4.286802	2.604336	1.503629
31	H	5.137677	5.235656	4.310099	3.443104	2.150222
32	H	6.164526	6.493002	5.255306	3.147227	2.140634
33	H	5.475109	5.707190	4.491427	2.740982	2.153176

		26	27	28	29	30
26	O	0.000000				
27	H	2.135124	0.000000			
28	H	2.144565	1.849122	0.000000		
29	H	2.125742	3.106164	2.449863	0.000000	
30	C	2.506598	2.833828	3.530505	2.218667	0.000000
31	H	2.924547	3.786506	4.331911	2.582739	1.094120
32	H	3.413836	3.311643	3.927956	2.566221	1.094394
33	H	2.687997	2.565608	3.795288	3.108501	1.092512

		31	32	33
31	H	0.000000		
32	H	1.768077	0.000000	
33	H	1.774150	1.777311	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.008134	1.867739	-0.215860
2	6	0	-3.825724	0.816787	0.048207
3	7	0	-3.023839	-0.320548	0.059392
4	6	0	-1.752950	0.042151	-0.193480
5	7	0	-1.725021	1.365389	-0.369297
6	6	0	-0.496087	2.146183	-0.623154
7	6	0	0.109656	2.731109	0.656940

8	1	0	-3.228780	2.916343	-0.319084
9	1	0	-4.886476	0.784482	0.218265
10	1	0	0.213562	1.461312	-1.089856
11	1	0	-0.737335	2.938097	-1.333286
12	1	0	-0.578727	3.466339	1.086412
13	1	0	0.223840	1.916562	1.387910
14	35	0	0.951874	-1.785334	-0.243283
15	1	0	-0.870698	-0.642758	-0.243991
16	6	0	-3.387987	-1.675985	0.297244
17	6	0	-4.620652	-2.084430	0.566547
18	1	0	-2.532247	-2.339227	0.235885
19	1	0	-4.800983	-3.136934	0.735032
20	1	0	-5.473016	-1.419454	0.629531
21	7	0	1.356189	3.394208	0.291688
22	1	0	1.679529	4.007009	1.030730
23	1	0	2.085206	2.700818	0.122516
24	6	0	3.193460	-0.130524	-1.085917
25	6	0	3.123021	-0.404059	0.351066
26	8	0	3.111442	0.960303	-0.142297
27	1	0	4.147802	-0.202494	-1.602646
28	1	0	2.302602	-0.288814	-1.686527
29	1	0	2.152360	-0.730223	0.718554
30	6	0	4.325223	-0.803537	1.161020
31	1	0	4.258653	-0.402802	2.176933
32	1	0	4.380462	-1.894038	1.234876
33	1	0	5.246860	-0.435886	0.703855

Rotational constants (GHZ): 0.5606114 0.2692082 0.1925052

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1360.4068164194 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 3.81D-06 NBF= 482

NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"

B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999061 -0.020329 0.006155 -0.037753 Ang= -4.97 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3205.58899522 A.U. after 13 cycles
NFock= 13 Conv=0.39D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000025924	-0.000407442	-0.000270628
2	6	-0.000141644	-0.000298377	0.000239676
3	7	-0.000085869	0.000205728	0.000514613
4	6	0.001594701	0.001947172	-0.001242721
5	7	-0.000180504	-0.000764364	0.000719707
6	6	0.000020360	-0.001640552	-0.001669958
7	6	0.002036129	0.000219340	0.000575917
8	1	0.000051849	-0.000040660	0.000100671
9	1	0.000085700	-0.000069878	0.000005950
10	1	0.000281657	0.000963512	0.000391193
11	1	-0.000017674	-0.000219099	0.000076468
12	1	-0.000079401	0.000165660	0.000067399
13	1	0.000160590	-0.000045250	0.000178920
14	35	-0.076919862	-0.053444292	-0.016699409
15	1	-0.002500044	0.001613144	0.000272783
16	6	0.000071804	0.000257217	-0.000053901
17	6	-0.000177319	-0.000288476	-0.000024321

18	1	-0.000223780	0.000020942	-0.000016913
19	1	-0.000052592	-0.000089982	-0.000003722
20	1	0.000095817	-0.000052515	0.000041254
21	7	-0.001416445	0.000648887	0.000140739
22	1	-0.000950901	0.000237208	0.000317852
23	1	0.000105404	-0.001556439	-0.000343172
24	6	0.007399900	0.003976953	0.000542228
25	6	0.029861960	0.016698051	0.011426177
26	8	0.002714725	0.012935484	-0.002717922
27	1	0.001549812	0.000095349	0.000018716
28	1	0.005527422	0.001663647	0.000139437
29	1	0.026534596	0.016998375	0.009175826
30	6	0.003067638	0.000247701	-0.002422418
31	1	-0.000172884	0.000371396	0.000085807
32	1	-0.000236071	-0.000053520	-0.000112932
33	1	0.002020850	-0.000294921	0.000546682

Cartesian Forces: Max 0.076919862 RMS 0.010906056

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.512398338 RMS 0.091708097
Search for a local minimum.
Step number 2 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 2 1
DE= 5.72D-02 DEPred=-1.13D-03 R=-5.09D+01
Trust test=-5.09D+01 RLast= 3.43D-01 DXMaxT set to 1.50D-01
ITU= -1 0
Use linear search instead of GDIIS.
Energy rises -- skip Quadratic/GDIIS search.
Quartic linear search produced a step of -0.86213.
Iteration 1 RMS(Cart)= 0.26964107 RMS(Int)= 0.00918628
Iteration 2 RMS(Cart)= 0.08749322 RMS(Int)= 0.00079809
Iteration 3 RMS(Cart)= 0.00242295 RMS(Int)= 0.00013539
Iteration 4 RMS(Cart)= 0.00000086 RMS(Int)= 0.00013539

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56522	-0.04482	0.00040	0.00000	0.00040	2.56562
R2	2.62003	0.02700	-0.00058	0.00000	-0.00058	2.61945
R3	2.03434	-0.00006	0.00001	0.00000	0.00001	2.03435

R4	2.62983	-0.05381	-0.00038	0.00000	-0.00037	2.62945
R5	2.03105	-0.00008	0.00019	0.00000	0.00019	2.03123
R6	2.54283	0.01307	0.00115	0.00000	0.00115	2.54397
R7	2.69005	0.00022	-0.00060	0.00000	-0.00060	2.68945
R8	2.52309	0.11254	0.00544	0.00000	0.00544	2.52852
R9	2.11280	-0.02701	0.00035	0.00000	0.00035	2.11314
R10	2.79294	0.08853	0.00625	0.00000	0.00625	2.79919
R11	2.89548	0.06592	-0.00063	0.00000	-0.00063	2.89485
R12	2.06185	-0.00063	0.00060	0.00000	0.00060	2.06245
R13	2.06111	-0.00020	0.00042	0.00000	0.00042	2.06153
R14	2.06913	0.00019	-0.00030	0.00000	-0.00030	2.06882
R15	2.07942	0.00017	-0.00018	0.00000	-0.00018	2.07924
R16	2.75599	0.08357	0.00497	0.00000	0.00497	2.76096
R17	4.06500	-0.03383	-0.00311	0.00000	-0.00311	4.06189
R18	2.50616	0.00024	-0.00060	0.00000	-0.00060	2.50556
R19	2.04924	-0.00018	0.00026	0.00000	0.00026	2.04950
R20	2.04289	0.00010	-0.00024	0.00000	-0.00024	2.04265
R21	2.04640	-0.00011	0.00029	0.00000	0.00029	2.04669
R22	1.91437	0.00004	0.00005	0.00000	0.00005	1.91442
R23	1.92796	0.02181	-0.00191	0.00000	-0.00192	1.92604
R24	3.85091	-0.01438	0.00070	0.00000	0.00070	3.85161
R25	2.76747	-0.04122	0.00093	0.00000	0.00114	2.76861
R26	2.73002	0.01145	-0.00043	0.00000	-0.00051	2.72950
R27	2.05534	0.00133	0.00039	0.00000	0.00039	2.05573
R28	2.05226	-0.00490	0.00000	0.00000	0.00000	2.05226
R29	2.74175	0.00000	-0.00111	0.00000	-0.00124	2.74051
R30	2.05591	-0.02480	-0.00017	0.00000	-0.00017	2.05574
R31	2.84145	0.00260	-0.00059	0.00000	-0.00059	2.84085
R32	2.06759	0.00024	0.00006	0.00000	0.00006	2.06765
R33	2.06811	0.00003	0.00001	0.00000	0.00001	2.06812
R34	2.06455	0.00140	-0.00021	0.00000	-0.00021	2.06433
A1	1.87383	0.06062	0.00172	0.00000	0.00172	1.87554
A2	2.27750	-0.03027	-0.00013	0.00000	-0.00013	2.27737
A3	2.13175	-0.03026	-0.00157	0.00000	-0.00157	2.13019
A4	1.86214	-0.01202	0.00134	0.00000	0.00135	1.86349
A5	2.27639	0.00603	-0.00049	0.00000	-0.00049	2.27589
A6	2.14463	0.00591	-0.00086	0.00000	-0.00086	2.14377
A7	1.89908	0.04244	-0.00167	0.00000	-0.00167	1.89742
A8	2.25508	-0.02100	-0.00055	0.00000	-0.00055	2.25453
A9	2.12899	-0.02138	0.00218	0.00000	0.00218	2.13117
A10	1.88771	-0.02198	0.00165	0.00000	0.00165	1.88937
A11	2.20019	-0.24246	-0.00103	0.00000	-0.00103	2.19916
A12	2.19527	0.26460	-0.00062	0.00000	-0.00062	2.19465
A13	1.90197	-0.06892	-0.00303	0.00000	-0.00303	1.89894

A14	2.21070	-0.31015	-0.00554	0.00000	-0.00554	2.20517
A15	2.16952	0.37957	0.00865	0.00000	0.00865	2.17817
A16	1.96807	-0.00752	0.00839	0.00000	0.00838	1.97645
A17	1.85738	0.07427	0.00156	0.00000	0.00157	1.85895
A18	1.88755	-0.06701	-0.00414	0.00000	-0.00414	1.88341
A19	1.91756	0.05426	0.00007	0.00000	0.00008	1.91763
A20	1.93287	-0.04902	-0.00593	0.00000	-0.00593	1.92694
A21	1.89770	-0.00163	0.00005	0.00000	0.00005	1.89775
A22	1.91292	-0.10746	-0.00431	0.00000	-0.00431	1.90861
A23	1.88958	0.00620	-0.00249	0.00000	-0.00249	1.88709
A24	1.87784	0.16714	0.00690	0.00000	0.00692	1.88475
A25	1.87731	0.02403	-0.00005	0.00000	-0.00004	1.87727
A26	1.90741	-0.12173	-0.00377	0.00000	-0.00377	1.90364
A27	1.99791	0.02418	0.00329	0.00000	0.00328	2.00119
A28	2.17117	0.00050	-0.00150	0.00000	-0.00150	2.16967
A29	1.95093	-0.00013	0.00069	0.00000	0.00069	1.95162
A30	2.16108	-0.00037	0.00078	0.00000	0.00078	2.16186
A31	2.07892	0.00004	-0.00002	0.00000	-0.00002	2.07890
A32	2.15830	-0.00003	-0.00015	0.00000	-0.00015	2.15814
A33	2.04596	-0.00001	0.00017	0.00000	0.00017	2.04614
A34	1.94458	-0.14069	-0.00560	0.00000	-0.00637	1.93821
A35	1.92119	0.51240	0.00335	0.00000	0.00318	1.92437
A36	1.87970	-0.20127	-0.00064	0.00000	-0.00046	1.87924
A37	2.08980	0.00388	0.00003	0.00000	-0.00020	2.08960
A38	2.06687	-0.00386	0.00007	0.00000	0.00032	2.06719
A39	1.99336	-0.00754	0.00022	0.00000	0.00034	1.99370
A40	2.00945	0.00423	0.00066	0.00000	0.00058	2.01003
A41	2.03463	-0.00054	-0.00030	0.00000	-0.00030	2.03433
A42	2.01568	-0.00805	0.00061	0.00000	0.00083	2.01651
A43	2.14090	0.00895	-0.00067	0.00000	-0.00089	2.14001
A44	1.97107	0.00114	0.00015	0.00000	0.00006	1.97113
A45	2.02571	-0.01043	-0.00059	0.00000	-0.00046	2.02525
A46	2.03951	-0.00062	0.00031	0.00000	0.00029	2.03981
A47	2.43163	-0.01745	-0.00173	0.00000	-0.00154	2.43009
A48	2.43876	0.00940	-0.00157	0.00000	-0.00135	2.43740
A49	1.93286	-0.00081	-0.00004	0.00000	-0.00004	1.93283
A50	1.91924	-0.00072	-0.00048	0.00000	-0.00048	1.91876
A51	1.93871	0.00252	0.00007	0.00000	0.00007	1.93878
A52	1.88112	0.00038	-0.00004	0.00000	-0.00004	1.88108
A53	1.89296	-0.00073	0.00026	0.00000	0.00026	1.89322
A54	1.89756	-0.00071	0.00024	0.00000	0.00024	1.89780
A55	3.03318	0.36127	0.09347	0.00000	0.09347	3.12665
A56	2.86830	0.43109	0.24051	0.00000	0.24084	3.10914
A57	3.12199	-0.01148	0.01690	0.00000	0.01690	3.13889

A58	3.18724	0.08879	-0.00025	0.00000	0.00011	3.18735
D1	0.00529	-0.01443	-0.00327	0.00000	-0.00327	0.00203
D2	-3.12833	-0.00256	-0.00268	0.00000	-0.00268	-3.13101
D3	3.13146	-0.00718	-0.00151	0.00000	-0.00151	3.12994
D4	-0.00217	0.00470	-0.00092	0.00000	-0.00092	-0.00309
D5	-0.00826	0.01648	0.00303	0.00000	0.00303	-0.00523
D6	-3.10345	-0.00701	0.00076	0.00000	0.00076	-3.10269
D7	-3.13600	0.01006	0.00144	0.00000	0.00144	-3.13455
D8	0.05200	-0.01343	-0.00083	0.00000	-0.00083	0.05118
D9	-0.00060	0.00811	0.00243	0.00000	0.00243	0.00184
D10	3.13301	0.01571	-0.00205	0.00000	-0.00205	3.13096
D11	3.13377	-0.00264	0.00190	0.00000	0.00190	3.13568
D12	-0.01580	0.00496	-0.00258	0.00000	-0.00258	-0.01838
D13	-0.00454	0.00208	-0.00057	0.00000	-0.00057	-0.00511
D14	3.13295	0.04439	-0.00048	0.00000	-0.00049	3.13247
D15	-3.13884	-0.00484	0.00354	0.00000	0.00354	-3.13530
D16	-0.00135	0.03748	0.00363	0.00000	0.00363	0.00228
D17	-0.00590	-0.00434	-0.00043	0.00000	-0.00043	-0.00632
D18	3.13979	-0.00440	0.00426	0.00000	0.00426	-3.13914
D19	3.12679	0.00439	-0.00546	0.00000	-0.00546	3.12133
D20	-0.01071	0.00432	-0.00077	0.00000	-0.00077	-0.01148
D21	0.00789	-0.01175	-0.00150	0.00000	-0.00150	0.00639
D22	3.10442	-0.01103	0.00027	0.00000	0.00027	3.10469
D23	-3.12962	-0.05242	-0.00158	0.00000	-0.00158	-3.13121
D24	-0.03309	-0.05169	0.00019	0.00000	0.00019	-0.03291
D25	1.44073	-0.11515	-0.01011	0.00000	-0.01011	1.43062
D26	-2.73894	-0.00354	-0.00397	0.00000	-0.00397	-2.74291
D27	-0.70261	-0.00033	-0.00515	0.00000	-0.00515	-0.70776
D28	-1.64773	-0.12703	-0.01236	0.00000	-0.01236	-1.66009
D29	0.45578	-0.01541	-0.00621	0.00000	-0.00622	0.44957
D30	2.49211	-0.01221	-0.00740	0.00000	-0.00740	2.48471
D31	-1.13690	0.11442	0.01755	0.00000	0.01755	-1.11935
D32	0.90608	0.08733	0.01374	0.00000	0.01373	0.91981
D33	3.07400	0.22324	0.02049	0.00000	0.02048	3.09448
D34	3.07759	-0.01084	0.01011	0.00000	0.01011	3.08770
D35	-1.16261	-0.03792	0.00629	0.00000	0.00629	-1.15632
D36	1.00531	0.09799	0.01304	0.00000	0.01304	1.01835
D37	0.98091	-0.01269	0.01376	0.00000	0.01376	0.99466
D38	3.02389	-0.03977	0.00994	0.00000	0.00994	3.03383
D39	-1.09137	0.09614	0.01669	0.00000	0.01669	-1.07469
D40	2.87570	-0.13037	-0.00604	0.00000	-0.00584	2.86986
D41	-1.32340	-0.13596	-0.00823	0.00000	-0.00842	-1.33182
D42	0.79989	-0.03028	-0.00274	0.00000	-0.00255	0.79734
D43	2.88397	-0.03587	-0.00494	0.00000	-0.00513	2.87884

D44	-1.30667	0.01205	-0.00212	0.00000	-0.00193	-1.30860
D45	0.77741	0.00646	-0.00432	0.00000	-0.00451	0.77290
D46	-3.13971	-0.00006	0.00428	0.00000	0.00428	-3.13543
D47	0.00193	-0.00008	0.00189	0.00000	0.00189	0.00382
D48	-0.00269	0.00002	-0.00096	0.00000	-0.00096	-0.00365
D49	3.13894	0.00000	-0.00335	0.00000	-0.00335	3.13559
D50	1.18514	-0.00448	0.04580	0.00000	0.04501	1.23015
D51	-0.45309	-0.17284	-0.08346	0.00000	-0.08358	-0.53667
D52	-3.02721	0.10183	0.07167	0.00000	0.07179	-2.95542
D53	1.61774	-0.06654	-0.05759	0.00000	-0.05679	1.56096
D54	-2.70429	0.00194	-0.00018	0.00000	-0.00019	-2.70448
D55	-0.01342	0.00212	0.00052	0.00000	0.00050	-0.01292
D56	-0.02502	0.00055	-0.00072	0.00000	-0.00070	-0.02573
D57	2.66584	0.00073	-0.00001	0.00000	-0.00001	2.66584
D58	2.00321	0.00288	0.00246	0.00000	0.00228	2.00549
D59	-0.41985	0.00785	0.00187	0.00000	0.00165	-0.41820
D60	0.45601	-0.03958	-0.00309	0.00000	-0.00287	0.45314
D61	-1.96741	-0.02741	-0.00305	0.00000	-0.00287	-1.97028
D62	2.55218	0.00525	0.00006	0.00000	0.00002	2.55220
D63	-1.65383	0.00476	-0.00032	0.00000	-0.00036	-1.65419
D64	0.44754	0.00503	-0.00029	0.00000	-0.00033	0.44721
D65	1.34899	-0.00843	0.00072	0.00000	0.00074	1.34973
D66	-2.85702	-0.00892	0.00034	0.00000	0.00036	-2.85666
D67	-0.75565	-0.00866	0.00037	0.00000	0.00039	-0.75526
D68	-1.04585	0.00371	0.00084	0.00000	0.00085	-1.04500
D69	1.03133	0.00322	0.00046	0.00000	0.00047	1.03180
D70	3.13269	0.00349	0.00049	0.00000	0.00050	3.13319

Item	Value	Threshold	Converged?
Maximum Force	0.512398	0.000450	NO
RMS Force	0.091708	0.000300	NO
Maximum Displacement	1.503894	0.001800	NO
RMS Displacement	0.352974	0.001200	NO

Predicted change in Energy=-5.041719D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.897530	2.117300	-0.252093
2	6	0	-3.826214	1.176022	0.055807
3	7	0	-3.159673	-0.044374	0.105626
4	6	0	-1.857387	0.163386	-0.164877

5	7	0	-1.679415	1.470295	-0.389944
6	6	0	-0.374093	2.108404	-0.678215
7	6	0	0.302888	2.689411	0.567097
8	1	0	-2.999565	3.179476	-0.394547
9	1	0	-4.882256	1.270861	0.232308
10	1	0	0.258636	1.335440	-1.117920
11	1	0	-0.539537	2.890159	-1.420904
12	1	0	-0.312301	3.500764	0.969314
13	1	0	0.350545	1.898945	1.330986
14	35	0	0.496991	-2.101378	-0.235317
15	1	0	-1.058954	-0.619006	-0.193147
16	6	0	-3.674299	-1.338510	0.398636
17	6	0	-4.942619	-1.589598	0.692384
18	1	0	-2.900766	-2.097802	0.361616
19	1	0	-5.241436	-2.605955	0.907139
20	1	0	-5.711317	-0.827745	0.733615
21	7	0	1.600273	3.228077	0.165526
22	1	0	1.976212	3.841399	0.878837
23	1	0	2.268312	2.471309	0.024700
24	6	0	3.806329	-0.204625	-1.058672
25	6	0	3.791480	-0.411053	0.391720
26	8	0	3.559347	0.906090	-0.168965
27	1	0	4.756198	-0.151407	-1.586234
28	1	0	2.947607	-0.533134	-1.636682
29	1	0	2.888204	-0.866943	0.791313
30	6	0	5.048668	-0.571937	1.200145
31	1	0	4.927731	-0.134745	2.195839
32	1	0	5.277127	-1.634644	1.327315
33	1	0	5.895929	-0.087115	0.709808

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357667	0.000000			
3	N	2.206698	1.391448	0.000000		
4	C	2.215239	2.224952	1.346211	0.000000	
5	N	1.386154	2.212247	2.175081	1.338036	0.000000
6	C	2.559178	3.650378	3.606705	2.499355	1.481266
7	C	3.352768	4.427329	4.435749	3.403436	2.516286
8	H	1.076533	2.213593	3.266346	3.233283	2.159657
9	H	2.211389	1.074882	2.170986	3.245626	3.268817
10	H	3.364868	4.253122	3.884043	2.599915	2.074650
11	H	2.742911	3.990136	4.219821	3.278662	2.092418
12	H	3.176353	4.311207	4.628336	3.848608	2.799891

13	H	3.619918	4.426513	4.195192	3.181940	2.695567
14	Br	5.414822	5.432882	4.209359	3.267601	4.185391
15	H	3.297151	3.307844	2.198292	1.118227	2.188351
16	C	3.601311	2.542338	1.423194	2.423717	3.534233
17	C	4.337686	3.049631	2.431234	3.650548	4.602487
18	H	4.259546	3.415831	2.085457	2.545349	3.845498
19	H	5.398783	4.126860	3.396742	4.502250	5.566528
20	H	4.190741	2.833394	2.742066	4.079510	4.774894
21	N	4.651716	5.802563	5.776644	4.632162	3.762273
22	H	5.291964	6.438149	6.486479	5.414204	4.538232
23	H	5.185350	6.230729	5.983163	4.731157	4.093716
24	C	7.140282	7.836068	7.064450	5.745606	5.774594
25	C	7.179827	7.788511	6.966695	5.705215	5.837907
26	O	6.570023	7.393910	6.791467	5.467416	5.273688
27	H	8.093609	8.838334	8.095360	6.771917	6.743748
28	H	6.565630	7.188211	6.369725	5.073393	5.193978
29	H	6.593111	7.056776	6.141955	4.949395	5.265092
30	C	8.513697	9.117477	8.297780	7.077964	7.208758
31	H	8.502869	9.106558	8.353638	7.190250	7.274394
32	H	9.132175	9.611836	8.671856	7.507386	7.809168
33	H	9.116447	9.825645	9.075836	7.806519	7.811582

		6	7	8	9	10
6	C	0.000000				
7	C	1.531886	0.000000			
8	H	2.849696	3.474352	0.000000		
9	H	4.674833	5.386101	2.753232	0.000000	
10	H	1.091403	2.162054	3.813084	5.315642	0.000000
11	H	1.090916	2.168439	2.681204	4.920818	1.773705
12	H	2.157971	1.094774	3.030633	5.138107	3.061232
13	H	2.146128	1.100287	3.980008	5.383660	2.514582
14	Br	4.321714	4.861399	6.335509	6.366079	3.556334
15	H	2.853610	3.657623	4.270246	4.286052	2.532016
16	C	4.892053	5.663085	4.636442	2.880215	4.991785
17	C	6.035329	6.770595	5.263169	2.897851	6.235872
18	H	5.015725	5.763942	5.332092	3.910359	4.894690
19	H	6.959135	7.674377	6.339684	3.951469	7.063020
20	H	6.253015	6.969130	4.968316	2.311449	6.614218
21	N	2.421506	1.461037	4.634065	6.771879	2.651283
22	H	3.309323	2.055304	5.178611	7.352840	3.635511
23	H	2.758278	2.050526	5.331773	7.253606	2.575767
24	C	4.792784	4.826248	7.629771	8.907031	3.868002
25	C	4.984418	4.670536	7.721944	8.836738	4.220218
26	O	4.144496	3.785043	6.945395	8.459004	3.461149
27	H	5.679008	5.704301	8.524480	9.911091	4.760052

28	H	4.350870	4.715504	7.120058	8.249501	3.315305
29	H	4.653470	4.402474	7.241933	8.078536	3.925594
30	C	6.333940	5.793062	9.021652	10.146716	5.652957
31	H	6.434380	5.658430	8.974196	10.102823	5.911251
32	H	7.068865	6.634639	9.728525	10.623279	6.323435
33	H	6.786758	6.245924	9.540442	10.873885	6.094532

		11	12	13	14	15
11	H	0.000000				
12	H	2.477422	0.000000			
13	H	3.057392	1.770874	0.000000		
14	Br	5.234065	5.787062	4.298527	0.000000	
15	H	3.753854	4.345263	3.263395	2.149458	0.000000
16	C	5.569479	5.920074	5.248787	4.287602	2.776314
17	C	6.627318	6.886823	6.371447	5.541833	4.099886
18	H	5.799356	6.197854	5.242584	3.449797	2.426287
19	H	7.598349	7.848074	7.193332	5.872764	4.759386
20	H	6.723992	6.923939	6.673670	6.411245	4.748362
21	N	2.685095	2.092456	2.164881	5.457197	4.690436
22	H	3.538737	2.315493	2.573006	6.224631	5.500600
23	H	3.185784	2.934559	2.389940	4.910667	4.546230
24	C	5.347471	5.899640	4.698714	3.902217	4.959014
25	C	5.739452	5.698855	4.249511	3.755533	4.889992
26	O	4.722788	4.797674	3.678590	4.292701	4.863662
27	H	6.109276	6.749730	5.667794	4.875264	5.997944
28	H	4.891386	5.804356	4.633227	3.229354	4.259542
29	H	5.546091	5.417728	3.792242	2.880225	4.075622
30	C	7.077007	6.736480	5.309871	5.011736	6.264704
31	H	7.219549	6.494553	5.082765	5.423063	6.463912
32	H	7.865121	7.598834	6.062794	5.050679	6.594638
33	H	7.404006	7.175119	5.922970	5.839438	7.033394

		16	17	18	19	20
16	C	0.000000				
17	C	1.325884	0.000000			
18	H	1.084550	2.129986	0.000000		
19	H	2.078681	1.080922	2.456533	0.000000	
20	H	2.126625	1.083060	3.106546	1.847412	0.000000
21	N	6.980628	8.142298	6.975872	9.021913	8.380440
22	H	7.680516	8.797768	7.702372	9.677997	8.995560
23	H	7.068887	8.302668	6.907217	9.107888	8.663764
24	C	7.705143	9.029310	7.112416	9.565189	9.704955
25	C	7.523169	8.818381	6.901607	9.310039	9.518071
26	O	7.595132	8.902461	7.144084	9.536574	9.474495
27	H	8.741979	10.066158	8.137055	10.592186	10.742811
28	H	6.974294	8.294355	6.375331	8.822020	8.982320

29	H	6.591132	7.864719	5.933955	8.314363	8.599804
30	C	8.793190	10.055807	8.137867	10.493299	10.773131
31	H	8.869831	10.089637	8.276674	10.544173	10.761398
32	H	9.004342	10.239550	8.247728	10.571668	11.034015
33	H	9.656711	10.942206	9.030279	11.420350	11.630875

		21	22	23	24	25
21	N	0.000000				
22	H	1.013068	0.000000			
23	H	1.019218	1.640738	0.000000		
24	C	4.260139	4.844954	3.271057	0.000000	
25	C	4.253918	4.649283	3.280664	1.465083	0.000000
26	O	3.056384	3.495747	2.038183	1.444391	1.450213
27	H	4.944637	5.454117	3.957691	1.087844	2.215942
28	H	4.382918	5.138870	3.499758	1.086010	2.200327
29	H	4.338152	4.796652	3.480788	2.168885	1.087850
30	C	5.234689	5.387092	4.286420	2.603954	1.503315
31	H	5.148079	5.124030	4.310205	3.443002	2.149944
32	H	6.206050	6.409697	5.254391	3.146607	2.140014
33	H	5.453384	5.552115	4.491604	2.740029	2.152864

		26	27	28	29	30
26	O	0.000000				
27	H	2.135275	0.000000			
28	H	2.144711	1.849125	0.000000		
29	H	2.125138	3.107108	2.451554	0.000000	
30	C	2.505414	2.833071	3.530376	2.218507	0.000000
31	H	2.923715	3.785997	4.332184	2.582339	1.094152
32	H	3.412470	3.310608	3.927502	2.565856	1.094400
33	H	2.686691	2.564162	3.794411	3.108244	1.092399

		31	32	33
31	H	0.000000		
32	H	1.768080	0.000000	
33	H	1.774250	1.777379	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.935023	2.085935	-0.242722

2	6	0	-3.857630	1.136120	0.057127
3	7	0	-3.182967	-0.080134	0.098144
4	6	0	-1.881882	0.138415	-0.169621
5	7	0	-1.712488	1.448179	-0.384482
6	6	0	-0.411236	2.097212	-0.666705
7	6	0	0.260817	2.673142	0.583625
8	1	0	-3.044058	3.148468	-0.377096
9	1	0	-4.914428	1.222526	0.233434
10	1	0	0.227018	1.331906	-1.111787
11	1	0	-0.581307	2.883530	-1.403507
12	1	0	-0.360124	3.477241	0.991531
13	1	0	0.313146	1.877161	1.341456
14	35	0	0.487678	-2.109926	-0.255420
15	1	0	-1.078200	-0.638373	-0.203210
16	6	0	-3.689148	-1.379901	0.380751
17	6	0	-4.955997	-1.641727	0.671457
18	1	0	-2.910514	-2.133690	0.338569
19	1	0	-5.248172	-2.661684	0.878135
20	1	0	-5.729817	-0.885377	0.717874
21	7	0	1.554892	3.223555	0.187334
22	1	0	1.926128	3.833876	0.905664
23	1	0	2.228102	2.472382	0.041276
24	6	0	3.784903	-0.184783	-1.061293
25	6	0	3.770251	-0.402456	0.387455
26	8	0	3.529755	0.917377	-0.163291
27	1	0	4.734825	-0.121150	-1.587604
28	1	0	2.928874	-0.514578	-1.642558
29	1	0	2.869724	-0.867442	0.782748
30	6	0	5.027827	-0.561132	1.195714
31	1	0	4.903149	-0.132431	2.194632
32	1	0	5.263299	-1.623232	1.314910
33	1	0	5.872221	-0.066891	0.709854

Rotational constants (GHZ): 0.5270100 0.2311934 0.1692755

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1293.9050256023 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 482 RedAO= T EigKep= 3.82D-06 NBF= 482
NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482
Lowest energy guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999979 -0.002890 0.000761 -0.005785 Ang= -0.75 deg.
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999324 0.017454 -0.005383 0.031905 Ang= 4.21 deg.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3205.64616933 A.U. after 11 cycles
NFock= 11 Conv=0.55D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000504791	-0.000035385	0.000027109
2	6	-0.000537499	0.000196113	-0.000086177
3	7	0.001667621	0.001814721	0.000108114
4	6	0.002733428	0.004257931	-0.001010440
5	7	0.000081470	-0.002179724	0.001728356
6	6	-0.000536956	-0.002311271	-0.002816884
7	6	0.000653755	0.000348224	0.001349803
8	1	-0.000183940	-0.000012388	0.000149792
9	1	0.000119869	0.000012933	-0.000131197
10	1	-0.000318554	0.000359775	0.000048570
11	1	0.000050775	-0.000556818	-0.000171408
12	1	-0.000015738	0.000090165	0.000390041
13	1	0.000492882	0.000253542	0.000410429
14	35	-0.000884300	-0.000782058	-0.000039662
15	1	-0.000769443	0.000299847	-0.000048665
16	6	0.000736539	-0.000016686	0.000164052
17	6	-0.000611082	-0.000221521	0.000117326
18	1	-0.000247522	0.000096871	-0.000165744
19	1	-0.000102415	-0.000166271	-0.000067925
20	1	0.000110825	-0.000177829	-0.000044790
21	7	-0.004068442	-0.001054218	0.000281324

22	1	-0.000336628	0.000080070	0.000073448
23	1	0.001605551	-0.000573470	-0.000384640
24	6	0.000273749	-0.000475172	-0.000104332
25	6	0.000453871	-0.000047940	0.000017431
26	8	-0.000829244	0.001022609	-0.000104100
27	1	-0.000008183	-0.000009950	0.000322316
28	1	0.000139322	0.000020340	0.000137331
29	1	0.000322983	-0.000044550	-0.000213436
30	6	0.000166054	-0.000327038	0.000078280
31	1	0.000044329	0.000043208	-0.000013816
32	1	0.000039289	0.000027333	-0.000001973
33	1	0.000262424	0.000068606	0.000001467

Cartesian Forces: Max 0.004257931 RMS 0.000927987

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.008090314 RMS 0.001324070
Search for a local minimum.
Step number 3 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 2 3 1
ITU= 0 -1 0
Use linear search instead of GDIIS.
Energy rises -- skip Quadratic/GDIIS search.
Quartic linear search produced a step of -0.58785.
Iteration 1 RMS(Cart)= 0.03194645 RMS(Int)= 0.00010107
Iteration 2 RMS(Cart)= 0.00024021 RMS(Int)= 0.00000511
Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00000511

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56562	-0.00139	0.00004	0.00000	0.00004	2.56566
R2	2.61945	0.00099	-0.00005	0.00000	-0.00005	2.61940
R3	2.03435	-0.00001	0.00000	0.00000	0.00000	2.03435
R4	2.62945	-0.00082	-0.00004	0.00000	-0.00004	2.62942
R5	2.03123	-0.00014	0.00002	0.00000	0.00002	2.03125
R6	2.54397	-0.00072	0.00011	0.00000	0.00011	2.54408
R7	2.68945	0.00048	-0.00006	0.00000	-0.00006	2.68939
R8	2.52852	-0.00407	0.00051	0.00000	0.00051	2.52903
R9	2.11314	-0.00084	0.00003	0.00000	0.00003	2.11318

R10	2.79919	-0.00261	0.00059	0.00000	0.00059	2.79977
R11	2.89485	0.00124	-0.00006	0.00000	-0.00006	2.89479
R12	2.06245	-0.00046	0.00006	0.00000	0.00006	2.06251
R13	2.06153	-0.00029	0.00004	0.00000	0.00004	2.06157
R14	2.06882	0.00022	-0.00003	0.00000	-0.00003	2.06879
R15	2.07924	0.00013	-0.00002	0.00000	-0.00002	2.07922
R16	2.76096	-0.00221	0.00047	0.00000	0.00047	2.76143
R17	4.06189	-0.00010	-0.00029	0.00000	-0.00029	4.06160
R18	2.50556	0.00068	-0.00006	0.00000	-0.00006	2.50550
R19	2.04950	-0.00024	0.00002	0.00000	0.00002	2.04953
R20	2.04265	0.00017	-0.00002	0.00000	-0.00002	2.04262
R21	2.04669	-0.00021	0.00003	0.00000	0.00003	2.04671
R22	1.91442	-0.00002	0.00000	0.00000	0.00000	1.91442
R23	1.92604	0.00189	-0.00018	0.00000	-0.00018	1.92587
R24	3.85161	0.00032	0.00006	0.00000	0.00006	3.85167
R25	2.76861	-0.00129	-0.00003	0.00000	-0.00003	2.76858
R26	2.72950	0.00068	0.00001	0.00000	0.00000	2.72951
R27	2.05573	-0.00016	0.00004	0.00000	0.00004	2.05576
R28	2.05226	-0.00019	0.00000	0.00000	0.00000	2.05226
R29	2.74051	0.00124	-0.00003	0.00000	-0.00003	2.74047
R30	2.05574	-0.00033	-0.00002	0.00000	-0.00002	2.05572
R31	2.84085	0.00048	-0.00006	0.00000	-0.00006	2.84080
R32	2.06765	0.00000	0.00001	0.00000	0.00001	2.06765
R33	2.06812	-0.00002	0.00000	0.00000	0.00000	2.06812
R34	2.06433	0.00023	-0.00002	0.00000	-0.00002	2.06431
A1	1.87554	0.00000	0.00016	0.00000	0.00016	1.87570
A2	2.27737	-0.00021	-0.00001	0.00000	-0.00001	2.27736
A3	2.13019	0.00021	-0.00015	0.00000	-0.00015	2.13004
A4	1.86349	-0.00133	0.00013	0.00000	0.00013	1.86361
A5	2.27589	0.00062	-0.00005	0.00000	-0.00005	2.27585
A6	2.14377	0.00071	-0.00008	0.00000	-0.00008	2.14369
A7	1.89742	0.00130	-0.00016	0.00000	-0.00016	1.89726
A8	2.25453	-0.00007	-0.00005	0.00000	-0.00005	2.25448
A9	2.13117	-0.00123	0.00020	0.00000	0.00020	2.13138
A10	1.88937	-0.00055	0.00015	0.00000	0.00015	1.88952
A11	2.19916	-0.00355	-0.00010	0.00000	-0.00010	2.19906
A12	2.19465	0.00410	-0.00006	0.00000	-0.00006	2.19460
A13	1.89894	0.00058	-0.00028	0.00000	-0.00028	1.89866
A14	2.20517	-0.00240	-0.00052	0.00000	-0.00052	2.20465
A15	2.17817	0.00182	0.00081	0.00000	0.00081	2.17898
A16	1.97645	-0.00392	0.00079	0.00000	0.00079	1.97724
A17	1.85895	0.00225	0.00014	0.00000	0.00014	1.85910
A18	1.88341	0.00006	-0.00039	0.00000	-0.00039	1.88302
A19	1.91763	0.00145	0.00000	0.00000	0.00000	1.91764

A20	1.92694	0.00095	-0.00056	0.00000	-0.00056	1.92639
A21	1.89775	-0.00070	0.00001	0.00000	0.00001	1.89776
A22	1.90861	-0.00071	-0.00040	0.00000	-0.00040	1.90820
A23	1.88709	0.00104	-0.00023	0.00000	-0.00023	1.88686
A24	1.88475	0.00040	0.00064	0.00000	0.00064	1.88539
A25	1.87727	-0.00008	-0.00001	0.00000	-0.00001	1.87726
A26	1.90364	-0.00120	-0.00035	0.00000	-0.00035	1.90329
A27	2.00119	0.00051	0.00031	0.00000	0.00031	2.00150
A28	2.16967	0.00067	-0.00014	0.00000	-0.00014	2.16953
A29	1.95162	-0.00027	0.00006	0.00000	0.00006	1.95168
A30	2.16186	-0.00039	0.00007	0.00000	0.00007	2.16193
A31	2.07890	0.00002	0.00000	0.00000	0.00000	2.07890
A32	2.15814	0.00003	-0.00001	0.00000	-0.00001	2.15813
A33	2.04614	-0.00005	0.00002	0.00000	0.00002	2.04615
A34	1.93821	-0.00216	-0.00008	0.00000	-0.00011	1.93810
A35	1.92437	0.00809	0.00041	0.00000	0.00040	1.92477
A36	1.87924	-0.00275	-0.00016	0.00000	-0.00015	1.87909
A37	2.08960	-0.00026	0.00014	0.00000	0.00013	2.08973
A38	2.06719	-0.00006	-0.00014	0.00000	-0.00013	2.06706
A39	1.99370	-0.00037	-0.00005	0.00000	-0.00004	1.99366
A40	2.01003	-0.00001	0.00011	0.00000	0.00010	2.01013
A41	2.03433	0.00019	-0.00002	0.00000	-0.00002	2.03430
A42	2.01651	-0.00028	-0.00008	0.00000	-0.00007	2.01644
A43	2.14001	0.00007	0.00007	0.00000	0.00006	2.14007
A44	1.97113	0.00004	0.00006	0.00000	0.00006	1.97119
A45	2.02525	-0.00018	-0.00013	0.00000	-0.00013	2.02512
A46	2.03981	0.00012	0.00004	0.00000	0.00003	2.03984
A47	2.43009	0.00014	-0.00027	0.00000	-0.00027	2.42982
A48	2.43740	0.00061	-0.00027	0.00000	-0.00026	2.43714
A49	1.93283	0.00000	0.00000	0.00000	0.00000	1.93282
A50	1.91876	0.00002	-0.00005	0.00000	-0.00005	1.91871
A51	1.93878	0.00018	0.00001	0.00000	0.00001	1.93879
A52	1.88108	-0.00001	0.00000	0.00000	0.00000	1.88108
A53	1.89322	-0.00010	0.00002	0.00000	0.00002	1.89324
A54	1.89780	-0.00010	0.00002	0.00000	0.00002	1.89783
A55	3.12665	0.00470	0.00879	0.00000	0.00879	3.13543
A56	3.10914	0.00555	0.02242	0.00000	0.02243	3.13157
A57	3.13889	-0.00080	0.00159	0.00000	0.00159	3.14048
A58	3.18735	0.00052	-0.00023	0.00000	-0.00022	3.18713
D1	0.00203	-0.00003	-0.00031	0.00000	-0.00031	0.00172
D2	-3.13101	0.00008	-0.00025	0.00000	-0.00025	-3.13126
D3	3.12994	0.00000	-0.00014	0.00000	-0.00014	3.12980
D4	-0.00309	0.00012	-0.00009	0.00000	-0.00009	-0.00318
D5	-0.00523	0.00006	0.00028	0.00000	0.00028	-0.00494

D6	-3.10269	-0.00006	0.00007	0.00000	0.00007	-3.10262
D7	-3.13455	0.00003	0.00014	0.00000	0.00014	-3.13442
D8	0.05118	-0.00008	-0.00008	0.00000	-0.00008	0.05110
D9	0.00184	-0.00001	0.00023	0.00000	0.00023	0.00207
D10	3.13096	0.00026	-0.00019	0.00000	-0.00019	3.13077
D11	3.13568	-0.00011	0.00018	0.00000	0.00018	3.13585
D12	-0.01838	0.00015	-0.00024	0.00000	-0.00024	-0.01863
D13	-0.00511	0.00004	-0.00005	0.00000	-0.00005	-0.00517
D14	3.13247	0.00051	-0.00005	0.00000	-0.00005	3.13242
D15	-3.13530	-0.00021	0.00033	0.00000	0.00033	-3.13497
D16	0.00228	0.00025	0.00034	0.00000	0.00034	0.00263
D17	-0.00632	-0.00002	-0.00004	0.00000	-0.00004	-0.00636
D18	-3.13914	-0.00024	0.00040	0.00000	0.00040	-3.13874
D19	3.12133	0.00030	-0.00051	0.00000	-0.00051	3.12082
D20	-0.01148	0.00008	-0.00007	0.00000	-0.00007	-0.01156
D21	0.00639	-0.00007	-0.00014	0.00000	-0.00014	0.00625
D22	3.10469	-0.00009	0.00003	0.00000	0.00003	3.10472
D23	-3.13121	-0.00051	-0.00015	0.00000	-0.00015	-3.13136
D24	-0.03291	-0.00053	0.00002	0.00000	0.00002	-0.03289
D25	1.43062	-0.00110	-0.00095	0.00000	-0.00095	1.42967
D26	-2.74291	-0.00014	-0.00037	0.00000	-0.00037	-2.74328
D27	-0.70776	0.00022	-0.00048	0.00000	-0.00048	-0.70825
D28	-1.66009	-0.00118	-0.00116	0.00000	-0.00116	-1.66125
D29	0.44957	-0.00022	-0.00058	0.00000	-0.00058	0.44898
D30	2.48471	0.00015	-0.00070	0.00000	-0.00070	2.48402
D31	-1.11935	0.00139	0.00165	0.00000	0.00165	-1.11770
D32	0.91981	0.00149	0.00129	0.00000	0.00129	0.92111
D33	3.09448	0.00301	0.00193	0.00000	0.00193	3.09641
D34	3.08770	0.00009	0.00095	0.00000	0.00095	3.08865
D35	-1.15632	0.00019	0.00059	0.00000	0.00059	-1.15573
D36	1.01835	0.00171	0.00123	0.00000	0.00123	1.01958
D37	0.99466	-0.00056	0.00129	0.00000	0.00129	0.99596
D38	3.03383	-0.00047	0.00094	0.00000	0.00094	3.03476
D39	-1.07469	0.00105	0.00157	0.00000	0.00157	-1.07312
D40	2.86986	-0.00190	-0.00068	0.00000	-0.00067	2.86919
D41	-1.33182	-0.00147	-0.00066	0.00000	-0.00067	-1.33250
D42	0.79734	-0.00060	-0.00037	0.00000	-0.00036	0.79698
D43	2.87884	-0.00017	-0.00035	0.00000	-0.00036	2.87848
D44	-1.30860	0.00005	-0.00031	0.00000	-0.00030	-1.30890
D45	0.77290	0.00048	-0.00029	0.00000	-0.00030	0.77260
D46	-3.13543	-0.00023	0.00040	0.00000	0.00040	-3.13503
D47	0.00382	-0.00008	0.00018	0.00000	0.00018	0.00399
D48	-0.00365	0.00002	-0.00009	0.00000	-0.00009	-0.00374
D49	3.13559	0.00017	-0.00031	0.00000	-0.00031	3.13528

D50	1.23015	0.00056	0.00477	0.00000	0.00474	1.23489
D51	-0.53667	-0.00179	-0.00778	0.00000	-0.00779	-0.54445
D52	-2.95542	0.00127	0.00667	0.00000	0.00667	-2.94874
D53	1.56096	-0.00108	-0.00589	0.00000	-0.00586	1.55510
D54	-2.70448	0.00025	-0.00001	0.00000	-0.00001	-2.70449
D55	-0.01292	0.00006	0.00006	0.00000	0.00006	-0.01286
D56	-0.02573	0.00000	-0.00008	0.00000	-0.00008	-0.02580
D57	2.66584	-0.00018	0.00000	0.00000	0.00000	2.66583
D58	2.00549	-0.00001	0.00034	0.00000	0.00033	2.00582
D59	-0.41820	0.00014	0.00031	0.00000	0.00030	-0.41790
D60	0.45314	-0.00035	-0.00042	0.00000	-0.00041	0.45273
D61	-1.97028	-0.00038	-0.00039	0.00000	-0.00039	-1.97067
D62	2.55220	0.00018	0.00003	0.00000	0.00002	2.55223
D63	-1.65419	0.00019	-0.00001	0.00000	-0.00001	-1.65420
D64	0.44721	0.00020	-0.00001	0.00000	-0.00001	0.44720
D65	1.34973	-0.00011	0.00005	0.00000	0.00005	1.34979
D66	-2.85666	-0.00011	0.00002	0.00000	0.00002	-2.85664
D67	-0.75526	-0.00010	0.00002	0.00000	0.00002	-0.75524
D68	-1.04500	-0.00010	0.00007	0.00000	0.00007	-1.04493
D69	1.03180	-0.00010	0.00004	0.00000	0.00004	1.03183
D70	3.13319	-0.00009	0.00004	0.00000	0.00004	3.13323

Item	Value	Threshold	Converged?
Maximum Force	0.008090	0.000450	NO
RMS Force	0.001324	0.000300	NO
Maximum Displacement	0.128779	0.001800	NO
RMS Displacement	0.031862	0.001200	NO

Predicted change in Energy=-5.705281D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.907614	2.120587	-0.250024
2	6	0	-3.843143	1.185577	0.056334
3	7	0	-3.185654	-0.039775	0.104243
4	6	0	-1.881780	0.159036	-0.165616
5	7	0	-1.694080	1.465230	-0.388529
6	6	0	-0.384278	2.095378	-0.675587
7	6	0	0.296538	2.671505	0.569864
8	1	0	-3.001953	3.183688	-0.390878
9	1	0	-4.898489	1.287848	0.232906
10	1	0	0.243738	1.318970	-1.116057

11	1	0	-0.544788	2.878961	-1.417461
12	1	0	-0.314479	3.485489	0.973083
13	1	0	0.340220	1.879911	1.332808
14	35	0	0.443381	-2.135277	-0.246440
15	1	0	-1.089073	-0.629141	-0.194993
16	6	0	-3.709865	-1.330449	0.395379
17	6	0	-4.979992	-1.572325	0.688915
18	1	0	-2.941976	-2.095427	0.357549
19	1	0	-5.286415	-2.586634	0.902575
20	1	0	-5.742909	-0.804719	0.731211
21	7	0	1.596616	3.204639	0.168720
22	1	0	1.975283	3.815562	0.882650
23	1	0	2.261392	2.445270	0.027126
24	6	0	3.847051	-0.201690	-1.058369
25	6	0	3.837077	-0.408845	0.391946
26	8	0	3.580867	0.904098	-0.168058
27	1	0	4.795333	-0.131101	-1.586786
28	1	0	2.993922	-0.545582	-1.635714
29	1	0	2.942483	-0.881123	0.792013
30	6	0	5.097532	-0.547171	1.199403
31	1	0	4.969390	-0.112602	2.195347
32	1	0	5.345274	-1.605615	1.326019
33	1	0	5.935505	-0.046908	0.708639

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357687	0.000000			
3	N	2.206802	1.391429	0.000000		
4	C	2.215207	2.224858	1.346268	0.000000	
5	N	1.386125	2.212370	2.175468	1.338307	0.000000
6	C	2.559095	3.650643	3.607593	2.500400	1.481577
7	C	3.352956	4.428166	4.437736	3.405657	2.517175
8	H	1.076533	2.213606	3.266437	3.233273	2.159545
9	H	2.211393	1.074892	2.170931	3.245546	3.268927
10	H	3.365059	4.253808	3.885363	2.601271	2.075048
11	H	2.742442	3.989833	4.220045	3.279124	2.092417
12	H	3.175421	4.310626	4.628825	3.849462	2.799773
13	H	3.621009	4.428545	4.198375	3.184960	2.696912
14	Br	5.416784	5.430840	4.205234	3.267533	4.189579
15	H	3.297139	3.307758	2.198305	1.118244	2.188579
16	C	3.601361	2.542262	1.423164	2.423876	3.534646
17	C	4.337506	3.049362	2.431090	3.650583	4.602701
18	H	4.259706	3.415818	2.085485	2.545647	3.846057

19	H	5.398621	4.126588	3.396618	4.502363	5.566814
20	H	4.190362	2.832992	2.741857	4.079392	4.774882
21	N	4.651731	5.803467	5.779316	4.635377	3.763608
22	H	5.291368	6.438455	6.488822	5.417193	4.539182
23	H	5.186604	6.233220	5.987630	4.736021	4.096218
24	C	7.188316	7.893424	7.129994	5.809185	5.825069
25	C	7.231943	7.851152	7.038305	5.773966	5.891943
26	O	6.602042	7.432733	6.837460	5.513224	5.309288
27	H	8.135873	8.891386	8.158681	6.832843	6.789445
28	H	6.622441	7.252957	6.439756	5.141025	5.251304
29	H	6.657307	7.131423	6.223741	5.027176	5.328861
30	C	8.561550	9.178491	8.370663	7.146524	7.259289
31	H	8.544832	9.160861	8.419190	7.251652	7.319002
32	H	9.191227	9.686582	8.759071	7.587442	7.869070
33	H	9.155208	9.877575	9.141165	7.868716	7.854992

		6	7	8	9	10
6	C	0.000000				
7	C	1.531855	0.000000			
8	H	2.849158	3.473528	0.000000		
9	H	4.674994	5.386683	2.753210	0.000000	
10	H	1.091433	2.162051	3.812816	5.316311	0.000000
11	H	1.090937	2.168024	2.680372	4.920372	1.773750
12	H	2.157637	1.094759	3.028860	5.137182	3.061032
13	H	2.145920	1.100278	3.980081	5.385573	2.514140
14	Br	4.332161	4.877813	6.338972	6.362635	3.567620
15	H	2.854945	3.660490	4.270263	4.285976	2.533748
16	C	4.893137	5.665452	4.636461	2.880052	4.993479
17	C	6.036100	6.772447	5.262914	2.897443	6.237376
18	H	5.017174	5.766861	5.332241	3.910246	4.896773
19	H	6.960084	7.676462	6.339432	3.951019	7.064786
20	H	6.253364	6.970300	4.967828	2.310885	6.615314
21	N	2.422242	1.461285	4.632540	6.772341	2.652674
22	H	3.309783	2.055453	5.176294	7.352567	3.636763
23	H	2.759674	2.050951	5.331303	7.255747	2.578052
24	C	4.829822	4.848972	7.669105	8.964964	3.911470
25	C	5.023006	4.696342	7.764756	8.900234	4.262805
26	O	4.171224	3.801984	6.969914	8.497501	3.493889
27	H	5.711029	5.722316	8.556617	9.964681	4.800137
28	H	4.394171	4.742373	7.169908	8.315248	3.363051
29	H	4.699015	4.435261	7.297824	8.154623	3.970436
30	C	6.367801	5.814270	9.058143	10.208910	5.692377
31	H	6.463682	5.677058	9.005353	10.158123	5.945299
32	H	7.108554	6.659975	9.775549	10.700547	6.367308
33	H	6.815066	6.261548	9.566810	10.926268	6.131179

		11	12	13	14	15
11	H	0.000000				
12	H	2.477019	0.000000			
13	H	3.057011	1.770851	0.000000		
14	Br	5.243123	5.801258	4.315831	0.000000	
15	H	3.754657	4.346789	3.266863	2.149304	0.000000
16	C	5.569850	5.920781	5.252463	4.278917	2.776495
17	C	6.627353	6.886890	6.374731	5.532158	4.100017
18	H	5.800147	6.199133	5.246642	3.439045	2.426633
19	H	7.598573	7.848298	7.196814	5.861272	4.759633
20	H	6.723596	6.923311	6.676347	6.402840	4.748354
21	N	2.684706	2.092406	2.165303	5.478778	4.695006
22	H	3.538148	2.315197	2.573484	6.247723	5.505177
23	H	3.185839	2.934621	2.390677	4.935728	4.552687
24	C	5.376578	5.919494	4.727436	3.997869	5.029259
25	C	5.769260	5.721798	4.283880	3.860735	4.965882
26	O	4.741532	4.810354	3.702243	4.368954	4.915271
27	H	6.132376	6.763345	5.693525	4.975213	6.067237
28	H	4.929259	5.831027	4.662325	3.310963	4.330532
29	H	5.584000	5.450494	3.832433	2.982750	4.158259
30	C	7.100854	6.753031	5.342335	5.125785	6.342329
31	H	7.239336	6.508414	5.113051	5.526146	6.533415
32	H	7.894994	7.620808	6.099140	5.175107	6.683398
33	H	7.421267	7.184014	5.950583	5.952890	7.106353

		16	17	18	19	20
16	C	0.000000				
17	C	1.325855	0.000000			
18	H	1.084563	2.130012	0.000000		
19	H	2.078643	1.080910	2.456569	0.000000	
20	H	2.126603	1.083074	3.106569	1.847423	0.000000
21	N	6.984063	8.145046	6.980342	9.025159	8.382122
22	H	7.683734	8.800154	7.706812	9.680948	8.996689
23	H	7.074431	8.307628	6.913910	9.113499	8.667583
24	C	7.777818	9.102106	7.189016	9.641237	9.774127
25	C	7.603006	8.898460	6.985793	9.393700	9.594162
26	O	7.646270	8.952955	7.198673	9.589586	9.521635
27	H	8.815090	10.139671	8.216141	10.670904	10.811170
28	H	7.048554	8.369075	6.450581	8.897909	9.055478
29	H	6.679292	7.953238	6.024130	8.404507	8.685940
30	C	8.878639	10.142388	8.230401	10.586494	10.853602
31	H	8.947207	10.168104	8.360550	10.628905	10.834023
32	H	9.106995	10.344957	8.358012	10.685247	11.132970
33	H	9.735440	11.021587	9.117531	11.507359	11.702997

		21	22	23	24	25

21	N	0.000000				
22	H	1.013070	0.000000			
23	H	1.019126	1.640572	0.000000		
24	C	4.263013	4.838323	3.270934	0.000000	
25	C	4.257553	4.642486	3.280525	1.465069	0.000000
26	O	3.056659	3.486905	2.038216	1.444394	1.450195
27	H	4.943759	5.443063	3.957683	1.087863	2.216028
28	H	4.390057	5.138030	3.499548	1.086010	2.200231
29	H	4.346643	4.796096	3.480493	2.168822	1.087841
30	C	5.234004	5.374216	4.286330	2.603958	1.503286
31	H	5.146543	5.110608	4.310121	3.443000	2.149918
32	H	6.207280	6.398638	5.254248	3.146584	2.139956
33	H	5.448856	5.534646	4.491605	2.740058	2.152834

		26	27	28	29	30
26	O	0.000000				
27	H	2.135264	0.000000			
28	H	2.144782	1.849127	0.000000		
29	H	2.125155	3.107132	2.451345	0.000000	
30	C	2.505274	2.833247	3.530307	2.218497	0.000000
31	H	2.923586	3.786181	4.332087	2.582310	1.094155
32	H	3.412339	3.310749	3.927390	2.565825	1.094400
33	H	2.686509	2.564382	3.794415	3.108223	1.092388

		31	32	33
31	H	0.000000		
32	H	1.768080	0.000000	
33	H	1.774259	1.777385	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.923055	2.107908	-0.245961
2	6	0	-3.856156	1.169392	0.057063
3	7	0	-3.195377	-0.054329	0.101235
4	6	0	-1.891957	0.148870	-0.167545
5	7	0	-1.707711	1.456280	-0.386176
6	6	0	-0.399522	2.090883	-0.670760
7	6	0	0.279330	2.664820	0.576772

8	1	0	-3.020218	3.171201	-0.383412
9	1	0	-4.911832	1.268244	0.233612
10	1	0	0.230730	1.317600	-1.113525
11	1	0	-0.561905	2.876423	-1.410154
12	1	0	-0.334013	3.475845	0.982414
13	1	0	0.324901	1.870886	1.337170
14	35	0	0.439415	-2.138886	-0.255001
15	1	0	-1.097116	-0.637065	-0.199202
16	6	0	-3.716197	-1.347346	0.388026
17	6	0	-4.985762	-1.593597	0.680355
18	1	0	-2.946233	-2.110123	0.347982
19	1	0	-5.289514	-2.609413	0.890637
20	1	0	-5.750761	-0.828193	0.724875
21	7	0	1.578095	3.202754	0.177786
22	1	0	1.954880	3.812386	0.893812
23	1	0	2.244965	2.445643	0.033963
24	6	0	3.838117	-0.193508	-1.059545
25	6	0	3.828230	-0.405373	0.390091
26	8	0	3.568660	0.908675	-0.165756
27	1	0	4.786377	-0.118654	-1.587414
28	1	0	2.986107	-0.537835	-1.638282
29	1	0	2.934784	-0.881354	0.788331
30	6	0	5.088792	-0.542905	1.197518
31	1	0	4.959153	-0.111903	2.194817
32	1	0	5.339349	-1.601080	1.320798
33	1	0	5.925571	-0.038800	0.708652

Rotational constants (GHZ): 0.5240208 0.2280547 0.1673077

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1289.1323279052 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 3.82D-06 NBF= 482

NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482

Lowest energy guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999996 -0.001192 0.000310 -0.002399 Ang= -0.31 deg.

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999993 0.001698 -0.000451 0.003386 Ang= 0.44 deg.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3205.64626919 A.U. after 7 cycles

NFock= 7 Conv=0.73D-08 -V/T= 2.0018

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000553284	0.000017766	0.000049816
2	6	-0.000551015	0.000241252	-0.000123036
3	7	0.001839891	0.001936538	0.000072908
4	6	0.002930776	0.004435403	-0.000953947
5	7	0.000078673	-0.002284660	0.001804858
6	6	-0.000617265	-0.002363866	-0.002922783
7	6	0.000565284	0.000392773	0.001429799
8	1	-0.000202664	-0.000008283	0.000154180
9	1	0.000122603	0.000022626	-0.000144290
10	1	-0.000357034	0.000335715	0.000018410
11	1	0.000058965	-0.000589950	-0.000195791
12	1	-0.000011487	0.000076865	0.000420574
13	1	0.000540182	0.000274534	0.000436409
14	35	-0.000034448	-0.000310926	0.000041950
15	1	-0.000765393	0.000140966	-0.000093678
16	6	0.000786564	-0.000059704	0.000197426
17	6	-0.000658378	-0.000196133	0.000129534
18	1	-0.000218557	0.000096101	-0.000196344
19	1	-0.000106428	-0.000174142	-0.000076991
20	1	0.000107358	-0.000190824	-0.000050253
21	7	-0.004303580	-0.001204794	0.000267482
22	1	-0.000322221	0.000061761	0.000066945
23	1	0.001727804	-0.000461274	-0.000394919
24	6	0.000187401	-0.000404622	-0.000147067
25	6	0.000226021	0.000044086	-0.000200835
26	8	-0.000844186	0.000464106	-0.000077623
27	1	-0.000088481	-0.000059399	0.000324911

28	1	0.000027252	0.000130801	0.000009490
29	1	0.000054341	-0.000059175	-0.000002712
30	6	0.000076066	-0.000433245	0.000209564
31	1	0.000046219	0.000034405	-0.000037121
32	1	0.000072358	0.000030899	0.000012051
33	1	0.000186665	0.000064399	-0.000028915

Cartesian Forces: Max 0.004435403 RMS 0.000959952

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.005480144 RMS 0.000845988
Search for a local minimum.
Step number 4 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Update second derivatives using D2CorX and points 2 3 1 4
ITU= 0 0 -1 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00217	0.00230	0.00230	0.00230	0.00334
Eigenvalues ---	0.00604	0.00723	0.00860	0.01385	0.01470
Eigenvalues ---	0.01842	0.01942	0.02083	0.02143	0.02260
Eigenvalues ---	0.02308	0.02354	0.02394	0.02407	0.02891
Eigenvalues ---	0.03061	0.03069	0.03070	0.03199	0.03933
Eigenvalues ---	0.04046	0.04352	0.04612	0.04654	0.05291
Eigenvalues ---	0.05679	0.05766	0.05904	0.07423	0.08562
Eigenvalues ---	0.09507	0.11238	0.12028	0.12319	0.12544
Eigenvalues ---	0.12758	0.12867	0.15453	0.15898	0.15998
Eigenvalues ---	0.15999	0.16000	0.16000	0.16000	0.16000
Eigenvalues ---	0.16000	0.16000	0.17091	0.17973	0.21393
Eigenvalues ---	0.22001	0.22598	0.23076	0.23504	0.24967
Eigenvalues ---	0.29127	0.29428	0.31679	0.31993	0.32200
Eigenvalues ---	0.33157	0.33653	0.34269	0.34309	0.34337
Eigenvalues ---	0.34537	0.34640	0.34701	0.35051	0.35058
Eigenvalues ---	0.35275	0.35445	0.35622	0.35883	0.36262
Eigenvalues ---	0.36416	0.36618	0.37912	0.41975	0.42368
Eigenvalues ---	0.44209	0.45340	0.45462	0.48939	0.53988
Eigenvalues ---	0.54677	0.60478	0.74071		

RFO step: Lambda=-8.86502810D-04 EMin= 2.16561425D-03
Quartic linear search produced a step of 0.01307.
Maximum step size (0.150) exceeded in Quadratic search.

-- Step size scaled by 0.511

Iteration 1 RMS(Cart)= 0.07465542 RMS(Int)= 0.00194290

Iteration 2 RMS(Cart)= 0.00382031 RMS(Int)= 0.00004629

Iteration 3 RMS(Cart)= 0.00000879 RMS(Int)= 0.00004611

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00004611

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56566	-0.00097	0.00000	-0.00088	-0.00088	2.56477
R2	2.61940	0.00075	0.00000	0.00108	0.00108	2.62048
R3	2.03435	-0.00001	0.00000	-0.00002	-0.00002	2.03433
R4	2.62942	-0.00019	0.00000	0.00022	0.00022	2.62964
R5	2.03125	-0.00014	0.00000	-0.00030	-0.00030	2.03095
R6	2.54408	-0.00099	0.00000	-0.00169	-0.00169	2.54239
R7	2.68939	0.00051	0.00000	0.00096	0.00096	2.69035
R8	2.52903	-0.00548	0.00000	-0.00815	-0.00816	2.52088
R9	2.11318	-0.00045	0.00000	-0.00091	-0.00091	2.11227
R10	2.79977	-0.00386	-0.00001	-0.00920	-0.00921	2.79057
R11	2.89479	0.00064	0.00000	0.00147	0.00147	2.89626
R12	2.06251	-0.00045	0.00000	-0.00100	-0.00100	2.06151
R13	2.06157	-0.00030	0.00000	-0.00067	-0.00067	2.06090
R14	2.06879	0.00022	0.00000	0.00049	0.00049	2.06929
R15	2.07922	0.00013	0.00000	0.00029	0.00029	2.07952
R16	2.76143	-0.00328	0.00000	-0.00732	-0.00732	2.75411
R17	4.06160	0.00019	0.00000	0.00381	0.00381	4.06540
R18	2.50550	0.00073	0.00000	0.00095	0.00095	2.50645
R19	2.04953	-0.00022	0.00000	-0.00046	-0.00046	2.04907
R20	2.04262	0.00018	0.00000	0.00039	0.00039	2.04301
R21	2.04671	-0.00021	0.00000	-0.00047	-0.00047	2.04625
R22	1.91442	-0.00004	0.00000	-0.00007	-0.00007	1.91436
R23	1.92587	0.00162	0.00000	0.00292	0.00293	1.92879
R24	3.85167	0.00010	0.00000	0.00082	0.00081	3.85248
R25	2.76858	-0.00034	0.00000	-0.00109	-0.00117	2.76741
R26	2.72951	0.00022	0.00000	0.00066	0.00069	2.73020
R27	2.05576	-0.00024	0.00000	-0.00056	-0.00056	2.05520
R28	2.05226	-0.00007	0.00000	-0.00010	-0.00010	2.05216
R29	2.74047	0.00067	0.00000	0.00148	0.00153	2.74200
R30	2.05572	-0.00002	0.00000	0.00007	0.00007	2.05579
R31	2.84080	0.00043	0.00000	0.00102	0.00102	2.84181
R32	2.06765	-0.00003	0.00000	-0.00007	-0.00007	2.06758
R33	2.06812	-0.00001	0.00000	-0.00002	-0.00002	2.06809
R34	2.06431	0.00019	0.00000	0.00039	0.00039	2.06471
A1	1.87570	-0.00075	0.00000	-0.00203	-0.00204	1.87367
A2	2.27736	0.00014	0.00000	-0.00013	-0.00013	2.27723
A3	2.13004	0.00061	0.00000	0.00214	0.00214	2.13218

A4	1.86361	-0.00125	0.00000	-0.00251	-0.00251	1.86110
A5	2.27585	0.00057	0.00000	0.00098	0.00098	2.27683
A6	2.14369	0.00068	0.00000	0.00153	0.00153	2.14522
A7	1.89726	0.00093	0.00000	0.00301	0.00300	1.90026
A8	2.25448	0.00020	0.00000	0.00065	0.00064	2.25512
A9	2.13138	-0.00113	0.00000	-0.00357	-0.00358	2.12779
A10	1.88952	-0.00039	0.00000	-0.00264	-0.00264	1.88688
A11	2.19906	-0.00100	0.00000	-0.00232	-0.00233	2.19674
A12	2.19460	0.00139	0.00000	0.00497	0.00497	2.19957
A13	1.89866	0.00146	0.00000	0.00416	0.00417	1.90283
A14	2.20465	0.00107	0.00000	0.00553	0.00553	2.21018
A15	2.17898	-0.00254	-0.00001	-0.00978	-0.00978	2.16920
A16	1.97724	-0.00386	-0.00001	-0.01412	-0.01411	1.96313
A17	1.85910	0.00132	0.00000	0.00222	0.00221	1.86131
A18	1.88302	0.00089	0.00000	0.00239	0.00241	1.88543
A19	1.91764	0.00104	0.00000	0.00311	0.00308	1.92072
A20	1.92639	0.00136	0.00001	0.00653	0.00652	1.93291
A21	1.89776	-0.00070	0.00000	0.00009	0.00006	1.89782
A22	1.90820	0.00045	0.00000	0.00298	0.00298	1.91118
A23	1.88686	0.00123	0.00000	0.00646	0.00646	1.89332
A24	1.88539	-0.00175	-0.00001	-0.00801	-0.00802	1.87738
A25	1.87726	-0.00040	0.00000	-0.00039	-0.00041	1.87686
A26	1.90329	0.00031	0.00000	0.00088	0.00089	1.90418
A27	2.00150	0.00021	0.00000	-0.00157	-0.00156	1.99995
A28	2.16953	0.00068	0.00000	0.00242	0.00242	2.17195
A29	1.95168	-0.00031	0.00000	-0.00104	-0.00105	1.95063
A30	2.16193	-0.00038	0.00000	-0.00132	-0.00133	2.16061
A31	2.07890	0.00001	0.00000	0.00006	0.00005	2.07896
A32	2.15813	0.00004	0.00000	0.00022	0.00022	2.15835
A33	2.04615	-0.00005	0.00000	-0.00027	-0.00027	2.04588
A34	1.93810	-0.00061	0.00000	0.00176	0.00199	1.94010
A35	1.92477	0.00163	0.00000	0.00369	0.00373	1.92851
A36	1.87909	-0.00038	0.00000	-0.00013	-0.00020	1.87889
A37	2.08973	-0.00041	0.00000	-0.00134	-0.00126	2.08847
A38	2.06706	0.00025	0.00000	0.00081	0.00071	2.06778
A39	1.99366	0.00002	0.00000	0.00008	0.00004	1.99370
A40	2.01013	-0.00024	0.00000	-0.00093	-0.00090	2.00923
A41	2.03430	0.00012	0.00000	0.00054	0.00054	2.03485
A42	2.01644	0.00010	0.00000	-0.00031	-0.00039	2.01605
A43	2.14007	-0.00014	0.00000	-0.00024	-0.00016	2.13991
A44	1.97119	-0.00017	0.00000	-0.00007	-0.00004	1.97115
A45	2.02512	0.00026	0.00000	0.00149	0.00144	2.02657
A46	2.03984	-0.00003	0.00000	-0.00034	-0.00034	2.03951
A47	2.42982	0.00024	0.00000	0.00170	0.00163	2.43145

A48	2.43714	0.00046	0.00000	0.00267	0.00259	2.43973
A49	1.93282	0.00001	0.00000	0.00004	0.00004	1.93286
A50	1.91871	0.00009	0.00000	0.00062	0.00062	1.91933
A51	1.93879	0.00007	0.00000	0.00014	0.00014	1.93892
A52	1.88108	-0.00003	0.00000	0.00005	0.00005	1.88112
A53	1.89324	-0.00007	0.00000	-0.00046	-0.00046	1.89278
A54	1.89783	-0.00009	0.00000	-0.00040	-0.00040	1.89743
A55	3.13543	0.00093	-0.00008	0.11004	0.10996	3.24539
A56	3.13157	0.00006	-0.00021	-0.06783	-0.06816	3.06341
A57	3.14048	-0.00037	-0.00001	-0.06575	-0.06576	3.07472
A58	3.18713	0.00011	0.00000	0.02316	0.02305	3.21018
D1	0.00172	0.00010	0.00000	0.00411	0.00411	0.00583
D2	-3.13126	0.00011	0.00000	0.00402	0.00402	-3.12725
D3	3.12980	0.00007	0.00000	0.00213	0.00213	3.13193
D4	-0.00318	0.00009	0.00000	0.00203	0.00204	-0.00114
D5	-0.00494	-0.00009	0.00000	-0.00341	-0.00342	-0.00837
D6	-3.10262	0.00003	0.00000	-0.00107	-0.00107	-3.10368
D7	-3.13442	-0.00006	0.00000	-0.00161	-0.00162	-3.13604
D8	0.05110	0.00005	0.00000	0.00073	0.00073	0.05183
D9	0.00207	-0.00009	0.00000	-0.00345	-0.00346	-0.00139
D10	3.13077	0.00013	0.00000	0.00478	0.00479	3.13556
D11	3.13585	-0.00010	0.00000	-0.00336	-0.00338	3.13248
D12	-0.01863	0.00012	0.00000	0.00486	0.00487	-0.01375
D13	-0.00517	0.00003	0.00000	0.00136	0.00136	-0.00380
D14	3.13242	0.00019	0.00000	0.00414	0.00413	3.13656
D15	-3.13497	-0.00018	0.00000	-0.00620	-0.00620	-3.14116
D16	0.00263	-0.00002	0.00000	-0.00343	-0.00343	-0.00080
D17	-0.00636	0.00001	0.00000	0.00033	0.00033	-0.00603
D18	-3.13874	-0.00023	0.00000	-0.00725	-0.00725	3.13719
D19	3.12082	0.00028	0.00000	0.00957	0.00957	3.13039
D20	-0.01156	0.00004	0.00000	0.00199	0.00199	-0.00957
D21	0.00625	0.00003	0.00000	0.00124	0.00124	0.00749
D22	3.10472	0.00003	0.00000	-0.00059	-0.00058	3.10414
D23	-3.13136	-0.00012	0.00000	-0.00151	-0.00151	-3.13287
D24	-0.03289	-0.00012	0.00000	-0.00334	-0.00333	-0.03622
D25	1.42967	-0.00005	0.00001	0.00166	0.00167	1.43134
D26	-2.74328	-0.00018	0.00000	-0.00148	-0.00147	-2.74476
D27	-0.70825	0.00011	0.00000	0.00093	0.00093	-0.70732
D28	-1.66125	-0.00003	0.00001	0.00394	0.00395	-1.65730
D29	0.44898	-0.00017	0.00001	0.00080	0.00081	0.44979
D30	2.48402	0.00013	0.00001	0.00321	0.00321	2.48723
D31	-1.11770	0.00004	-0.00002	0.01212	0.01210	-1.10560
D32	0.92111	0.00050	-0.00001	0.01689	0.01689	0.93800
D33	3.09641	0.00042	-0.00002	0.01400	0.01399	3.11040

D34	3.08865	0.00016	-0.00001	0.01635	0.01634	3.10499
D35	-1.15573	0.00061	-0.00001	0.02112	0.02113	-1.13460
D36	1.01958	0.00054	-0.00001	0.01824	0.01823	1.03781
D37	0.99596	-0.00049	-0.00001	0.01015	0.01012	1.00608
D38	3.03476	-0.00004	-0.00001	0.01492	0.01491	3.04967
D39	-1.07312	-0.00011	-0.00001	0.01204	0.01201	-1.06111
D40	2.86919	-0.00046	0.00001	-0.00648	-0.00654	2.86265
D41	-1.33250	-0.00027	0.00001	-0.00313	-0.00307	-1.33557
D42	0.79698	-0.00018	0.00000	-0.00596	-0.00602	0.79096
D43	2.87848	0.00002	0.00000	-0.00262	-0.00255	2.87593
D44	-1.30890	-0.00003	0.00000	-0.00505	-0.00511	-1.31401
D45	0.77260	0.00017	0.00000	-0.00171	-0.00164	0.77096
D46	-3.13503	-0.00024	0.00000	-0.00690	-0.00691	3.14125
D47	0.00399	-0.00009	0.00000	-0.00308	-0.00308	0.00092
D48	-0.00374	0.00003	0.00000	0.00158	0.00158	-0.00217
D49	3.13528	0.00018	0.00000	0.00540	0.00541	3.14068
D50	1.23489	0.00016	-0.00004	-0.01738	-0.01715	1.21774
D51	-0.54445	-0.00019	0.00007	0.01809	0.01816	-0.52629
D52	-2.94874	0.00010	-0.00006	-0.02667	-0.02675	-2.97549
D53	1.55510	-0.00025	0.00005	0.00879	0.00857	1.56367
D54	-2.70449	0.00011	0.00000	0.00121	0.00121	-2.70328
D55	-0.01286	-0.00005	0.00000	-0.00105	-0.00104	-0.01390
D56	-0.02580	0.00004	0.00000	0.00137	0.00136	-0.02444
D57	2.66583	-0.00012	0.00000	-0.00089	-0.00089	2.66494
D58	2.00582	-0.00002	0.00000	-0.00232	-0.00225	2.00357
D59	-0.41790	0.00005	0.00000	-0.00217	-0.00209	-0.41999
D60	0.45273	-0.00005	0.00000	0.00286	0.00278	0.45551
D61	-1.97067	-0.00010	0.00000	0.00170	0.00164	-1.96903
D62	2.55223	0.00006	0.00000	0.00024	0.00025	2.55248
D63	-1.65420	0.00009	0.00000	0.00071	0.00072	-1.65348
D64	0.44720	0.00009	0.00000	0.00071	0.00072	0.44792
D65	1.34979	-0.00007	0.00000	-0.00069	-0.00070	1.34909
D66	-2.85664	-0.00004	0.00000	-0.00021	-0.00022	-2.85686
D67	-0.75524	-0.00004	0.00000	-0.00022	-0.00023	-0.75547
D68	-1.04493	-0.00007	0.00000	-0.00204	-0.00205	-1.04697
D69	1.03183	-0.00004	0.00000	-0.00157	-0.00157	1.03026
D70	3.13323	-0.00004	0.00000	-0.00157	-0.00158	3.13166

Item	Value	Threshold	Converged?
Maximum Force	0.005480	0.000450	NO
RMS Force	0.000846	0.000300	NO
Maximum Displacement	0.300432	0.001800	NO
RMS Displacement	0.077485	0.001200	NO

Predicted change in Energy=-3.493475D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.875591	2.124570	-0.243214
2	6	0	-3.792830	1.173812	0.067881
3	7	0	-3.111175	-0.038608	0.110104
4	6	0	-1.814084	0.181258	-0.171409
5	7	0	-1.653618	1.486680	-0.394239
6	6	0	-0.356225	2.126680	-0.690597
7	6	0	0.314876	2.698783	0.562912
8	1	0	-2.988763	3.186230	-0.380944
9	1	0	-4.848578	1.256852	0.251040
10	1	0	0.276888	1.358009	-1.135998
11	1	0	-0.527515	2.910689	-1.429079
12	1	0	-0.310101	3.494703	0.981225
13	1	0	0.383638	1.900289	1.316989
14	35	0	0.352296	-2.259569	-0.208634
15	1	0	-1.011544	-0.595804	-0.210140
16	6	0	-3.608572	-1.341174	0.397773
17	6	0	-4.872676	-1.613135	0.693245
18	1	0	-2.826203	-2.090299	0.348132
19	1	0	-5.156861	-2.636092	0.897233
20	1	0	-5.652179	-0.863194	0.743031
21	7	0	1.596456	3.262030	0.157510
22	1	0	1.967748	3.877306	0.871525
23	1	0	2.279907	2.520000	0.002400
24	6	0	3.758022	-0.200816	-1.057079
25	6	0	3.732859	-0.398058	0.393808
26	8	0	3.532498	0.921432	-0.175587
27	1	0	4.711213	-0.173132	-1.580012
28	1	0	2.894350	-0.512361	-1.637006
29	1	0	2.817901	-0.831441	0.791937
30	6	0	4.983299	-0.584683	1.208090
31	1	0	4.869429	-0.139008	2.200813
32	1	0	5.186293	-1.651700	1.342078
33	1	0	5.843956	-0.122879	0.718425

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357220	0.000000			

3	N	2.204466	1.391546	0.000000		
4	C	2.215494	2.226624	1.345375	0.000000	
5	N	1.386697	2.210806	2.169179	1.333990	0.000000
6	C	2.558781	3.646025	3.594349	2.485875	1.476705
7	C	3.340456	4.409517	4.408648	3.377815	2.502060
8	H	1.076522	2.213095	3.264306	3.233207	2.161309
9	H	2.211312	1.074732	2.171785	3.247079	3.267564
10	H	3.364937	4.248041	3.870695	2.585989	2.072105
11	H	2.745491	3.989976	4.212213	3.269066	2.089690
12	H	3.155670	4.283705	4.592293	3.816994	2.780125
13	H	3.620374	4.419381	4.174879	3.162338	2.692543
14	Br	5.444366	5.389493	4.126729	3.263775	4.253531
15	H	3.297908	3.308230	2.195786	1.117764	2.186983
16	C	3.599931	2.543214	1.423670	2.421147	3.527873
17	C	4.340016	3.053559	2.433531	3.649994	4.599327
18	H	4.256436	3.415748	2.085019	2.540527	3.836776
19	H	5.400806	4.130832	3.398724	4.500401	5.562181
20	H	4.196290	2.839437	2.745403	4.081427	4.775330
21	N	4.631803	5.780405	5.749630	4.607725	3.744232
22	H	5.269977	6.413967	6.458297	5.389874	4.520127
23	H	5.176471	6.220502	5.968404	4.718124	4.086281
24	C	7.076342	7.756965	6.969541	5.654977	5.707263
25	C	7.102187	7.694998	6.859336	5.605681	5.760850
26	O	6.520408	7.333717	6.718757	5.397575	5.221410
27	H	8.039033	8.766331	8.004020	6.685003	6.683720
28	H	6.495251	7.104097	6.272414	4.979803	5.121002
29	H	6.498107	6.946010	6.020583	4.838273	5.174474
30	C	8.438512	9.022905	8.186835	6.978116	7.134891
31	H	8.431037	9.017074	8.250526	7.099250	7.206060
32	H	9.042529	9.499038	8.542119	7.392946	7.723251
33	H	9.055731	9.745371	8.976164	7.715561	7.748698

		6	7	8	9	10
6	C	0.000000				
7	C	1.532634	0.000000			
8	H	2.854608	3.470231	0.000000		
9	H	4.671672	5.370074	2.753327	0.000000	
10	H	1.090903	2.164582	3.817981	5.310792	0.000000
11	H	1.090581	2.173145	2.689285	4.922354	1.773070
12	H	2.160696	1.095020	3.020909	5.112624	3.064743
13	H	2.151524	1.100433	3.988698	5.378322	2.514480
14	Br	4.469168	5.018161	6.391329	6.294887	3.735312
15	H	2.841162	3.634736	4.271106	4.285774	2.516874
16	C	4.877327	5.634002	4.635510	2.882514	4.973413
17	C	6.024912	6.746876	5.266584	2.903955	6.220276

18	H	4.996265	5.731302	5.329140	3.911886	4.870589
19	H	6.946316	7.649351	6.343013	3.958234	7.043614
20	H	6.248341	6.951681	4.975433	2.320006	6.604417
21	N	2.412731	1.457410	4.617349	6.750404	2.653247
22	H	3.302389	2.053325	5.158805	7.328989	3.638134
23	H	2.753932	2.051215	5.324444	7.243802	2.580360
24	C	4.741158	4.784068	7.579469	8.826638	3.815031
25	C	4.926545	4.615368	7.656864	8.740719	4.167471
26	O	4.103660	3.749326	6.906398	8.398628	3.422278
27	H	5.635523	5.671666	8.486030	9.838049	4.712195
28	H	4.292606	4.669558	7.061749	8.163809	3.255826
29	H	4.585135	4.333598	7.157840	7.964198	3.868769
30	C	6.282278	5.743829	8.960948	10.048532	5.605275
31	H	6.387570	5.610679	8.914811	10.009481	5.870843
32	H	7.009096	6.577575	9.654321	10.504698	6.269088
33	H	6.744487	6.209403	9.496091	10.791311	6.051790

		11	12	13	14	15
11	H	0.000000				
12	H	2.489560	0.000000			
13	H	3.064637	1.770922	0.000000		
14	Br	5.384712	5.913220	4.430906	0.000000	
15	H	3.743741	4.317826	3.241780	2.151319	0.000000
16	C	5.559554	5.882689	5.223963	4.110918	2.769420
17	C	6.621909	6.854928	6.353114	5.341497	4.093826
18	H	5.783799	6.158232	5.212155	3.231330	2.416231
19	H	7.590083	7.815675	7.173011	5.631653	4.751074
20	H	6.724763	6.898246	6.663134	6.237727	4.745053
21	N	2.674314	2.089881	2.160939	5.671865	4.671158
22	H	3.528947	2.312361	2.572244	6.437209	5.482234
23	H	3.175436	2.935351	2.389147	5.157955	4.537296
24	C	5.309019	5.861840	4.630045	4.069066	4.860255
25	C	5.693989	5.643063	4.165566	3.905940	4.786775
26	O	4.691704	4.767127	3.619567	4.498172	4.790774
27	H	6.080872	6.725068	5.605318	5.023351	5.899589
28	H	4.844550	5.760226	4.566251	3.399269	4.159197
29	H	5.488922	5.341886	3.696440	3.019918	3.965392
30	C	7.038562	6.686773	5.229132	5.124309	6.160327
31	H	7.183577	6.443506	5.006215	5.541364	6.372378
32	H	7.819354	7.538303	5.973504	5.112899	6.475915
33	H	7.376310	7.143415	5.853764	5.965167	6.934246

		16	17	18	19	20
16	C	0.000000				
17	C	1.326359	0.000000			
18	H	1.084322	2.129517	0.000000		

19	H	2.079296	1.081116	2.455885	0.000000	
20	H	2.126969	1.082827	3.106102	1.847237	0.000000
21	N	6.952664	8.118123	6.945767	8.996795	8.360802
22	H	7.651949	8.773148	7.672563	9.653241	8.975084
23	H	7.052600	8.289724	6.888160	9.093488	8.655202
24	C	7.594980	8.918926	6.992623	9.445901	9.603698
25	C	7.401763	8.696052	6.773999	9.180923	9.403044
26	O	7.512856	8.821897	7.055345	9.450497	9.401438
27	H	8.631036	9.954509	8.012859	10.468132	10.642960
28	H	6.864055	8.183427	6.257427	8.703712	8.878672
29	H	6.458696	7.730833	5.799793	8.177083	8.470281
30	C	8.663090	9.922854	7.999670	10.350254	10.649283
31	H	8.750580	9.967669	8.152467	10.414473	10.646774
32	H	8.850863	10.079947	8.085813	10.399411	10.883614
33	H	9.536107	10.819783	8.898287	11.285663	11.519973

		21	22	23	24	25
21	N	0.000000				
22	H	1.013035	0.000000			
23	H	1.020674	1.641677	0.000000		
24	C	4.258979	4.853419	3.272638	0.000000	
25	C	4.244561	4.650007	3.283188	1.464449	0.000000
26	O	3.055751	3.504579	2.038647	1.444760	1.451003
27	H	4.951872	5.471991	3.958312	1.087565	2.214437
28	H	4.376168	5.140087	3.501486	1.085958	2.200084
29	H	4.318673	4.785540	3.484962	2.168035	1.087876
30	C	5.231791	5.395940	4.289647	2.603776	1.503823
31	H	5.143394	5.130062	4.313811	3.442806	2.150388
32	H	6.199587	6.414854	5.257841	3.146582	2.140865
33	H	5.460174	5.572245	4.494435	2.740367	2.153562

		26	27	28	29	30
26	O	0.000000				
27	H	2.135380	0.000000			
28	H	2.144468	1.849139	0.000000		
29	H	2.125868	3.105501	2.451004	0.000000	
30	C	2.507543	2.831416	3.530370	2.218788	0.000000
31	H	2.925610	3.784288	4.332342	2.583246	1.094117
32	H	3.414580	3.309150	3.927599	2.566078	1.094387
33	H	2.689364	2.562897	3.794723	3.108773	1.092596

		31	32	33
31	H	0.000000		
32	H	1.768069	0.000000	
33	H	1.774103	1.777290	0.000000

Stoichiometry C10H18BrN3O

Framework group C1[X(C10H18BrN3O)]

Deg. of freedom 93

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.851795	2.170804	-0.229657
2	6	0	-3.776764	1.224360	0.071543
3	7	0	-3.105114	0.005983	0.100571
4	6	0	-1.806322	0.218157	-0.178992
5	7	0	-1.635156	1.524523	-0.387892
6	6	0	-0.332602	2.156948	-0.677804
7	6	0	0.343485	2.710056	0.581539
8	1	0	-2.956247	3.234774	-0.355982
9	1	0	-4.831750	1.314129	0.255919
10	1	0	0.294051	1.387899	-1.131608
11	1	0	-0.497598	2.950201	-1.407799
12	1	0	-0.274815	3.506574	1.008546
13	1	0	0.405841	1.902998	1.327007
14	35	0	0.339862	-2.239895	-0.243030
15	1	0	-1.010221	-0.565031	-0.226293
16	6	0	-3.613161	-1.295446	0.374446
17	6	0	-4.879395	-1.560130	0.667398
18	1	0	-2.837003	-2.050416	0.316540
19	1	0	-5.171952	-2.582836	0.860520
20	1	0	-5.652679	-0.804370	0.725457
21	7	0	1.629567	3.267033	0.181774
22	1	0	2.006084	3.871552	0.902213
23	1	0	2.306844	2.521100	0.018513
24	6	0	3.762239	-0.200305	-1.070495
25	6	0	3.735791	-0.412849	0.378207
26	8	0	3.546177	0.914265	-0.176972
27	1	0	4.715504	-0.174879	-1.593408
28	1	0	2.895894	-0.498500	-1.653444
29	1	0	2.817386	-0.842917	0.771971
30	6	0	4.984841	-0.618473	1.190043
31	1	0	4.874880	-0.182525	2.187515
32	1	0	5.179066	-1.688499	1.312540
33	1	0	5.849160	-0.158561	0.705069

Rotational constants (GHZ): 0.4959602 0.2380749 0.1694121

Standard basis: 6-311++G(d,p) (5D, 7F)
There are 499 symmetry adapted cartesian basis functions of A symmetry.
There are 482 symmetry adapted basis functions of A symmetry.
482 basis functions, 760 primitive gaussians, 499 cartesian basis functions
71 alpha electrons 71 beta electrons
nuclear repulsion energy 1290.8056779431 Hartrees.
NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 482 RedAO= T EigKep= 3.81D-06 NBF= 482
NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999969 -0.000041 -0.000640 0.007806 Ang= -0.90 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3205.64650369 A.U. after 11 cycles
NFock= 11 Conv=0.91D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Atomic Forces (Hartrees/Bohr)
Number Number X Y Z
---
1 6 -0.000274370 0.000479291 -0.000478093

2	6	0.000596692	-0.000431779	0.000158155
3	7	-0.000005289	-0.000471426	0.000511137
4	6	0.001911080	0.003305777	-0.000874952
5	7	-0.000247827	0.000005487	0.000299488
6	6	-0.001440158	-0.001268937	-0.000226590
7	6	0.001141062	0.000604387	-0.000347907
8	1	-0.000017052	-0.000014575	0.000051176
9	1	0.000056735	-0.000118809	0.000024763
10	1	0.000009762	0.000527164	-0.000121115
11	1	0.000566190	-0.000057651	0.000133345
12	1	-0.000141981	-0.000183815	0.000024940
13	1	-0.000119913	-0.000006228	0.000065906
14	35	0.000319316	-0.000234152	0.000067486
15	1	-0.002039259	-0.001022323	0.000418724
16	6	-0.000292569	-0.000882994	0.000018327
17	6	-0.000154905	0.000374605	-0.000129101
18	1	0.000639357	-0.000192363	-0.000081760
19	1	0.000080180	-0.000038407	0.000033086
20	1	-0.000141376	0.000019143	0.000039810
21	7	-0.000400497	-0.000176446	0.000366443
22	1	-0.000129792	0.000111353	0.000022327
23	1	0.000236129	0.000199013	0.000151352
24	6	0.000129259	-0.000261477	-0.000051813
25	6	0.000218897	-0.000180076	0.000119951
26	8	-0.000764045	0.000599041	-0.000146521
27	1	-0.000141025	-0.000046258	0.000066506
28	1	0.000272014	-0.000161682	-0.000194781
29	1	0.000249255	-0.000363602	0.000142628
30	6	-0.000069413	-0.000234721	0.000080995
31	1	0.000015504	0.000019252	-0.000048653
32	1	-0.000091770	0.000072654	-0.000067928
33	1	0.000029810	0.000030555	-0.000027330

Cartesian Forces: Max 0.003305777 RMS 0.000572913

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.002474948 RMS 0.000379785

Search for a local minimum.

Step number 5 out of a maximum of 172

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.
Update second derivatives using D2CorX and points 2 3 1 4 5
DE= -2.34D-04 DEPred=-3.49D-04 R= 6.71D-01
TightC=F SS= 1.41D+00 RLast= 1.63D-01 DXNew= 2.5227D-01 4.9002D-01
Trust test= 6.71D-01 RLast= 1.63D-01 DXMaxT set to 2.52D-01
ITU= 1 0 0 -1 0

Eigenvalues ---	0.00222	0.00230	0.00230	0.00301	0.00404
Eigenvalues ---	0.00600	0.00723	0.00855	0.01385	0.01467
Eigenvalues ---	0.01816	0.01918	0.02083	0.02163	0.02265
Eigenvalues ---	0.02325	0.02367	0.02388	0.02393	0.02949
Eigenvalues ---	0.03060	0.03070	0.03075	0.03194	0.03937
Eigenvalues ---	0.04041	0.04419	0.04590	0.04659	0.05403
Eigenvalues ---	0.05743	0.05766	0.05900	0.07961	0.08593
Eigenvalues ---	0.09497	0.10987	0.11892	0.12202	0.12527
Eigenvalues ---	0.12787	0.12837	0.13853	0.15502	0.15998
Eigenvalues ---	0.16000	0.16000	0.16000	0.16000	0.16000
Eigenvalues ---	0.16000	0.16025	0.17134	0.19733	0.21548
Eigenvalues ---	0.22030	0.22946	0.23026	0.24884	0.26265
Eigenvalues ---	0.29115	0.29520	0.31653	0.32064	0.32120
Eigenvalues ---	0.33651	0.34050	0.34282	0.34327	0.34344
Eigenvalues ---	0.34538	0.34664	0.34720	0.35053	0.35059
Eigenvalues ---	0.35276	0.35591	0.35739	0.35891	0.36416
Eigenvalues ---	0.36576	0.36628	0.38317	0.41957	0.42455
Eigenvalues ---	0.44409	0.45182	0.45463	0.48741	0.54589
Eigenvalues ---	0.55564	0.60495	0.85942		

En-DIIS/RFO-DIIS IScMMF= 0 using points: 5 4
RFO step: Lambda=-6.29234945D-05.
DidBck=F Rises=F RFO-DIIS coefs: 1.03290 -0.03290
Iteration 1 RMS(Cart)= 0.07636737 RMS(Int)= 0.00289663
Iteration 2 RMS(Cart)= 0.00567712 RMS(Int)= 0.00005864
Iteration 3 RMS(Cart)= 0.00003705 RMS(Int)= 0.00005441
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00005441

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56477	0.00049	-0.00003	0.00062	0.00059	2.56537
R2	2.62048	0.00021	0.00004	0.00119	0.00123	2.62171
R3	2.03433	-0.00002	0.00000	-0.00006	-0.00006	2.03427
R4	2.62964	-0.00030	0.00001	-0.00059	-0.00059	2.62905
R5	2.03095	-0.00006	-0.00001	-0.00034	-0.00035	2.03060
R6	2.54239	-0.00052	-0.00006	-0.00205	-0.00211	2.54028
R7	2.69035	0.00058	0.00003	0.00194	0.00197	2.69232
R8	2.52088	-0.00101	-0.00027	-0.00627	-0.00654	2.51433
R9	2.11227	-0.00038	-0.00003	-0.00178	-0.00181	2.11046
R10	2.79057	-0.00070	-0.00030	-0.00696	-0.00726	2.78331

R11	2.89626	0.00032	0.00005	0.00204	0.00209	2.89835
R12	2.06151	-0.00031	-0.00003	-0.00148	-0.00151	2.05999
R13	2.06090	-0.00022	-0.00002	-0.00102	-0.00104	2.05986
R14	2.06929	-0.00004	0.00002	0.00014	0.00016	2.06944
R15	2.07952	0.00004	0.00001	0.00028	0.00029	2.07981
R16	2.75411	-0.00067	-0.00024	-0.00572	-0.00596	2.74815
R17	4.06540	0.00038	0.00013	0.01023	0.01035	4.07576
R18	2.50645	0.00012	0.00003	0.00072	0.00076	2.50721
R19	2.04907	0.00060	-0.00001	0.00147	0.00145	2.05053
R20	2.04301	0.00002	0.00001	0.00027	0.00028	2.04330
R21	2.04625	0.00012	-0.00002	0.00009	0.00007	2.04632
R22	1.91436	0.00003	0.00000	0.00004	0.00004	1.91440
R23	1.92879	0.00030	0.00010	0.00231	0.00241	1.93121
R24	3.85248	0.00034	0.00003	0.00916	0.00918	3.86167
R25	2.76741	-0.00024	-0.00004	-0.00076	-0.00092	2.76649
R26	2.73020	0.00059	0.00002	0.00172	0.00180	2.73200
R27	2.05520	-0.00016	-0.00002	-0.00076	-0.00078	2.05442
R28	2.05216	-0.00007	0.00000	-0.00026	-0.00026	2.05190
R29	2.74200	0.00090	0.00005	0.00291	0.00303	2.74503
R30	2.05579	-0.00001	0.00000	-0.00004	-0.00004	2.05575
R31	2.84181	-0.00011	0.00003	0.00020	0.00023	2.84205
R32	2.06758	-0.00004	0.00000	-0.00014	-0.00015	2.06744
R33	2.06809	-0.00010	0.00000	-0.00030	-0.00030	2.06779
R34	2.06471	0.00005	0.00001	0.00036	0.00037	2.06508
A1	1.87367	-0.00049	-0.00007	-0.00255	-0.00262	1.87105
A2	2.27723	0.00022	0.00000	0.00052	0.00051	2.27774
A3	2.13218	0.00027	0.00007	0.00209	0.00215	2.13434
A4	1.86110	0.00024	-0.00008	0.00019	0.00011	1.86122
A5	2.27683	0.00000	0.00003	0.00050	0.00053	2.27737
A6	2.14522	-0.00024	0.00005	-0.00071	-0.00066	2.14456
A7	1.90026	-0.00042	0.00010	-0.00040	-0.00031	1.89995
A8	2.25512	0.00072	0.00002	0.00346	0.00347	2.25859
A9	2.12779	-0.00030	-0.00012	-0.00302	-0.00315	2.12464
A10	1.88688	0.00073	-0.00009	0.00109	0.00100	1.88789
A11	2.19674	-0.00247	-0.00008	-0.01691	-0.01699	2.17974
A12	2.19957	0.00175	0.00016	0.01582	0.01598	2.21555
A13	1.90283	-0.00006	0.00014	0.00170	0.00183	1.90466
A14	2.21018	0.00125	0.00018	0.00744	0.00761	2.21779
A15	2.16920	-0.00119	-0.00032	-0.00933	-0.00966	2.15954
A16	1.96313	-0.00055	-0.00046	-0.00963	-0.01009	1.95304
A17	1.86131	0.00023	0.00007	0.00295	0.00301	1.86432
A18	1.88543	0.00061	0.00008	0.00721	0.00729	1.89272
A19	1.92072	0.00001	0.00010	0.00001	0.00011	1.92083
A20	1.93291	-0.00004	0.00021	0.00270	0.00293	1.93584

A21	1.89782	-0.00022	0.00000	-0.00304	-0.00305	1.89477
A22	1.91118	-0.00027	0.00010	-0.00038	-0.00028	1.91089
A23	1.89332	-0.00017	0.00021	0.00253	0.00274	1.89605
A24	1.87738	0.00054	-0.00026	-0.00074	-0.00100	1.87638
A25	1.87686	0.00001	-0.00001	-0.00202	-0.00203	1.87482
A26	1.90418	0.00009	0.00003	0.00221	0.00224	1.90642
A27	1.99995	-0.00023	-0.00005	-0.00156	-0.00161	1.99834
A28	2.17195	-0.00024	0.00008	0.00020	0.00028	2.17222
A29	1.95063	-0.00019	-0.00003	-0.00203	-0.00207	1.94856
A30	2.16061	0.00043	-0.00004	0.00184	0.00179	2.16240
A31	2.07896	-0.00017	0.00000	-0.00105	-0.00105	2.07791
A32	2.15835	0.00018	0.00001	0.00123	0.00124	2.15959
A33	2.04588	-0.00001	-0.00001	-0.00019	-0.00019	2.04569
A34	1.94010	-0.00005	0.00007	-0.00101	-0.00119	1.93891
A35	1.92851	-0.00026	0.00012	0.00221	0.00228	1.93078
A36	1.87889	0.00019	-0.00001	0.00078	0.00082	1.87971
A37	2.08847	-0.00029	-0.00004	-0.00268	-0.00263	2.08584
A38	2.06778	0.00032	0.00002	0.00216	0.00208	2.06985
A39	1.99370	-0.00016	0.00000	0.00006	0.00001	1.99370
A40	2.00923	0.00017	-0.00003	0.00218	0.00217	2.01140
A41	2.03485	-0.00013	0.00002	-0.00102	-0.00100	2.03385
A42	2.01605	0.00034	-0.00001	0.00076	0.00065	2.01670
A43	2.13991	-0.00023	-0.00001	-0.00176	-0.00168	2.13823
A44	1.97115	0.00025	0.00000	0.00347	0.00350	1.97465
A45	2.02657	-0.00006	0.00005	0.00211	0.00210	2.02867
A46	2.03951	-0.00021	-0.00001	-0.00193	-0.00195	2.03756
A47	2.43145	0.00045	0.00005	0.00677	0.00668	2.43813
A48	2.43973	0.00046	0.00009	0.00758	0.00751	2.44724
A49	1.93286	0.00002	0.00000	0.00020	0.00020	1.93307
A50	1.91933	-0.00013	0.00002	-0.00056	-0.00054	1.91879
A51	1.93892	0.00000	0.00000	0.00011	0.00011	1.93904
A52	1.88112	0.00006	0.00000	0.00047	0.00047	1.88159
A53	1.89278	-0.00001	-0.00002	-0.00026	-0.00027	1.89251
A54	1.89743	0.00006	-0.00001	0.00005	0.00004	1.89747
A55	3.24539	-0.00045	0.00362	-0.05556	-0.05194	3.19345
A56	3.06341	-0.00023	-0.00224	0.04533	0.04287	3.10628
A57	3.07472	-0.00016	-0.00216	-0.11273	-0.11489	2.95983
A58	3.21018	-0.00022	0.00076	-0.05313	-0.05227	3.15791
D1	0.00583	-0.00008	0.00014	-0.00157	-0.00144	0.00439
D2	-3.12725	-0.00005	0.00013	0.00012	0.00026	-3.12698
D3	3.13193	0.00005	0.00007	0.00263	0.00271	3.13464
D4	-0.00114	0.00008	0.00007	0.00433	0.00441	0.00327
D5	-0.00837	0.00011	-0.00011	0.00278	0.00267	-0.00570
D6	-3.10368	0.00020	-0.00004	0.00781	0.00781	-3.09588

D7	-3.13604	-0.00001	-0.00005	-0.00099	-0.00105	-3.13709
D8	0.05183	0.00008	0.00002	0.00404	0.00409	0.05592
D9	-0.00139	0.00003	-0.00011	-0.00016	-0.00027	-0.00166
D10	3.13556	0.00009	0.00016	0.00760	0.00778	-3.13984
D11	3.13248	0.00000	-0.00011	-0.00169	-0.00180	3.13067
D12	-0.01375	0.00006	0.00016	0.00607	0.00625	-0.00750
D13	-0.00380	0.00003	0.00004	0.00189	0.00193	-0.00187
D14	3.13656	-0.00007	0.00014	-0.00089	-0.00072	3.13584
D15	-3.14116	-0.00003	-0.00020	-0.00521	-0.00540	3.13662
D16	-0.00080	-0.00013	-0.00011	-0.00799	-0.00806	-0.00886
D17	-0.00603	-0.00001	0.00001	0.00032	0.00032	-0.00571
D18	3.13719	0.00000	-0.00024	-0.00352	-0.00376	3.13343
D19	3.13039	0.00006	0.00031	0.00897	0.00929	3.13968
D20	-0.00957	0.00007	0.00007	0.00514	0.00521	-0.00436
D21	0.00749	-0.00008	0.00004	-0.00287	-0.00283	0.00466
D22	3.10414	-0.00010	-0.00002	-0.00721	-0.00721	3.09693
D23	-3.13287	0.00003	-0.00005	-0.00006	-0.00008	-3.13295
D24	-0.03622	0.00002	-0.00011	-0.00440	-0.00446	-0.04068
D25	1.43134	0.00015	0.00005	0.01678	0.01683	1.44817
D26	-2.74476	-0.00002	-0.00005	0.01302	0.01297	-2.73179
D27	-0.70732	0.00014	0.00003	0.01460	0.01464	-0.69268
D28	-1.65730	0.00021	0.00013	0.02216	0.02229	-1.63501
D29	0.44979	0.00004	0.00003	0.01840	0.01842	0.46822
D30	2.48723	0.00020	0.00011	0.01998	0.02010	2.50733
D31	-1.10560	-0.00005	0.00040	-0.00631	-0.00591	-1.11151
D32	0.93800	-0.00029	0.00056	-0.00751	-0.00695	0.93105
D33	3.11040	-0.00033	0.00046	-0.00832	-0.00786	3.10254
D34	3.10499	0.00001	0.00054	-0.00385	-0.00331	3.10168
D35	-1.13460	-0.00022	0.00070	-0.00504	-0.00435	-1.13895
D36	1.03781	-0.00027	0.00060	-0.00585	-0.00526	1.03255
D37	1.00608	0.00032	0.00033	-0.00179	-0.00146	1.00462
D38	3.04967	0.00008	0.00049	-0.00299	-0.00250	3.04717
D39	-1.06111	0.00004	0.00040	-0.00380	-0.00341	-1.06452
D40	2.86265	-0.00003	-0.00022	-0.00856	-0.00872	2.85393
D41	-1.33557	0.00001	-0.00010	-0.00680	-0.00696	-1.34253
D42	0.79096	-0.00007	-0.00020	-0.00891	-0.00904	0.78192
D43	2.87593	-0.00003	-0.00008	-0.00714	-0.00729	2.86864
D44	-1.31401	0.00000	-0.00017	-0.00688	-0.00698	-1.32099
D45	0.77096	0.00004	-0.00005	-0.00511	-0.00523	0.76573
D46	3.14125	0.00004	-0.00023	-0.00227	-0.00250	3.13875
D47	0.00092	-0.00001	-0.00010	-0.00191	-0.00201	-0.00109
D48	-0.00217	0.00004	0.00005	0.00202	0.00207	-0.00010
D49	3.14068	-0.00002	0.00018	0.00238	0.00256	-3.13995
D50	1.21774	0.00019	-0.00056	0.00892	0.00837	1.22610

D51	-0.52629	-0.00009	0.00060	-0.03255	-0.03225	-0.55854
D52	-2.97549	0.00012	-0.00088	0.03185	0.03127	-2.94422
D53	1.56367	-0.00016	0.00028	-0.00962	-0.00935	1.55432
D54	-2.70328	0.00025	0.00004	0.00574	0.00579	-2.69749
D55	-0.01390	-0.00001	-0.00003	-0.00184	-0.00187	-0.01577
D56	-0.02444	-0.00002	0.00004	0.00184	0.00188	-0.02256
D57	2.66494	-0.00028	-0.00003	-0.00574	-0.00577	2.65917
D58	2.00357	-0.00023	-0.00007	-0.00984	-0.00984	1.99372
D59	-0.41999	-0.00003	-0.00007	-0.01089	-0.01086	-0.43086
D60	0.45551	0.00009	0.00009	0.01261	0.01262	0.46813
D61	-1.96903	0.00019	0.00005	0.00896	0.00894	-1.96008
D62	2.55248	0.00005	0.00001	0.00137	0.00139	2.55387
D63	-1.65348	0.00006	0.00002	0.00172	0.00176	-1.65172
D64	0.44792	0.00005	0.00002	0.00148	0.00152	0.44944
D65	1.34909	0.00001	-0.00002	0.00046	0.00043	1.34952
D66	-2.85686	0.00002	-0.00001	0.00081	0.00079	-2.85607
D67	-0.75547	0.00000	-0.00001	0.00058	0.00056	-0.75491
D68	-1.04697	-0.00008	-0.00007	-0.00566	-0.00573	-1.05270
D69	1.03026	-0.00007	-0.00005	-0.00530	-0.00536	1.02490
D70	3.13166	-0.00009	-0.00005	-0.00554	-0.00559	3.12606

Item	Value	Threshold	Converged?
Maximum Force	0.002475	0.000450	NO
RMS Force	0.000380	0.000300	NO
Maximum Displacement	0.634139	0.001800	NO
RMS Displacement	0.080596	0.001200	NO

Predicted change in Energy=-1.224861D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.905959	2.139627	-0.290771
2	6	0	-3.827638	1.194321	0.025137
3	7	0	-3.146760	-0.016595	0.100125
4	6	0	-1.846979	0.198479	-0.166984
5	7	0	-1.682520	1.496335	-0.409531
6	6	0	-0.376320	2.117239	-0.688180
7	6	0	0.274434	2.675947	0.583324
8	1	0	-3.016391	3.198811	-0.448132
9	1	0	-4.886004	1.279557	0.190223
10	1	0	0.255428	1.341824	-1.121710
11	1	0	-0.519257	2.903227	-1.429773

12	1	0	-0.347255	3.481442	0.988208
13	1	0	0.312046	1.877017	1.339360
14	35	0	0.305186	-2.235748	0.126938
15	1	0	-1.057184	-0.591092	-0.174441
16	6	0	-3.645503	-1.317806	0.396630
17	6	0	-4.914784	-1.591039	0.669683
18	1	0	-2.858107	-2.063936	0.369820
19	1	0	-5.198401	-2.612982	0.880227
20	1	0	-5.698802	-0.844509	0.694291
21	7	0	1.572705	3.214443	0.209994
22	1	0	1.933530	3.828497	0.930429
23	1	0	2.249986	2.460952	0.076116
24	6	0	3.810518	-0.186870	-1.075289
25	6	0	3.814962	-0.422268	0.369620
26	8	0	3.551424	0.903576	-0.162121
27	1	0	4.754975	-0.107981	-1.607907
28	1	0	2.954001	-0.520156	-1.653475
29	1	0	2.926671	-0.907139	0.768706
30	6	0	5.085299	-0.581650	1.158730
31	1	0	4.971133	-0.167868	2.165047
32	1	0	5.331429	-1.643085	1.259294
33	1	0	5.919252	-0.073201	0.668626

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357533	0.000000			
3	N	2.204559	1.391236	0.000000		
4	C	2.214682	2.225224	1.344260	0.000000	
5	N	1.387347	2.209453	2.166266	1.330528	0.000000
6	C	2.560763	3.643103	3.584692	2.473080	1.472863
7	C	3.341643	4.397020	4.380392	3.346820	2.491368
8	H	1.076488	2.213614	3.264417	3.232423	2.163128
9	H	2.211708	1.074549	2.170966	3.245304	3.266344
10	H	3.364716	4.243636	3.861744	2.576597	2.070438
11	H	2.752591	3.997813	4.215415	3.266978	2.091272
12	H	3.159623	4.274517	4.567515	3.789655	2.770787
13	H	3.616883	4.396617	4.133378	3.122171	2.679894
14	Br	5.443330	5.371776	4.103814	3.262464	4.262302
15	H	3.299747	3.301961	2.184436	1.116805	2.191726
16	C	3.601845	2.545969	1.424713	2.418981	3.524568
17	C	4.344620	3.058685	2.434990	3.648810	4.598272
18	H	4.255422	3.416876	2.085105	2.535559	3.829481
19	H	5.404981	4.135907	3.399855	4.498110	5.559800

20	H	4.204211	2.847077	2.747979	4.082420	4.777917
21	N	4.632971	5.768776	5.720579	4.575193	3.732586
22	H	5.269180	6.399179	6.425223	5.354773	4.506694
23	H	5.178959	6.208419	5.938323	4.686470	4.078105
24	C	7.151163	7.839647	7.057926	5.742890	5.783588
25	C	7.222894	7.819295	6.978737	5.721088	5.874557
26	O	6.575877	7.387161	6.766177	5.444257	5.273210
27	H	8.091755	8.833124	8.084747	6.764316	6.741756
28	H	6.578035	7.193595	6.367730	5.076958	5.206819
29	H	6.665196	7.112645	6.174677	4.988551	5.330063
30	C	8.565431	9.158579	8.319059	7.100887	7.251265
31	H	8.567622	9.157137	8.377767	7.215208	7.325921
32	H	9.195987	9.667603	8.710272	7.546865	7.863614
33	H	9.148846	9.850003	9.083995	7.815779	7.836632

		6	7	8	9	10
6	C	0.000000				
7	C	1.533739	0.000000			
8	H	2.863109	3.488096	0.000000		
9	H	4.670177	5.360461	2.754357	0.000000	
10	H	1.090102	2.165037	3.821897	5.306539	0.000000
11	H	1.090031	2.175812	2.699382	4.932460	1.770034
12	H	2.161520	1.095103	3.044214	5.107379	3.064791
13	H	2.154640	1.100589	4.002594	5.356976	2.519226
14	Br	4.480778	4.932949	6.395155	6.269755	3.789541
15	H	2.839465	3.608456	4.275132	4.276934	2.521196
16	C	4.864556	5.599180	4.637804	2.885782	4.959460
17	C	6.016043	6.718825	5.272197	2.910504	6.208209
18	H	4.976028	5.685498	5.328283	3.914533	4.849532
19	H	6.934505	7.616616	6.348436	3.965546	7.027979
20	H	6.245958	6.934369	4.984867	2.329460	6.597784
21	N	2.410242	1.454256	4.636073	6.742336	2.648651
22	H	3.299046	2.049745	5.176741	7.317857	3.634672
23	H	2.756768	2.050924	5.343594	7.234021	2.581762
24	C	4.794621	4.842584	7.646100	8.909625	3.870108
25	C	5.013470	4.709560	7.774851	8.867649	4.243391
26	O	4.144501	3.799428	6.963195	8.453146	3.460702
27	H	5.668129	5.712005	8.524909	9.904898	4.752289
28	H	4.356454	4.732698	7.136466	8.252507	3.321452
29	H	4.709472	4.461752	7.325264	8.133521	3.970774
30	C	6.365875	5.838447	9.083571	10.189651	5.676955
31	H	6.477489	5.713853	9.053384	10.156678	5.943048
32	H	7.107116	6.684623	9.800273	10.680856	6.351744
33	H	6.802439	6.279257	9.581175	10.900109	6.106267

		11	12	13	14	15

11	H	0.000000					
12	H	2.492097	0.000000				
13	H	3.067942	1.769793	0.000000			
14	Br	5.432507	5.818396	4.287756	0.000000		
15	H	3.751731	4.294332	3.202803	2.156798	0.000000	
16	C	5.561140	5.853305	5.172796	4.064886	2.748387	
17	C	6.627730	6.833290	6.308378	5.287562	4.073514	
18	H	5.777670	6.118660	5.149853	3.177252	2.389312	
19	H	7.593356	7.790204	7.122915	5.567694	4.727583	
20	H	6.736829	6.887619	6.629714	6.189128	4.729010	
21	N	2.676190	2.088816	2.157183	5.596256	4.641788	
22	H	3.527441	2.307762	2.569963	6.330258	5.449575	
23	H	3.183082	2.935809	2.385870	5.083682	4.507230	
24	C	5.331165	5.916216	4.725407	4.234455	4.966835	
25	C	5.751712	5.739831	4.300875	3.958046	4.905335	
26	O	4.709139	4.813351	3.700757	4.525149	4.844940	
27	H	6.075906	6.756961	5.689131	5.228547	6.005781	
28	H	4.881918	5.821475	4.656547	3.623445	4.275767	
29	H	5.588078	5.479636	3.861791	3.008197	4.106155	
30	C	7.089130	6.786047	5.372301	5.162375	6.285502	
31	H	7.245601	6.556498	5.154649	5.495551	6.480195	
32	H	7.882295	7.653870	6.131210	5.186193	6.631491	
33	H	7.397081	7.211569	5.974445	6.040511	7.046249	

		16	17	18	19	20
16	C	0.000000				
17	C	1.326759	0.000000			
18	H	1.085091	2.131542	0.000000		
19	H	2.079144	1.081265	2.457426	0.000000	
20	H	2.128062	1.082865	3.108349	1.847287	0.000000
21	N	6.914174	8.086500	6.893397	8.958569	8.341729
22	H	7.608875	8.737206	7.615434	9.610390	8.952387
23	H	7.009888	8.252568	6.830335	9.048197	8.630842
24	C	7.683607	9.008192	7.076883	9.532612	9.694899
25	C	7.514071	8.812748	6.872039	9.289815	9.528662
26	O	7.552648	8.865194	7.083161	9.487470	9.452826
27	H	8.720658	10.044457	8.105318	10.561038	10.729587
28	H	6.956482	8.274155	6.344886	8.789837	8.971522
29	H	6.595495	7.871844	5.912777	8.302959	8.626021
30	C	8.794864	10.062788	8.118944	10.486103	10.797298
31	H	8.871081	10.099153	8.253175	10.537967	10.792056
32	H	9.024152	10.263296	8.248441	10.581196	11.073525
33	H	9.649226	10.939843	9.005239	11.406027	11.643657

		21	22	23	24	25
21	N	0.000000				

22	H	1.013057	0.000000			
23	H	1.021950	1.643221	0.000000		
24	C	4.269507	4.865096	3.282066	0.000000	
25	C	4.275379	4.682232	3.293669	1.463965	0.000000
26	O	3.064947	3.516590	2.043506	1.445710	1.452606
27	H	4.946727	5.468049	3.963624	1.087154	2.212015
28	H	4.396331	5.160301	3.517687	1.085818	2.200852
29	H	4.374107	4.841356	3.504514	2.168016	1.087856
30	C	5.258207	5.425418	4.297497	2.602260	1.503946
31	H	5.177989	5.169356	4.321917	3.441971	2.150584
32	H	6.230940	6.449192	5.266718	3.143884	2.140464
33	H	5.469133	5.583706	4.498501	2.738780	2.153901

		26	27	28	29	30
26	O	0.000000				
27	H	2.135903	0.000000			
28	H	2.146640	1.848099	0.000000		
29	H	2.129658	3.103166	2.453052	0.000000	
30	C	2.510641	2.826262	3.529123	2.217598	0.000000
31	H	2.929040	3.779615	4.332902	2.583818	1.094040
32	H	3.416771	3.302981	3.923947	2.562257	1.094229
33	H	2.692739	2.557216	3.792708	3.108216	1.092794

		31	32	33
31	H	0.000000		
32	H	1.768182	0.000000	
33	H	1.774025	1.777346	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.881816	2.181154	-0.211937
2	6	0	-3.804354	1.218616	0.043682
3	7	0	-3.126434	0.003784	0.031591
4	6	0	-1.827559	0.233561	-0.227565
5	7	0	-1.660844	1.544597	-0.381504
6	6	0	-0.354488	2.180024	-0.624387
7	6	0	0.304841	2.648675	0.678689
8	1	0	-2.990178	3.248895	-0.295683

9	1	0	-4.861548	1.294860	0.220265
10	1	0	0.272696	1.434653	-1.113656
11	1	0	-0.499345	3.015351	-1.309524
12	1	0	-0.312360	3.425995	1.141385
13	1	0	0.344419	1.799697	1.377950
14	35	0	0.319435	-2.220226	-0.113507
15	1	0	-1.040012	-0.555524	-0.293644
16	6	0	-3.627138	-1.313499	0.241038
17	6	0	-4.895642	-1.601779	0.501963
18	1	0	-2.841976	-2.057915	0.158645
19	1	0	-5.180924	-2.635073	0.643570
20	1	0	-5.677436	-0.856822	0.582168
21	7	0	1.602516	3.208398	0.335744
22	1	0	1.969025	3.770744	1.094508
23	1	0	2.276952	2.464245	0.146660
24	6	0	3.823733	-0.102116	-1.192448
25	6	0	3.835520	-0.436046	0.232874
26	8	0	3.572724	0.923765	-0.205210
27	1	0	4.765443	0.010851	-1.723791
28	1	0	2.963108	-0.392925	-1.787221
29	1	0	2.948109	-0.945016	0.602849
30	6	0	5.109758	-0.652195	1.001934
31	1	0	5.002311	-0.308117	2.034885
32	1	0	5.353494	-1.718612	1.028088
33	1	0	5.942393	-0.113331	0.543084

Rotational constants (GHZ): 0.5060212 0.2336841 0.1673423

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1288.2292005792 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 3.83D-06 NBF= 482

NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999981 -0.005951 -0.000727 -0.001357 Ang= -0.70 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3205.64644702 A.U. after 12 cycles
NFock= 12 Conv=0.79D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000101169	-0.000060161	0.000102822
2	6	0.000442724	-0.000461755	0.000241340
3	7	-0.001533431	-0.001064811	0.000660544
4	6	0.000201600	-0.000847746	-0.001803305
5	7	-0.000153098	0.001151378	-0.001295113
6	6	-0.000567845	0.000151848	0.001281244
7	6	0.000533808	0.000060869	-0.000522754
8	1	0.000166430	-0.000028827	0.000049108
9	1	-0.000084012	-0.000011549	0.000131234
10	1	0.000297157	0.000084965	-0.000045929
11	1	0.000175269	0.000385911	0.000245011
12	1	-0.000159534	-0.000061818	-0.000212014
13	1	-0.000382800	-0.000212576	-0.000416134
14	35	0.000516004	-0.000286690	-0.000221874
15	1	-0.000553604	0.000435619	0.001510949
16	6	-0.000727748	-0.000659525	-0.000449375
17	6	0.000349226	0.000327495	-0.000244587
18	1	0.000358904	0.000048062	0.000553700

19	1	0.000095787	0.000054363	0.000088291
20	1	-0.000052716	0.000111665	0.000077629
21	7	0.001928224	0.000061065	0.000404078
22	1	0.000216778	0.000078992	-0.000132384
23	1	-0.000222792	0.001257521	-0.000072011
24	6	0.000463644	0.000483424	0.000470413
25	6	0.000016449	-0.000413805	0.000297269
26	8	-0.000548049	-0.001577864	-0.000288459
27	1	-0.000085290	0.000073605	-0.000342171
28	1	-0.000025288	0.000299363	-0.000371537
29	1	-0.000437863	0.000362201	0.000457295
30	6	0.000031340	0.000363401	-0.000108762
31	1	-0.000061398	-0.000073894	-0.000070863
32	1	-0.000097262	-0.000026027	0.000006118
33	1	0.000000555	-0.000004698	0.000020226

Cartesian Forces: Max 0.001928224 RMS 0.000554123

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.004067941 RMS 0.000677391
Search for a local minimum.
Step number 6 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 2 3 1 4 5
6
DE= 5.67D-05 DEPred=-1.22D-04 R=-4.63D-01
Trust test=-4.63D-01 RLast= 1.67D-01 DXMaxT set to 1.26D-01
ITU= -1 1 0 0 -1 0

Eigenvalues ---	0.00203	0.00230	0.00235	0.00374	0.00464
Eigenvalues ---	0.00721	0.00782	0.00838	0.01349	0.01449
Eigenvalues ---	0.01785	0.01869	0.02083	0.02163	0.02303
Eigenvalues ---	0.02333	0.02374	0.02382	0.02444	0.02988
Eigenvalues ---	0.03070	0.03076	0.03090	0.03243	0.03967
Eigenvalues ---	0.04080	0.04446	0.04500	0.04696	0.05420
Eigenvalues ---	0.05739	0.05766	0.05904	0.08233	0.08651
Eigenvalues ---	0.09286	0.10160	0.11418	0.12115	0.12384
Eigenvalues ---	0.12677	0.12773	0.13415	0.15515	0.15999
Eigenvalues ---	0.16000	0.16000	0.16000	0.16000	0.16000

Eigenvalues --- 0.16009 0.16024 0.17193 0.21018 0.21458
Eigenvalues --- 0.22045 0.22997 0.23003 0.24933 0.27671
Eigenvalues --- 0.29072 0.29695 0.31621 0.32072 0.32553
Eigenvalues --- 0.33654 0.34272 0.34303 0.34332 0.34534
Eigenvalues --- 0.34594 0.34691 0.34912 0.35058 0.35112
Eigenvalues --- 0.35279 0.35596 0.35765 0.35893 0.36416
Eigenvalues --- 0.36618 0.37839 0.38851 0.41931 0.42568
Eigenvalues --- 0.44858 0.45459 0.45680 0.48846 0.54634
Eigenvalues --- 0.57768 0.60657 1.24802
En-DIIS/RFO-DIIS IScMMF= 0 using points: 6 5 4
RFO step: Lambda=-1.32273495D-04.
DidBck=T Rises=F RFO-DIIS coefs: 0.37035 0.98501 -0.35536
Iteration 1 RMS(Cart)= 0.12215716 RMS(Int)= 0.00355635
Iteration 2 RMS(Cart)= 0.01263961 RMS(Int)= 0.00005006
Iteration 3 RMS(Cart)= 0.00005853 RMS(Int)= 0.00003802
Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00003802

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56537	0.00089	-0.00069	0.00119	0.00050	2.56587
R2	2.62171	-0.00012	-0.00039	0.00113	0.00074	2.62245
R3	2.03427	-0.00005	0.00003	-0.00010	-0.00007	2.03420
R4	2.62905	-0.00006	0.00045	-0.00098	-0.00053	2.62852
R5	2.03060	0.00010	0.00011	-0.00025	-0.00014	2.03046
R6	2.54028	0.00104	0.00073	-0.00148	-0.00075	2.53953
R7	2.69232	0.00011	-0.00090	0.00208	0.00118	2.69350
R8	2.51433	0.00163	0.00122	-0.00422	-0.00300	2.51133
R9	2.11046	-0.00013	0.00082	-0.00205	-0.00123	2.10923
R10	2.78331	0.00138	0.00130	-0.00445	-0.00316	2.78015
R11	2.89835	0.00002	-0.00079	0.00228	0.00149	2.89984
R12	2.05999	0.00013	0.00060	-0.00139	-0.00079	2.05920
R13	2.05986	0.00009	0.00041	-0.00096	-0.00054	2.05932
R14	2.06944	-0.00003	0.00008	0.00001	0.00009	2.06953
R15	2.07981	-0.00014	-0.00008	0.00016	0.00008	2.07989
R16	2.74815	0.00131	0.00115	-0.00366	-0.00250	2.74564
R17	4.07576	0.00051	-0.00517	0.01262	0.00745	4.08321
R18	2.50721	-0.00049	-0.00014	0.00041	0.00027	2.50748
R19	2.05053	0.00022	-0.00108	0.00199	0.00091	2.05144
R20	2.04330	-0.00006	-0.00004	0.00017	0.00013	2.04343
R21	2.04632	0.00011	-0.00021	0.00030	0.00009	2.04641
R22	1.91440	0.00003	-0.00005	0.00008	0.00004	1.91444
R23	1.93121	-0.00120	-0.00048	0.00141	0.00093	1.93213
R24	3.86167	-0.00010	-0.00549	0.00978	0.00428	3.86595
R25	2.76649	0.00101	0.00016	-0.00016	0.00001	2.76650
R26	2.73200	-0.00072	-0.00088	0.00138	0.00049	2.73249

R27	2.05442	0.00010	0.00029	-0.00067	-0.00038	2.05404
R28	2.05190	0.00012	0.00013	-0.00022	-0.00009	2.05181
R29	2.74503	-0.00081	-0.00136	0.00274	0.00137	2.74640
R30	2.05575	0.00036	0.00005	0.00008	0.00012	2.05587
R31	2.84205	-0.00021	0.00021	-0.00018	0.00003	2.84208
R32	2.06744	-0.00009	0.00007	-0.00020	-0.00014	2.06730
R33	2.06779	0.00000	0.00018	-0.00034	-0.00016	2.06763
R34	2.06508	-0.00001	-0.00010	0.00032	0.00022	2.06530
A1	1.87105	0.00021	0.00093	-0.00203	-0.00110	1.86995
A2	2.27774	0.00005	-0.00037	0.00066	0.00029	2.27803
A3	2.13434	-0.00026	-0.00059	0.00144	0.00085	2.13519
A4	1.86122	0.00066	-0.00096	0.00127	0.00031	1.86153
A5	2.27737	-0.00029	0.00001	0.00021	0.00022	2.27759
A6	2.14456	-0.00037	0.00096	-0.00149	-0.00053	2.14403
A7	1.89995	-0.00079	0.00126	-0.00186	-0.00061	1.89935
A8	2.25859	0.00020	-0.00195	0.00398	0.00202	2.26061
A9	2.12464	0.00059	0.00071	-0.00213	-0.00143	2.12321
A10	1.88789	0.00058	-0.00157	0.00265	0.00109	1.88897
A11	2.17974	0.00000	0.00987	-0.02111	-0.01124	2.16850
A12	2.21555	-0.00058	-0.00830	0.01843	0.01013	2.22568
A13	1.90466	-0.00066	0.00033	0.00000	0.00033	1.90498
A14	2.21779	0.00155	-0.00283	0.00702	0.00419	2.22197
A15	2.15954	-0.00090	0.00260	-0.00736	-0.00476	2.15478
A16	1.95304	0.00160	0.00134	-0.00570	-0.00436	1.94868
A17	1.86432	-0.00085	-0.00111	0.00294	0.00183	1.86614
A18	1.89272	0.00024	-0.00374	0.00808	0.00435	1.89708
A19	1.92083	-0.00062	0.00103	-0.00114	-0.00012	1.92071
A20	1.93584	-0.00068	0.00047	-0.00021	0.00026	1.93610
A21	1.89477	0.00030	0.00194	-0.00375	-0.00182	1.89295
A22	1.91089	-0.00021	0.00124	-0.00236	-0.00113	1.90977
A23	1.89605	-0.00088	0.00057	-0.00003	0.00053	1.89659
A24	1.87638	0.00093	-0.00222	0.00330	0.00109	1.87746
A25	1.87482	0.00023	0.00114	-0.00234	-0.00121	1.87362
A26	1.90642	0.00041	-0.00109	0.00267	0.00157	1.90799
A27	1.99834	-0.00049	0.00046	-0.00138	-0.00092	1.99742
A28	2.17222	-0.00049	0.00069	-0.00093	-0.00025	2.17198
A29	1.94856	0.00010	0.00093	-0.00205	-0.00113	1.94744
A30	2.16240	0.00040	-0.00160	0.00298	0.00138	2.16377
A31	2.07791	-0.00007	0.00068	-0.00135	-0.00067	2.07724
A32	2.15959	0.00001	-0.00071	0.00141	0.00070	2.16029
A33	2.04569	0.00006	0.00003	-0.00006	-0.00003	2.04566
A34	1.93891	0.00142	0.00146	0.00083	0.00201	1.94092
A35	1.93078	-0.00407	-0.00011	0.00017	0.00001	1.93079
A36	1.87971	0.00118	-0.00059	0.00040	-0.00013	1.87958

A37	2.08584	0.00009	0.00121	-0.00201	-0.00081	2.08503
A38	2.06985	0.00044	-0.00105	0.00287	0.00183	2.07169
A39	1.99370	0.00053	0.00001	-0.00018	-0.00017	1.99354
A40	2.01140	-0.00035	-0.00169	0.00215	0.00046	2.01186
A41	2.03385	-0.00034	0.00082	-0.00186	-0.00104	2.03281
A42	2.01670	0.00068	-0.00055	0.00197	0.00143	2.01813
A43	2.13823	-0.00052	0.00100	-0.00185	-0.00086	2.13737
A44	1.97465	-0.00032	-0.00222	0.00291	0.00068	1.97534
A45	2.02867	0.00040	-0.00081	0.00163	0.00083	2.02949
A46	2.03756	-0.00005	0.00111	-0.00221	-0.00110	2.03646
A47	2.43813	0.00029	-0.00363	0.00879	0.00517	2.44330
A48	2.44724	-0.00037	-0.00381	0.00809	0.00428	2.45153
A49	1.93307	-0.00008	-0.00012	0.00009	-0.00002	1.93304
A50	1.91879	-0.00012	0.00056	-0.00105	-0.00049	1.91831
A51	1.93904	0.00008	-0.00002	0.00029	0.00027	1.93930
A52	1.88159	0.00004	-0.00028	0.00048	0.00019	1.88179
A53	1.89251	0.00003	0.00001	-0.00008	-0.00007	1.89244
A54	1.89747	0.00005	-0.00017	0.00029	0.00012	1.89759
A55	3.19345	-0.00047	0.07178	0.04738	0.11916	3.31261
A56	3.10628	-0.00388	-0.05121	-0.01756	-0.06879	3.03749
A57	2.95983	0.00128	0.04897	0.00101	0.04998	3.00981
A58	3.15791	0.00088	0.04111	0.04737	0.08859	3.24650
D1	0.00439	0.00003	0.00237	-0.00325	-0.00089	0.00350
D2	-3.12698	-0.00017	0.00126	-0.00259	-0.00133	-3.12832
D3	3.13464	0.00020	-0.00095	0.00407	0.00312	3.13776
D4	0.00327	-0.00001	-0.00205	0.00473	0.00267	0.00594
D5	-0.00570	0.00007	-0.00290	0.00533	0.00243	-0.00326
D6	-3.09588	0.00031	-0.00529	0.01293	0.00765	-3.08822
D7	-3.13709	-0.00008	0.00008	-0.00124	-0.00117	-3.13826
D8	0.05592	0.00016	-0.00231	0.00635	0.00405	0.05997
D9	-0.00166	-0.00012	-0.00106	0.00013	-0.00094	-0.00260
D10	-3.13984	-0.00025	-0.00320	0.00579	0.00261	-3.13724
D11	3.13067	0.00006	-0.00006	-0.00046	-0.00053	3.13015
D12	-0.00750	-0.00007	-0.00220	0.00521	0.00301	-0.00449
D13	-0.00187	0.00016	-0.00073	0.00319	0.00246	0.00059
D14	3.13584	-0.00039	0.00192	-0.00388	-0.00195	3.13388
D15	3.13662	0.00028	0.00120	-0.00194	-0.00074	3.13588
D16	-0.00886	-0.00027	0.00385	-0.00902	-0.00516	-0.01401
D17	-0.00571	0.00013	-0.00008	0.00295	0.00287	-0.00284
D18	3.13343	0.00046	-0.00021	0.00370	0.00349	3.13692
D19	3.13968	-0.00001	-0.00245	0.00925	0.00680	-3.13670
D20	-0.00436	0.00032	-0.00257	0.01000	0.00742	0.00307
D21	0.00466	-0.00014	0.00222	-0.00525	-0.00302	0.00164
D22	3.09693	-0.00029	0.00433	-0.01203	-0.00769	3.08924

D23	-3.13295	0.00042	-0.00049	0.00212	0.00164	-3.13131
D24	-0.04068	0.00027	0.00162	-0.00466	-0.00302	-0.04370
D25	1.44817	0.00023	-0.01000	0.01331	0.00331	1.45147
D26	-2.73179	-0.00014	-0.00869	0.01046	0.00177	-2.73002
D27	-0.69268	-0.00011	-0.00889	0.01172	0.00283	-0.68985
D28	-1.63501	0.00049	-0.01263	0.02166	0.00903	-1.62598
D29	0.46822	0.00011	-0.01131	0.01880	0.00749	0.47571
D30	2.50733	0.00014	-0.01151	0.02006	0.00855	2.51588
D31	-1.11151	-0.00050	0.00802	-0.01799	-0.00997	-1.12147
D32	0.93105	-0.00084	0.01038	-0.02213	-0.01174	0.91931
D33	3.10254	-0.00140	0.00992	-0.02177	-0.01185	3.09069
D34	3.10168	-0.00004	0.00789	-0.01730	-0.00940	3.09228
D35	-1.13895	-0.00038	0.01025	-0.02144	-0.01118	-1.15013
D36	1.03255	-0.00095	0.00979	-0.02108	-0.01129	1.02126
D37	1.00462	0.00043	0.00452	-0.01173	-0.00722	0.99740
D38	3.04717	0.00009	0.00687	-0.01587	-0.00900	3.03818
D39	-1.06452	-0.00047	0.00641	-0.01551	-0.00911	-1.07362
D40	2.85393	0.00067	0.00317	-0.01236	-0.00913	2.84480
D41	-1.34253	0.00041	0.00329	-0.01120	-0.00797	-1.35050
D42	0.78192	0.00016	0.00355	-0.01289	-0.00927	0.77264
D43	2.86864	-0.00010	0.00368	-0.01173	-0.00812	2.86053
D44	-1.32099	-0.00010	0.00258	-0.01091	-0.00826	-1.32925
D45	0.76573	-0.00036	0.00271	-0.00975	-0.00710	0.75863
D46	3.13875	0.00028	-0.00088	0.00171	0.00083	3.13958
D47	-0.00109	0.00011	0.00017	-0.00013	0.00004	-0.00105
D48	-0.00010	-0.00009	-0.00074	0.00088	0.00014	0.00004
D49	-3.13995	-0.00025	0.00031	-0.00096	-0.00065	-3.14060
D50	1.22610	0.00011	-0.01136	0.01556	0.00401	1.23012
D51	-0.55854	0.00090	0.02676	0.00114	0.02776	-0.53078
D52	-2.94422	-0.00057	-0.02920	-0.00232	-0.03137	-2.97559
D53	1.55432	0.00023	0.00893	-0.01673	-0.00762	1.54670
D54	-2.69749	-0.00041	-0.00321	0.00369	0.00048	-2.69701
D55	-0.01577	-0.00014	0.00080	-0.00182	-0.00101	-0.01678
D56	-0.02256	-0.00005	-0.00070	0.00087	0.00018	-0.02239
D57	2.65917	0.00022	0.00332	-0.00463	-0.00132	2.65785
D58	1.99372	-0.00011	0.00540	-0.01300	-0.00761	1.98611
D59	-0.43086	0.00021	0.00610	-0.01234	-0.00626	-0.43711
D60	0.46813	0.00031	-0.00696	0.01514	0.00819	0.47632
D61	-1.96008	0.00029	-0.00505	0.01318	0.00815	-1.95193
D62	2.55387	-0.00023	-0.00078	0.00058	-0.00020	2.55366
D63	-1.65172	-0.00031	-0.00085	0.00056	-0.00029	-1.65201
D64	0.44944	-0.00027	-0.00070	0.00042	-0.00028	0.44916
D65	1.34952	0.00014	-0.00052	0.00024	-0.00027	1.34925
D66	-2.85607	0.00006	-0.00058	0.00022	-0.00036	-2.85642

D67	-0.75491	0.00010	-0.00043	0.00008	-0.00035	-0.75526
D68	-1.05270	0.00022	0.00288	-0.00397	-0.00109	-1.05379
D69	1.02490	0.00014	0.00281	-0.00399	-0.00117	1.02373
D70	3.12606	0.00018	0.00296	-0.00413	-0.00117	3.12490

Item	Value	Threshold	Converged?
Maximum Force	0.004068	0.000450	NO
RMS Force	0.000677	0.000300	NO
Maximum Displacement	0.669288	0.001800	NO
RMS Displacement	0.133330	0.001200	NO

Predicted change in Energy=-2.598906D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.884762	2.148819	-0.227763
2	6	0	-3.767102	1.172034	0.105377
3	7	0	-3.054152	-0.022253	0.117027
4	6	0	-1.774750	0.233336	-0.205105
5	7	0	-1.652668	1.539360	-0.418359
6	6	0	-0.372806	2.194057	-0.730988
7	6	0	0.317753	2.720517	0.534217
8	1	0	-3.027822	3.208757	-0.349480
9	1	0	-4.818226	1.225363	0.321688
10	1	0	0.255248	1.447347	-1.216150
11	1	0	-0.557437	3.002008	-1.438568
12	1	0	-0.298350	3.505404	0.985569
13	1	0	0.389779	1.899563	1.263760
14	35	0	0.255390	-2.318754	-0.227234
15	1	0	-0.975046	-0.542975	-0.265233
16	6	0	-3.504610	-1.344854	0.398805
17	6	0	-4.753571	-1.660547	0.716777
18	1	0	-2.697802	-2.066824	0.319491
19	1	0	-4.999602	-2.695287	0.911895
20	1	0	-5.556197	-0.937699	0.794126
21	7	0	1.596158	3.283300	0.134261
22	1	0	1.973397	3.885567	0.856263
23	1	0	2.277931	2.541314	-0.039015
24	6	0	3.729710	-0.230369	-1.047790
25	6	0	3.666421	-0.418460	0.402666
26	8	0	3.493281	0.901717	-0.179855
27	1	0	4.696924	-0.217841	-1.543579

28	1	0	2.880637	-0.537342	-1.650896
29	1	0	2.739821	-0.843978	0.782035
30	6	0	4.896101	-0.618546	1.245141
31	1	0	4.766962	-0.166672	2.233016
32	1	0	5.080362	-1.687627	1.387479
33	1	0	5.774140	-0.171064	0.772636

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357798	0.000000			
3	N	2.204796	1.390954	0.000000		
4	C	2.213982	2.224189	1.343861	0.000000	
5	N	1.387741	2.209086	2.165509	1.328939	0.000000
6	C	2.562266	3.642154	3.580610	2.467069	1.471194
7	C	3.341190	4.389504	4.366529	3.333352	2.486984
8	H	1.076452	2.213972	3.264620	3.231743	2.163950
9	H	2.212001	1.074474	2.170343	3.244129	3.266041
10	H	3.365804	4.242821	3.858654	2.572340	2.070044
11	H	2.758699	4.004313	4.218959	3.266318	2.092773
12	H	3.162597	4.272188	4.559952	3.782048	2.769570
13	H	3.606852	4.376163	4.107192	3.101461	2.670366
14	Br	5.460748	5.336354	4.042957	3.261154	4.308394
15	H	3.300633	3.297603	2.177144	1.116155	2.195162
16	C	3.603131	2.547494	1.425337	2.418223	3.523654
17	C	4.346939	3.061118	2.435515	3.648291	4.598210
18	H	4.255125	3.417520	2.085245	2.533369	3.826394
19	H	5.407101	4.138321	3.400251	4.497132	5.559117
20	H	4.208018	2.850650	2.748952	4.082783	4.779485
21	N	4.636458	5.763925	5.705467	4.558560	3.728482
22	H	5.271917	6.393780	6.410442	5.339841	4.503076
23	H	5.181031	6.199855	5.918389	4.666752	4.073993
24	C	7.077021	7.713541	6.886283	5.587864	5.700712
25	C	7.064444	7.607583	6.738299	5.513672	5.727115
26	O	6.498999	7.271010	6.618968	5.310323	5.190786
27	H	8.050740	8.734446	7.929378	6.624020	6.683651
28	H	6.517714	7.085118	6.213903	4.935270	5.136409
29	H	6.450772	6.845598	5.889617	4.745146	5.139572
30	C	8.388658	8.919435	8.052001	6.879620	7.092965
31	H	8.364557	8.896585	8.103584	6.992742	7.152061
32	H	8.987243	9.386111	8.399871	7.295135	7.681679
33	H	9.019936	9.658388	8.853852	7.622681	7.713721

		6	7	8	9	10
6	C	0.000000				

7	C	1.534528	0.000000			
8	H	2.867799	3.494591	0.000000		
9	H	4.669930	5.353403	2.754971	0.000000	
10	H	1.089683	2.165329	3.825210	5.306068	0.000000
11	H	1.089745	2.176483	2.707704	4.940576	1.768304
12	H	2.161421	1.095148	3.052928	5.105741	3.064251
13	H	2.155756	1.100630	3.999565	5.335293	2.524391
14	Br	4.584088	5.096857	6.430225	6.213184	3.893774
15	H	2.840944	3.600115	4.277438	4.271010	2.525718
16	C	4.858860	5.581759	4.639248	2.887481	4.953887
17	C	6.012079	6.704131	5.274963	2.913547	6.203506
18	H	4.966308	5.662006	5.328056	3.915954	4.840258
19	H	6.929069	7.599200	6.351120	3.968972	7.021642
20	H	6.245111	6.924838	4.989350	2.333803	6.595646
21	N	2.410793	1.452931	4.649811	6.739031	2.644309
22	H	3.299279	2.049930	5.188842	7.313590	3.632058
23	H	2.761489	2.050124	5.356574	7.226152	2.583342
24	C	4.775861	4.780369	7.614425	8.778487	3.861990
25	C	4.942244	4.591739	7.650838	8.642797	4.211639
26	O	4.113456	3.728527	6.919247	8.332913	3.443323
27	H	5.672717	5.668185	8.534585	9.803067	4.754844
28	H	4.346454	4.685802	7.115956	8.140682	3.319739
29	H	4.605143	4.316648	7.139376	7.849724	3.926324
30	C	6.291041	5.711044	8.943132	9.930806	5.644766
31	H	6.385576	5.569312	8.878145	9.872525	5.904013
32	H	7.020856	6.545399	9.629863	10.373209	6.315748
33	H	6.755711	6.179826	9.495097	10.693530	6.085449

		11	12	13	14	15
11	H	0.000000				
12	H	2.489372	0.000000			
13	H	3.068417	1.769078	0.000000		
14	Br	5.517113	5.974808	4.476083	0.000000	
15	H	3.757395	4.290897	3.188504	2.160742	0.000000
16	C	5.563900	5.843748	5.142047	3.934210	2.735444
17	C	6.632682	6.827026	6.279141	5.139463	4.060857
18	H	5.776244	6.103339	5.114393	3.013921	2.373164
19	H	7.597150	7.781759	7.090972	5.390207	4.713293
20	H	6.744910	6.886419	6.604940	6.060118	4.718579
21	N	2.681583	2.088831	2.155423	5.771598	4.627209
22	H	3.528746	2.306963	2.572569	6.528331	5.437191
23	H	3.195357	2.935382	2.382055	5.267481	4.488415
24	C	5.383364	5.857970	4.586394	4.135888	4.779628
25	C	5.738530	5.608556	4.105009	3.955127	4.690928
26	O	4.733276	4.744878	3.565312	4.567014	4.696847

27	H	6.163341	6.723980	5.560220	5.086632	5.823325
28	H	4.938870	5.779334	4.542918	3.477379	4.097119
29	H	5.531239	5.309335	3.644417	3.060390	3.871383
30	C	7.074728	6.637519	5.162185	5.157014	6.062780
31	H	7.202103	6.379471	4.936448	5.571227	6.273237
32	H	7.859008	7.487300	5.906337	5.126986	6.380412
33	H	7.419345	7.101894	5.789650	6.005741	6.838640

		16	17	18	19	20
16	C	0.000000				
17	C	1.326903	0.000000			
18	H	1.085574	2.132857	0.000000		
19	H	2.078926	1.081337	2.458494	0.000000	
20	H	2.128629	1.082913	3.109762	1.847372	0.000000
21	N	6.892577	8.068457	6.862669	8.936010	8.331172
22	H	7.587827	8.719572	7.585458	9.588193	8.942177
23	H	6.980814	8.226109	6.791273	9.016026	8.612271
24	C	7.461240	8.782093	6.823118	9.279929	9.493210
25	C	7.230623	8.516907	6.574752	8.974588	9.245514
26	O	7.372408	8.682149	6.884119	9.287595	9.285749
27	H	8.503421	9.823566	7.846766	10.304839	10.540851
28	H	6.754608	8.071468	6.110706	8.562873	8.793098
29	H	6.276198	7.538034	5.592588	7.958824	8.296556
30	C	8.474417	9.720138	7.785994	10.116761	10.466890
31	H	8.554025	9.755572	7.936930	10.174725	10.451435
32	H	8.648510	9.856816	7.860295	10.141363	10.679459
33	H	9.360168	10.632703	8.693277	11.066374	11.356264

		21	22	23	24	25
21	N	0.000000				
22	H	1.013076	0.000000			
23	H	1.022440	1.643557	0.000000		
24	C	4.277284	4.863227	3.287478	0.000000	
25	C	4.249831	4.647228	3.298977	1.463969	0.000000
26	O	3.060994	3.505274	2.045773	1.445970	1.453333
27	H	4.968691	5.478576	3.965876	1.086953	2.211347
28	H	4.408399	5.164402	3.526973	1.085769	2.201978
29	H	4.331512	4.791817	3.513924	2.169021	1.087922
30	C	5.229539	5.383349	4.299834	2.601668	1.503964
31	H	5.134304	5.110782	4.323261	3.441458	2.150527
32	H	6.198416	6.402805	5.269957	3.142992	2.140063
33	H	5.458543	5.559576	4.498805	2.738094	2.154196

		26	27	28	29	30
26	O	0.000000				
27	H	2.135863	0.000000			
28	H	2.147134	1.847294	0.000000		

29	H	2.130818	3.103350	2.456218	0.000000	
30	C	2.511915	2.824392	3.529265	2.216941	0.000000
31	H	2.930131	3.777591	4.333635	2.583291	1.093967
32	H	3.417612	3.301272	3.923477	2.560555	1.094143
33	H	2.694516	2.554884	3.792100	3.108053	1.092911

		31	32	33
31	H	0.000000		
32	H	1.768179	0.000000	
33	H	1.774018	1.777449	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.834406	2.214057	-0.201558
2	6	0	-3.727417	1.242957	0.119551
3	7	0	-3.027932	0.040687	0.114886
4	6	0	-1.745985	0.286093	-0.205038
5	7	0	-1.609389	1.593350	-0.401257
6	6	0	-0.322487	2.237675	-0.706446
7	6	0	0.374919	2.739695	0.564922
8	1	0	-2.965631	3.277041	-0.309233
9	1	0	-4.777708	1.305247	0.337506
10	1	0	0.296759	1.490389	-1.201933
11	1	0	-0.498565	3.056866	-1.403200
12	1	0	-0.231973	3.525462	1.027092
13	1	0	0.438270	1.908480	1.283570
14	35	0	0.255313	-2.288131	-0.262492
15	1	0	-0.955106	-0.498296	-0.276074
16	6	0	-3.493017	-1.280354	0.379707
17	6	0	-4.745203	-1.586144	0.694655
18	1	0	-2.694439	-2.010239	0.290193
19	1	0	-5.002705	-2.620526	0.876412
20	1	0	-5.539591	-0.855403	0.782211
21	7	0	1.659264	3.293282	0.171210
22	1	0	2.043806	3.881746	0.900703
23	1	0	2.332518	2.546022	-0.012405
24	6	0	3.752265	-0.228316	-1.058770

25	6	0	3.687979	-0.434703	0.389152
26	8	0	3.529247	0.894867	-0.175848
27	1	0	4.719177	-0.220148	-1.555238
28	1	0	2.899331	-0.517791	-1.665073
29	1	0	2.756944	-0.854728	0.763756
30	6	0	4.915977	-0.659629	1.227804
31	1	0	4.792686	-0.219336	2.221638
32	1	0	5.088316	-1.732488	1.355941
33	1	0	5.798630	-0.215875	0.760404

Rotational constants (GHZ): 0.4781678 0.2453740 0.1712129

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1292.5325678868 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 3.86D-06 NBF= 482

NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999974 0.004581 0.000066 0.005630 Ang= 0.83 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3205.64659557 A.U. after 12 cycles

NFock= 12 Conv=0.73D-08 -V/T= 2.0018

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000033607	-0.000075718	0.000272246
2	6	0.000587872	-0.000496933	0.000017020
3	7	-0.001850715	-0.001214089	0.000336917
4	6	0.000398008	-0.001997892	0.000631536
5	7	-0.000494503	0.002083350	-0.002200685
6	6	-0.000086973	0.000809607	0.002170605
7	6	0.000489363	0.000218533	-0.000957617
8	1	0.000188724	-0.000027330	-0.000086048
9	1	-0.000156282	-0.000000233	0.000084049
10	1	0.000339375	-0.000138069	-0.000265095
11	1	-0.000069174	0.000480031	0.000190108
12	1	-0.000033346	-0.000069902	-0.000205956
13	1	-0.000491601	-0.000347879	-0.000332696
14	35	0.000708251	-0.000405909	0.000132557
15	1	-0.001036647	0.000205449	0.000067303
16	6	-0.001151666	-0.000958858	0.000033432
17	6	0.000474930	0.000716347	-0.000200233
18	1	0.000647367	-0.000135399	0.000055708
19	1	0.000119657	0.000073052	0.000039743
20	1	-0.000160539	0.000130678	0.000020765
21	7	0.002913737	0.000468079	-0.000168363
22	1	0.000153735	0.000037467	-0.000186134
23	1	-0.000992190	0.001249805	0.000807505
24	6	0.000112401	0.000072830	0.000274509
25	6	0.000221068	-0.000154148	-0.000273288
26	8	-0.000670537	-0.000997680	-0.000019378
27	1	0.000137621	0.000113271	-0.000271038
28	1	-0.000011136	-0.000034344	-0.000083287
29	1	-0.000019861	0.000079308	0.000097733
30	6	-0.000042176	0.000432600	-0.000043584
31	1	0.000028794	-0.000019311	0.000058892
32	1	-0.000092524	-0.000038406	-0.000047636
33	1	-0.000127424	-0.000058306	0.000050410

Cartesian Forces: Max 0.002913737 RMS 0.000686759

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.003492240 RMS 0.000636916
Search for a local minimum.
Step number 7 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 2 3 1 4 5
6 7
DE= -1.49D-04 DEPred=-2.60D-04 R= 5.72D-01
TightC=F SS= 1.41D+00 RLast= 1.84D-01 DXNew= 2.1213D-01 5.5149D-01
Trust test= 5.72D-01 RLast= 1.84D-01 DXMaxT set to 2.12D-01
ITU= 1 -1 1 0 0 -1 0

Eigenvalues ---	0.00207	0.00230	0.00238	0.00373	0.00555
Eigenvalues ---	0.00723	0.00819	0.01307	0.01405	0.01487
Eigenvalues ---	0.01776	0.01868	0.02097	0.02163	0.02304
Eigenvalues ---	0.02348	0.02371	0.02393	0.02634	0.02997
Eigenvalues ---	0.03071	0.03079	0.03117	0.03253	0.03961
Eigenvalues ---	0.04087	0.04440	0.04452	0.04738	0.05426
Eigenvalues ---	0.05725	0.05765	0.05907	0.07785	0.08658
Eigenvalues ---	0.09345	0.10872	0.11460	0.12305	0.12372
Eigenvalues ---	0.12691	0.12768	0.13919	0.15526	0.15999
Eigenvalues ---	0.16000	0.16000	0.16000	0.16000	0.16009
Eigenvalues ---	0.16016	0.16030	0.17328	0.21192	0.21753
Eigenvalues ---	0.22373	0.22984	0.23234	0.25049	0.28114
Eigenvalues ---	0.29047	0.29670	0.31629	0.32069	0.32513
Eigenvalues ---	0.33657	0.34273	0.34310	0.34339	0.34540
Eigenvalues ---	0.34657	0.34708	0.35032	0.35067	0.35219
Eigenvalues ---	0.35283	0.35605	0.35815	0.35902	0.36416
Eigenvalues ---	0.36619	0.38048	0.39939	0.41901	0.42377
Eigenvalues ---	0.44938	0.45464	0.47084	0.49382	0.54476
Eigenvalues ---	0.59890	0.62463	0.91152		

En-DIIS/RFO-DIIS IScMMF= 0 using points: 7 6 5 4
RFO step: Lambda=-9.53939483D-05.
DidBck=T Rises=F RFO-DIIS coefs: 0.69214 0.08680 0.00121 0.21984
Iteration 1 RMS(Cart)= 0.06201913 RMS(Int)= 0.00104858
Iteration 2 RMS(Cart)= 0.00253850 RMS(Int)= 0.00003860
Iteration 3 RMS(Cart)= 0.00000309 RMS(Int)= 0.00003858
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00003858

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56587	0.00079	-0.00009	0.00034	0.00025	2.56612
R2	2.62245	-0.00024	-0.00074	0.00067	-0.00007	2.62238
R3	2.03420	-0.00004	0.00004	-0.00011	-0.00007	2.03412
R4	2.62852	-0.00010	0.00024	-0.00082	-0.00058	2.62795
R5	2.03046	0.00017	0.00019	0.00009	0.00027	2.03074
R6	2.53953	0.00141	0.00107	0.00071	0.00178	2.54131
R7	2.69350	0.00016	-0.00101	0.00121	0.00020	2.69370
R8	2.51133	0.00349	0.00416	-0.00037	0.00380	2.51513
R9	2.10923	-0.00011	0.00098	-0.00145	-0.00047	2.10876
R10	2.78015	0.00230	0.00460	-0.00055	0.00405	2.78420
R11	2.89984	-0.00004	-0.00124	0.00174	0.00049	2.90033
R12	2.05920	0.00041	0.00080	-0.00010	0.00070	2.05990
R13	2.05932	0.00024	0.00054	-0.00012	0.00043	2.05975
R14	2.06953	-0.00012	-0.00017	0.00004	-0.00013	2.06940
R15	2.07989	0.00000	-0.00015	0.00017	0.00001	2.07990
R16	2.74564	0.00179	0.00370	-0.00069	0.00301	2.74865
R17	4.08321	0.00074	-0.00542	0.01361	0.00819	4.09140
R18	2.50748	-0.00066	-0.00046	-0.00015	-0.00061	2.50688
R19	2.05144	0.00056	-0.00050	0.00123	0.00073	2.05217
R20	2.04343	-0.00009	-0.00019	0.00007	-0.00012	2.04331
R21	2.04641	0.00021	0.00006	0.00022	0.00028	2.04669
R22	1.91444	-0.00006	-0.00001	-0.00008	-0.00008	1.91435
R23	1.93213	-0.00153	-0.00146	-0.00040	-0.00186	1.93027
R24	3.86595	0.00024	-0.00353	0.00655	0.00302	3.86897
R25	2.76650	0.00007	0.00046	0.00037	0.00083	2.76733
R26	2.73249	-0.00002	-0.00070	0.00020	-0.00050	2.73198
R27	2.05404	0.00025	0.00041	0.00004	0.00045	2.05449
R28	2.05181	0.00006	0.00011	-0.00003	0.00007	2.05188
R29	2.74640	-0.00035	-0.00143	0.00029	-0.00114	2.74526
R30	2.05587	0.00002	-0.00004	-0.00005	-0.00009	2.05578
R31	2.84208	-0.00022	-0.00029	0.00005	-0.00024	2.84184
R32	2.06730	0.00004	0.00009	-0.00001	0.00008	2.06738
R33	2.06763	0.00002	0.00012	-0.00007	0.00006	2.06769
R34	2.06530	-0.00015	-0.00024	0.00003	-0.00021	2.06510
A1	1.86995	0.00053	0.00137	0.00010	0.00146	1.87141
A2	2.27803	-0.00006	-0.00017	0.00014	-0.00003	2.27800
A3	2.13519	-0.00047	-0.00121	-0.00024	-0.00144	2.13374
A4	1.86153	0.00096	0.00043	0.00051	0.00094	1.86246
A5	2.27759	-0.00047	-0.00040	-0.00011	-0.00051	2.27708
A6	2.14403	-0.00049	-0.00003	-0.00039	-0.00041	2.14362
A7	1.89935	-0.00076	-0.00040	-0.00076	-0.00116	1.89819
A8	2.26061	-0.00022	-0.00153	0.00060	-0.00092	2.25969

A9	2.12321	0.00099	0.00192	0.00015	0.00209	2.12530
A10	1.88897	0.00031	0.00002	0.00105	0.00107	1.89004
A11	2.16850	0.00005	0.00773	-0.01029	-0.00256	2.16594
A12	2.22568	-0.00036	-0.00774	0.00924	0.00150	2.22717
A13	1.90498	-0.00103	-0.00142	-0.00090	-0.00232	1.90266
A14	2.22197	0.00041	-0.00419	0.00207	-0.00211	2.21987
A15	2.15478	0.00061	0.00575	-0.00156	0.00419	2.15897
A16	1.94868	0.00286	0.00667	0.00034	0.00700	1.95568
A17	1.86614	-0.00105	-0.00171	0.00174	0.00004	1.86618
A18	1.89708	-0.00056	-0.00348	0.00110	-0.00238	1.89470
A19	1.92071	-0.00090	-0.00066	-0.00022	-0.00088	1.91982
A20	1.93610	-0.00087	-0.00216	-0.00128	-0.00346	1.93264
A21	1.89295	0.00047	0.00122	-0.00162	-0.00039	1.89257
A22	1.90977	-0.00017	-0.00024	-0.00166	-0.00191	1.90786
A23	1.89659	-0.00104	-0.00219	-0.00124	-0.00343	1.89315
A24	1.87746	0.00113	0.00165	0.00290	0.00455	1.88202
A25	1.87362	0.00026	0.00091	-0.00094	-0.00003	1.87358
A26	1.90799	0.00001	-0.00118	0.00041	-0.00076	1.90723
A27	1.99742	-0.00021	0.00098	0.00038	0.00135	1.99878
A28	2.17198	-0.00099	-0.00052	-0.00189	-0.00240	2.16957
A29	1.94744	0.00019	0.00103	-0.00076	0.00028	1.94771
A30	2.16377	0.00080	-0.00053	0.00265	0.00213	2.16590
A31	2.07724	-0.00012	0.00043	-0.00077	-0.00034	2.07689
A32	2.16029	0.00007	-0.00054	0.00070	0.00016	2.16045
A33	2.04566	0.00005	0.00011	0.00007	0.00018	2.04584
A34	1.94092	0.00077	-0.00079	0.00085	-0.00021	1.94071
A35	1.93079	-0.00252	-0.00133	-0.00043	-0.00182	1.92897
A36	1.87958	0.00080	-0.00010	-0.00008	-0.00011	1.87947
A37	2.08503	-0.00003	0.00111	-0.00079	0.00035	2.08537
A38	2.07169	0.00020	-0.00118	0.00209	0.00089	2.07257
A39	1.99354	0.00002	0.00004	-0.00036	-0.00033	1.99320
A40	2.01186	0.00007	-0.00042	-0.00008	-0.00049	2.01137
A41	2.03281	-0.00012	0.00042	-0.00074	-0.00032	2.03249
A42	2.01813	0.00024	-0.00050	0.00198	0.00146	2.01959
A43	2.13737	-0.00016	0.00067	-0.00051	0.00019	2.13756
A44	1.97534	0.00004	-0.00098	-0.00024	-0.00120	1.97413
A45	2.02949	-0.00010	-0.00104	0.00011	-0.00094	2.02855
A46	2.03646	-0.00004	0.00084	-0.00098	-0.00013	2.03633
A47	2.44330	0.00021	-0.00343	0.00660	0.00319	2.44649
A48	2.45153	0.00011	-0.00355	0.00705	0.00352	2.45505
A49	1.93304	0.00010	-0.00005	0.00042	0.00037	1.93341
A50	1.91831	-0.00018	0.00013	-0.00084	-0.00071	1.91760
A51	1.93930	0.00000	-0.00014	0.00038	0.00024	1.93954
A52	1.88179	0.00002	-0.00017	0.00008	-0.00009	1.88170

A53	1.89244	-0.00001	0.00018	-0.00009	0.00010	1.89253
A54	1.89759	0.00007	0.00004	0.00005	0.00009	1.89768
A55	3.31261	-0.00151	-0.04938	0.06457	0.01520	3.32781
A56	3.03749	-0.00164	0.02668	-0.05196	-0.02534	3.01215
A57	3.00981	-0.00008	0.02447	-0.06323	-0.03876	2.97105
A58	3.24650	-0.00064	-0.02078	-0.05616	-0.07684	3.16965
D1	0.00350	0.00007	-0.00031	0.00229	0.00198	0.00548
D2	-3.12832	0.00002	-0.00053	0.00120	0.00067	-3.12765
D3	3.13776	-0.00002	-0.00203	0.00216	0.00012	3.13788
D4	0.00594	-0.00007	-0.00225	0.00107	-0.00119	0.00475
D5	-0.00326	-0.00014	-0.00059	-0.00325	-0.00383	-0.00709
D6	-3.08822	-0.00002	-0.00385	0.00445	0.00055	-3.08768
D7	-3.13826	-0.00006	0.00095	-0.00313	-0.00217	-3.14042
D8	0.05997	0.00005	-0.00231	0.00457	0.00221	0.06218
D9	-0.00260	0.00003	0.00111	-0.00059	0.00052	-0.00208
D10	-3.13724	-0.00009	-0.00358	0.00179	-0.00181	-3.13905
D11	3.13015	0.00007	0.00130	0.00039	0.00170	3.13185
D12	-0.00449	-0.00005	-0.00338	0.00277	-0.00063	-0.00512
D13	0.00059	-0.00011	-0.00148	-0.00143	-0.00292	-0.00233
D14	3.13388	-0.00024	-0.00015	-0.00211	-0.00229	3.13159
D15	3.13588	-0.00001	0.00279	-0.00358	-0.00081	3.13507
D16	-0.01401	-0.00014	0.00412	-0.00426	-0.00019	-0.01420
D17	-0.00284	0.00003	-0.00103	0.00329	0.00227	-0.00057
D18	3.13692	0.00018	0.00135	0.00420	0.00555	-3.14071
D19	-3.13670	-0.00009	-0.00625	0.00594	-0.00031	-3.13701
D20	0.00307	0.00005	-0.00387	0.00684	0.00296	0.00603
D21	0.00164	0.00015	0.00128	0.00288	0.00416	0.00580
D22	3.08924	0.00004	0.00409	-0.00431	-0.00026	3.08898
D23	-3.13131	0.00028	-0.00016	0.00371	0.00354	-3.12777
D24	-0.04370	0.00017	0.00265	-0.00348	-0.00089	-0.04460
D25	1.45147	0.00031	-0.00511	0.00825	0.00315	1.45462
D26	-2.73002	0.00021	-0.00309	0.00929	0.00621	-2.72381
D27	-0.68985	-0.00008	-0.00431	0.00888	0.00456	-0.68530
D28	-1.62598	0.00049	-0.00857	0.01692	0.00835	-1.61763
D29	0.47571	0.00039	-0.00656	0.01796	0.01142	0.48713
D30	2.51588	0.00010	-0.00778	0.01755	0.00976	2.52564
D31	-1.12147	-0.00019	0.00171	-0.00275	-0.00104	-1.12252
D32	0.91931	-0.00057	0.00144	-0.00551	-0.00408	0.91523
D33	3.09069	-0.00076	0.00231	-0.00400	-0.00169	3.08900
D34	3.09228	-0.00011	0.00004	-0.00499	-0.00495	3.08732
D35	-1.15013	-0.00049	-0.00024	-0.00775	-0.00799	-1.15811
D36	1.02126	-0.00068	0.00063	-0.00624	-0.00560	1.01566
D37	0.99740	0.00045	0.00032	-0.00200	-0.00168	0.99571
D38	3.03818	0.00007	0.00004	-0.00476	-0.00472	3.03346

D39	-1.07362	-0.00011	0.00092	-0.00325	-0.00233	-1.07595
D40	2.84480	0.00057	0.00617	-0.01012	-0.00388	2.84093
D41	-1.35050	0.00041	0.00467	-0.00996	-0.00535	-1.35585
D42	0.77264	0.00012	0.00618	-0.01003	-0.00379	0.76886
D43	2.86053	-0.00004	0.00467	-0.00986	-0.00526	2.85527
D44	-1.32925	-0.00008	0.00521	-0.00937	-0.00410	-1.33335
D45	0.75863	-0.00023	0.00370	-0.00921	-0.00557	0.75306
D46	3.13958	0.00015	0.00181	0.00101	0.00282	-3.14078
D47	-0.00105	0.00008	0.00111	0.00075	0.00186	0.00081
D48	0.00004	-0.00001	-0.00085	0.00000	-0.00085	-0.00081
D49	-3.14060	-0.00008	-0.00155	-0.00026	-0.00181	3.14078
D50	1.23012	-0.00006	0.00069	-0.02336	-0.02280	1.20731
D51	-0.53078	0.00021	-0.00541	-0.00984	-0.01543	-0.54621
D52	-2.97559	-0.00009	0.00862	-0.01013	-0.00133	-2.97691
D53	1.54670	0.00019	0.00253	0.00339	0.00605	1.55275
D54	-2.69701	-0.00009	-0.00169	-0.00137	-0.00306	-2.70008
D55	-0.01678	-0.00001	0.00095	-0.00042	0.00054	-0.01624
D56	-0.02239	0.00002	-0.00077	-0.00023	-0.00100	-0.02338
D57	2.65785	0.00010	0.00188	0.00072	0.00260	2.66045
D58	1.98611	-0.00030	0.00502	-0.01320	-0.00817	1.97794
D59	-0.43711	-0.00023	0.00479	-0.01144	-0.00664	-0.44375
D60	0.47632	0.00023	-0.00592	0.01111	0.00516	0.48148
D61	-1.95193	0.00038	-0.00485	0.01289	0.00803	-1.94391
D62	2.55366	-0.00003	-0.00030	-0.00087	-0.00116	2.55250
D63	-1.65201	-0.00006	-0.00046	-0.00104	-0.00149	-1.65350
D64	0.44916	-0.00008	-0.00041	-0.00129	-0.00169	0.44747
D65	1.34925	0.00000	0.00014	-0.00071	-0.00057	1.34868
D66	-2.85642	-0.00003	-0.00002	-0.00088	-0.00090	-2.85732
D67	-0.75526	-0.00005	0.00003	-0.00113	-0.00110	-0.75635
D68	-1.05379	0.00011	0.00205	0.00082	0.00286	-1.05092
D69	1.02373	0.00009	0.00189	0.00064	0.00253	1.02626
D70	3.12490	0.00006	0.00194	0.00039	0.00233	3.12723

Item	Value	Threshold	Converged?
Maximum Force	0.003492	0.000450	NO
RMS Force	0.000637	0.000300	NO
Maximum Displacement	0.423735	0.001800	NO
RMS Displacement	0.063694	0.001200	NO

Predicted change in Energy=-7.894560D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-2.869902	2.131118	-0.284461
2	6	0	-3.757450	1.156978	0.043083
3	7	0	-3.039893	-0.032495	0.107681
4	6	0	-1.750991	0.223950	-0.177734
5	7	0	-1.628479	1.526482	-0.422321
6	6	0	-0.343152	2.187004	-0.709313
7	6	0	0.313060	2.746964	0.560098
8	1	0	-3.014748	3.186845	-0.436528
9	1	0	-4.815400	1.209554	0.224149
10	1	0	0.304372	1.437219	-1.164011
11	1	0	-0.515576	2.980299	-1.436629
12	1	0	-0.320133	3.537382	0.976631
13	1	0	0.367886	1.941804	1.308505
14	35	0	0.245318	-2.347316	-0.003003
15	1	0	-0.946942	-0.549748	-0.189620
16	6	0	-3.494231	-1.349604	0.408835
17	6	0	-4.752495	-1.660002	0.692110
18	1	0	-2.681524	-2.069284	0.379233
19	1	0	-5.002372	-2.689432	0.908873
20	1	0	-5.559119	-0.937822	0.720935
21	7	0	1.600212	3.310739	0.184544
22	1	0	1.950818	3.933471	0.902535
23	1	0	2.290758	2.569806	0.052137
24	6	0	3.665201	-0.205906	-1.058917
25	6	0	3.651493	-0.419749	0.389729
26	8	0	3.472771	0.911956	-0.162583
27	1	0	4.614300	-0.193858	-1.589060
28	1	0	2.791705	-0.491389	-1.637263
29	1	0	2.734100	-0.840095	0.796137
30	6	0	4.907951	-0.646570	1.184334
31	1	0	4.819075	-0.210577	2.183769
32	1	0	5.084950	-1.719910	1.301909
33	1	0	5.773554	-0.200444	0.688432

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357931	0.000000			
3	N	2.205424	1.390650	0.000000		
4	C	2.213739	2.223776	1.344803	0.000000	
5	N	1.387704	2.210352	2.168733	1.330948	0.000000
6	C	2.562828	3.644789	3.586930	2.473493	1.473336
7	C	3.350193	4.400502	4.378626	3.342200	2.494854

8	H	1.076413	2.214044	3.265110	3.231533	2.163042
9	H	2.211995	1.074619	2.169948	3.243998	3.267236
10	H	3.366173	4.246647	3.867993	2.582496	2.072193
11	H	2.755259	4.002973	4.223032	3.272388	2.093073
12	H	3.173209	4.284039	4.571235	3.789294	2.777148
13	H	3.613399	4.385846	4.117377	3.106375	2.674644
14	Br	5.462617	5.320183	4.020356	3.259937	4.323570
15	H	3.300578	3.296365	2.176324	1.115905	2.197584
16	C	3.603592	2.546765	1.425445	2.420542	3.527567
17	C	4.344011	3.057241	2.433791	3.648962	4.599469
18	H	4.256684	3.417511	2.085828	2.536736	3.831570
19	H	5.404551	4.134523	3.398903	4.498887	5.561399
20	H	4.202511	2.844939	2.746306	4.081563	4.778050
21	N	4.646869	5.776092	5.719588	4.570566	3.738488
22	H	5.281740	6.405615	6.424008	5.350787	4.512228
23	H	5.190198	6.211037	5.932191	4.678848	4.083387
24	C	6.983484	7.626770	6.808033	5.504217	5.606199
25	C	7.034917	7.582788	6.708515	5.470210	5.685538
26	O	6.459931	7.237294	6.586336	5.268896	5.144691
27	H	7.944858	8.635673	7.841660	6.533248	6.579752
28	H	6.384466	6.959318	6.104338	4.824730	5.008583
29	H	6.434333	6.833419	5.870706	4.711333	5.110520
30	C	8.388558	8.924372	8.043910	6.852338	7.073076
31	H	8.408095	8.944804	8.130512	6.995090	7.167986
32	H	8.979235	9.383452	8.383712	7.259341	7.653898
33	H	9.005112	9.648789	8.834157	7.586115	7.681545

		6	7	8	9	10
6	C	0.000000				
7	C	1.534788	0.000000			
8	H	2.865575	3.501581	0.000000		
9	H	4.672019	5.364475	2.754726	0.000000	
10	H	1.090053	2.165193	3.821909	5.309509	0.000000
11	H	1.089970	2.174397	2.699764	4.937834	1.768539
12	H	2.160198	1.095078	3.062816	5.117854	3.063175
13	H	2.153436	1.100637	4.004682	5.345883	2.524277
14	Br	4.626579	5.125755	6.437617	6.189813	3.959057
15	H	2.850343	3.608045	4.277723	4.269815	2.542294
16	C	4.866945	5.594660	4.639387	2.885982	4.966852
17	C	6.017121	6.715551	5.271196	2.908143	6.213684
18	H	4.976837	5.674196	5.329484	3.915132	4.857237
19	H	6.935883	7.611166	6.347548	3.963066	7.034744
20	H	6.246315	6.934407	4.982611	2.326185	6.601089
21	N	2.416283	1.454524	4.658212	6.751045	2.647240
22	H	3.303105	2.051174	5.196863	7.325410	3.634924

23	H	2.768361	2.049560	5.363574	7.237219	2.589884
24	C	4.681361	4.751579	7.517969	8.693123	3.742469
25	C	4.894921	4.604588	7.624237	8.623823	4.131060
26	O	4.060287	3.724687	6.880267	8.302523	3.364151
27	H	5.569451	5.636309	8.423767	9.704459	4.627802
28	H	4.226370	4.632386	6.977540	8.014119	3.182816
29	H	4.571563	4.334067	7.126357	7.843671	3.864184
30	C	6.260122	5.746195	8.949381	9.945386	5.572238
31	H	6.384897	5.629167	8.931809	9.933780	5.857082
32	H	6.983788	6.578312	9.628267	10.380764	6.237159
33	H	6.713248	6.206503	9.485438	10.692502	6.002120

		11	12	13	14	15
11	H	0.000000				
12	H	2.484425	0.000000			
13	H	3.065084	1.769006	0.000000		
14	Br	5.569356	5.992420	4.486828	0.000000	
15	H	3.768599	4.296238	3.190764	2.165078	0.000000
16	C	5.570115	5.854906	5.153515	3.892206	2.736166
17	C	6.634410	6.836635	6.290568	5.092515	4.061077
18	H	5.786793	6.112918	5.123600	2.964762	2.375155
19	H	7.601220	7.791095	7.102655	5.337303	4.715023
20	H	6.741222	6.894912	6.615653	6.016830	4.717191
21	N	2.685880	2.089616	2.157753	5.821039	4.640188
22	H	3.530344	2.306425	2.576281	6.570922	5.448767
23	H	3.203192	2.933879	2.381235	5.325876	4.502528
24	C	5.270054	5.834257	4.592345	4.170875	4.705929
25	C	5.679822	5.637123	4.147669	3.933419	4.636610
26	O	4.669920	4.751504	3.586781	4.589638	4.655230
27	H	6.034413	6.697280	5.566773	5.122593	5.745650
28	H	4.799060	5.722497	4.524695	3.549558	4.009558
29	H	5.490086	5.340714	3.687879	3.017346	3.821791
30	C	7.031235	6.699363	5.227551	5.103181	6.014723
31	H	7.193572	6.474244	5.021147	5.501534	6.244594
32	H	7.807526	7.547176	5.971507	5.051582	6.322789
33	H	7.361126	7.154539	5.847646	5.970640	6.786609

		16	17	18	19	20
16	C	0.000000				
17	C	1.326582	0.000000			
18	H	1.085959	2.134086	0.000000		
19	H	2.078380	1.081272	2.459966	0.000000	
20	H	2.128552	1.083059	3.110871	1.847546	0.000000
21	N	6.908144	8.082250	6.878649	8.951022	8.342302
22	H	7.602840	8.733019	7.600363	9.602589	8.953303
23	H	6.996792	8.240646	6.808211	9.032348	8.623880

24	C	7.397284	8.719983	6.769149	9.228592	9.422933
25	C	7.205996	8.500393	6.544325	8.961604	9.231115
26	O	7.347128	8.660280	6.859789	9.270709	9.261604
27	H	8.430635	9.751418	7.785914	10.244409	10.458872
28	H	6.666036	7.981640	6.042537	8.488924	8.688881
29	H	6.261127	7.532076	5.568995	7.955234	8.294136
30	C	8.467131	9.725921	7.763533	10.122433	10.481370
31	H	8.576644	9.794939	7.935372	10.209353	10.505983
32	H	8.633485	9.856509	7.828890	10.141426	10.688565
33	H	9.342943	10.626760	8.664671	11.061837	11.356684

		21	22	23	24	25
21	N	0.000000				
22	H	1.013031	0.000000			
23	H	1.021453	1.642656	0.000000		
24	C	4.263469	4.890895	3.290610	0.000000	
25	C	4.262205	4.701679	3.301970	1.464408	0.000000
26	O	3.062864	3.546882	2.047371	1.445704	1.452731
27	H	4.951020	5.507906	3.966134	1.087191	2.212155
28	H	4.381188	5.170788	3.532128	1.085808	2.202967
29	H	4.346167	4.838572	3.518169	2.170339	1.087874
30	C	5.253666	5.459013	4.298446	2.602074	1.503839
31	H	5.172779	5.200153	4.320506	3.441869	2.150716
32	H	6.220879	6.476342	5.269830	3.143469	2.139461
33	H	5.477143	5.634572	4.495445	2.738323	2.154173

		26	27	28	29	30
26	O	0.000000				
27	H	2.135592	0.000000			
28	H	2.146604	1.847349	0.000000		
29	H	2.129427	3.105147	2.458932	0.000000	
30	C	2.510564	2.825402	3.530438	2.216704	0.000000
31	H	2.928819	3.778420	4.334671	2.582428	1.094011
32	H	3.416223	3.302734	3.925171	2.560542	1.094172
33	H	2.693560	2.555560	3.792748	3.107899	1.092802

		31	32	33
31	H	0.000000		
32	H	1.768179	0.000000	
33	H	1.774026	1.777444	0.000000

Stoichiometry C10H18BrN3O

Framework group C1[X(C10H18BrN3O)]

Deg. of freedom 93

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.808472	2.228636	-0.219184
2	6	0	-3.710443	1.254157	0.065096
3	7	0	-3.012263	0.051475	0.067747
4	6	0	-1.720613	0.300646	-0.211620
5	7	0	-1.577793	1.611424	-0.392964
6	6	0	-0.283078	2.264271	-0.654158
7	6	0	0.387949	2.750771	0.637590
8	1	0	-2.936616	3.292745	-0.318757
9	1	0	-4.766560	1.314957	0.254106
10	1	0	0.349979	1.527222	-1.148340
11	1	0	-0.445695	3.094875	-1.340953
12	1	0	-0.230282	3.530033	1.095561
13	1	0	0.432884	1.909192	1.345493
14	35	0	0.233900	-2.308108	-0.173196
15	1	0	-0.929459	-0.484475	-0.265518
16	6	0	-3.486846	-1.271249	0.306634
17	6	0	-4.748761	-1.574693	0.581066
18	1	0	-2.686228	-2.001698	0.237632
19	1	0	-5.014559	-2.609306	0.748628
20	1	0	-5.543260	-0.841808	0.649381
21	7	0	1.682500	3.311301	0.283209
22	1	0	2.046521	3.892411	1.028884
23	1	0	2.360164	2.566635	0.111135
24	6	0	3.683766	-0.173334	-1.141370
25	6	0	3.673048	-0.457515	0.295160
26	8	0	3.513774	0.902328	-0.190520
27	1	0	4.630544	-0.150759	-1.675304
28	1	0	2.803104	-0.415996	-1.728336
29	1	0	2.750699	-0.882308	0.685407
30	6	0	4.929159	-0.743259	1.071088
31	1	0	4.851955	-0.355281	2.091074
32	1	0	5.089008	-1.823793	1.135180
33	1	0	5.799748	-0.287504	0.592988

Rotational constants (GHZ): 0.4752983 0.2482848 0.1712578

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1293.2998271317 Hartrees.
NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 482 RedAO= T EigKep= 3.83D-06 NBF= 482
NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999991 -0.003087 -0.000663 0.002685 Ang= -0.47 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3205.64670659 A.U. after 11 cycles
NFock= 11 Conv=0.68D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000117397	0.000096638	-0.000027203
2	6	0.000509757	-0.000188211	0.000127730
3	7	-0.000438536	-0.000244405	0.000013062
4	6	0.000653113	-0.001208535	-0.000197511
5	7	-0.000227155	0.001191807	-0.000792202
6	6	-0.000097624	0.000565229	0.001056602

7	6	-0.000063552	-0.000046144	-0.000171395
8	1	0.000072337	0.000006681	-0.000079743
9	1	-0.000042685	0.000037324	0.000042863
10	1	0.000086621	0.000059605	-0.000157396
11	1	-0.000105240	0.000194974	0.000032231
12	1	0.000033239	-0.000071288	-0.000083520
13	1	-0.000149125	-0.000094242	-0.000159080
14	35	0.000700753	-0.000447201	0.000072415
15	1	-0.001329022	0.000224972	0.000286066
16	6	-0.000750731	-0.000894228	0.000121433
17	6	0.000120516	0.000586720	-0.000129494
18	1	0.000590132	-0.000081132	0.000104314
19	1	0.000063249	0.000023093	0.000004606
20	1	-0.000111292	0.000035905	0.000020851
21	7	0.001628097	0.000003470	0.000208838
22	1	-0.000138089	0.000191183	-0.000079355
23	1	-0.000564513	0.000683528	-0.000198160
24	6	0.000398496	0.000235541	0.000625864
25	6	0.000157547	-0.000139828	0.000041855
26	8	-0.000803441	-0.000452501	-0.000209231
27	1	-0.000080757	0.000010141	-0.000246825
28	1	0.000114785	-0.000143420	-0.000150499
29	1	0.000071309	-0.000240389	0.000034997
30	6	0.000026613	0.000144449	-0.000073922
31	1	-0.000064409	-0.000030358	-0.000038878
32	1	-0.000074498	0.000002707	-0.000005611
33	1	-0.000068499	-0.000012082	0.000006299

Cartesian Forces: Max 0.001628097 RMS 0.000406503

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.001814661 RMS 0.000322409
Search for a local minimum.
Step number 8 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 2 3 1 4 5
6 7 8
DE= -1.11D-04 DEPred=-7.89D-05 R= 1.41D+00

TightC=F SS= 1.41D+00 RLast= 1.02D-01 DXNew= 3.5676D-01 3.0687D-01

Trust test= 1.41D+00 RLast= 1.02D-01 DXMaxT set to 3.07D-01

ITU= 1 1 -1 1 0 0 -1 0

Eigenvalues ---	0.00175	0.00231	0.00340	0.00424	0.00712
Eigenvalues ---	0.00724	0.01121	0.01292	0.01372	0.01471
Eigenvalues ---	0.01747	0.01910	0.02104	0.02173	0.02329
Eigenvalues ---	0.02364	0.02391	0.02453	0.02658	0.02895
Eigenvalues ---	0.03070	0.03077	0.03096	0.03207	0.03878
Eigenvalues ---	0.04142	0.04285	0.04426	0.04770	0.05403
Eigenvalues ---	0.05734	0.05762	0.05913	0.07789	0.08643
Eigenvalues ---	0.09434	0.10962	0.11365	0.12283	0.12371
Eigenvalues ---	0.12795	0.12866	0.13817	0.15594	0.16000
Eigenvalues ---	0.16000	0.16000	0.16000	0.16006	0.16011
Eigenvalues ---	0.16017	0.16089	0.17270	0.21213	0.21719
Eigenvalues ---	0.22517	0.22936	0.23402	0.25130	0.25632
Eigenvalues ---	0.29045	0.29824	0.31667	0.32070	0.32944
Eigenvalues ---	0.33659	0.34280	0.34310	0.34341	0.34542
Eigenvalues ---	0.34660	0.34712	0.34989	0.35064	0.35185
Eigenvalues ---	0.35285	0.35439	0.35637	0.35888	0.36418
Eigenvalues ---	0.36620	0.37530	0.38074	0.41822	0.42350
Eigenvalues ---	0.44668	0.45465	0.45727	0.49124	0.54932
Eigenvalues ---	0.56842	0.60550	1.35533		

En-DIIS/RFO-DIIS IScMMF= 0 using points: 8 7 6 5 4

RFO step: Lambda=-4.38839261D-05.

DidBck=T Rises=F RFO-DIIS coefs: 0.75350 0.50269 -0.10524 -0.80373 0.65278

Iteration 1 RMS(Cart)= 0.05232949 RMS(Int)= 0.00082446

Iteration 2 RMS(Cart)= 0.00151481 RMS(Int)= 0.00011602

Iteration 3 RMS(Cart)= 0.00000140 RMS(Int)= 0.00011601

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00011601

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56612	0.00019	0.00073	-0.00073	0.00000	2.56612
R2	2.62238	-0.00024	-0.00031	0.00078	0.00047	2.62285
R3	2.03412	0.00001	0.00000	-0.00013	-0.00013	2.03400
R4	2.62795	0.00005	-0.00023	-0.00093	-0.00117	2.62678
R5	2.03074	0.00005	0.00004	0.00027	0.00031	2.03104
R6	2.54131	0.00033	0.00015	0.00198	0.00213	2.54344
R7	2.69370	0.00035	-0.00008	0.00176	0.00168	2.69538
R8	2.51513	0.00181	0.00263	0.00048	0.00312	2.51825
R9	2.10876	-0.00030	0.00012	-0.00243	-0.00231	2.10644
R10	2.78420	0.00057	0.00311	-0.00120	0.00190	2.78611
R11	2.90033	-0.00024	-0.00038	0.00209	0.00170	2.90203
R12	2.05990	0.00008	0.00005	0.00041	0.00046	2.06036

R13	2.05975	0.00014	0.00004	0.00036	0.00040	2.06015
R14	2.06940	-0.00010	-0.00024	0.00014	-0.00011	2.06929
R15	2.07990	-0.00005	-0.00013	0.00024	0.00012	2.08002
R16	2.74865	0.00064	0.00250	-0.00103	0.00147	2.75012
R17	4.09140	0.00076	-0.00103	0.02753	0.02649	4.11790
R18	2.50688	-0.00024	-0.00029	-0.00032	-0.00060	2.50627
R19	2.05217	0.00049	0.00057	0.00144	0.00201	2.05418
R20	2.04331	-0.00004	-0.00015	0.00014	-0.00001	2.04330
R21	2.04669	0.00011	0.00027	0.00013	0.00040	2.04709
R22	1.91435	0.00001	0.00008	-0.00021	-0.00014	1.91422
R23	1.93027	-0.00060	-0.00085	-0.00104	-0.00190	1.92837
R24	3.86897	0.00033	0.00121	0.01094	0.01215	3.88112
R25	2.76733	-0.00032	0.00042	0.00022	0.00057	2.76790
R26	2.73198	0.00006	0.00007	-0.00056	-0.00046	2.73153
R27	2.05449	0.00005	0.00004	0.00036	0.00040	2.05489
R28	2.05188	0.00003	-0.00002	0.00006	0.00004	2.05192
R29	2.74526	0.00036	0.00009	-0.00025	-0.00011	2.74516
R30	2.05578	0.00005	0.00001	-0.00011	-0.00011	2.05568
R31	2.84184	-0.00022	-0.00056	0.00033	-0.00023	2.84161
R32	2.06738	-0.00004	-0.00003	0.00002	-0.00001	2.06737
R33	2.06769	-0.00001	-0.00008	0.00008	0.00000	2.06768
R34	2.06510	-0.00006	-0.00009	-0.00006	-0.00015	2.06495
A1	1.87141	0.00001	0.00029	0.00071	0.00100	1.87241
A2	2.27800	0.00009	0.00025	0.00002	0.00026	2.27826
A3	2.13374	-0.00010	-0.00050	-0.00077	-0.00128	2.13247
A4	1.86246	0.00058	0.00150	-0.00033	0.00117	1.86363
A5	2.27708	-0.00032	-0.00038	-0.00044	-0.00081	2.27626
A6	2.14362	-0.00026	-0.00113	0.00079	-0.00034	2.14328
A7	1.89819	-0.00029	-0.00188	0.00088	-0.00098	1.89720
A8	2.25969	-0.00022	0.00085	-0.00205	-0.00118	2.25850
A9	2.12530	0.00051	0.00098	0.00116	0.00217	2.12747
A10	1.89004	-0.00008	0.00189	-0.00118	0.00071	1.89075
A11	2.16594	-0.00001	-0.00330	-0.00744	-0.01074	2.15520
A12	2.22717	0.00008	0.00139	0.00862	0.01001	2.23718
A13	1.90266	-0.00023	-0.00179	-0.00016	-0.00196	1.90070
A14	2.21987	0.00018	-0.00087	0.00016	-0.00073	2.21913
A15	2.15897	0.00004	0.00268	-0.00068	0.00197	2.16094
A16	1.95568	0.00096	0.00485	0.00008	0.00491	1.96059
A17	1.86618	-0.00043	-0.00053	0.00209	0.00157	1.86776
A18	1.89470	-0.00014	0.00123	-0.00314	-0.00192	1.89278
A19	1.91982	-0.00036	-0.00181	0.00139	-0.00042	1.91940
A20	1.93264	-0.00019	-0.00289	0.00028	-0.00264	1.93001
A21	1.89257	0.00013	-0.00087	-0.00072	-0.00158	1.89099
A22	1.90786	0.00000	-0.00180	-0.00084	-0.00266	1.90520

A23	1.89315	-0.00026	-0.00282	0.00003	-0.00280	1.89035
A24	1.88202	0.00013	0.00424	0.00047	0.00472	1.88674
A25	1.87358	0.00005	-0.00034	-0.00021	-0.00056	1.87302
A26	1.90723	0.00021	0.00035	-0.00054	-0.00019	1.90704
A27	1.99878	-0.00014	0.00021	0.00101	0.00120	1.99998
A28	2.16957	-0.00070	-0.00101	-0.00352	-0.00452	2.16505
A29	1.94771	0.00005	0.00002	-0.00065	-0.00063	1.94708
A30	2.16590	0.00065	0.00097	0.00417	0.00514	2.17104
A31	2.07689	-0.00010	-0.00028	-0.00081	-0.00109	2.07580
A32	2.16045	0.00010	0.00019	0.00077	0.00096	2.16141
A33	2.04584	0.00000	0.00009	0.00004	0.00014	2.04598
A34	1.94071	0.00038	-0.00091	0.00125	-0.00048	1.94024
A35	1.92897	-0.00140	-0.00164	0.00051	-0.00130	1.92767
A36	1.87947	0.00058	0.00025	0.00088	0.00136	1.88083
A37	2.08537	0.00001	0.00013	-0.00037	-0.00033	2.08505
A38	2.07257	0.00013	0.00010	0.00264	0.00281	2.07538
A39	1.99320	-0.00007	0.00001	-0.00053	-0.00050	1.99271
A40	2.01137	0.00011	0.00116	-0.00118	-0.00006	2.01131
A41	2.03249	-0.00019	-0.00069	-0.00082	-0.00151	2.03098
A42	2.01959	0.00028	0.00036	0.00245	0.00288	2.02247
A43	2.13756	-0.00021	-0.00042	-0.00022	-0.00072	2.13684
A44	1.97413	0.00020	0.00103	-0.00116	-0.00017	1.97396
A45	2.02855	-0.00011	-0.00018	-0.00051	-0.00067	2.02788
A46	2.03633	-0.00009	-0.00033	-0.00076	-0.00107	2.03525
A47	2.44649	0.00044	0.00048	0.01137	0.01166	2.45815
A48	2.45505	0.00020	-0.00033	0.01175	0.01121	2.46626
A49	1.93341	-0.00007	-0.00009	0.00036	0.00027	1.93368
A50	1.91760	-0.00008	-0.00044	-0.00088	-0.00132	1.91628
A51	1.93954	0.00000	-0.00006	0.00074	0.00068	1.94022
A52	1.88170	0.00004	0.00011	-0.00019	-0.00008	1.88162
A53	1.89253	0.00006	0.00022	-0.00005	0.00017	1.89270
A54	1.89768	0.00006	0.00028	0.00000	0.00028	1.89796
A55	3.32781	-0.00132	-0.05284	0.00426	-0.04858	3.27923
A56	3.01215	-0.00065	0.03959	-0.03645	0.00305	3.01520
A57	2.97105	0.00032	0.04795	-0.08094	-0.03299	2.93805
A58	3.16965	0.00045	0.01870	0.04839	0.06740	3.23706
D1	0.00548	-0.00001	-0.00361	0.00771	0.00408	0.00956
D2	-3.12765	-0.00006	-0.00309	0.00445	0.00135	-3.12630
D3	3.13788	0.00002	-0.00021	0.00253	0.00230	3.14018
D4	0.00475	-0.00003	0.00032	-0.00074	-0.00042	0.00433
D5	-0.00709	0.00004	0.00421	-0.00988	-0.00565	-0.01274
D6	-3.08768	0.00012	0.00370	0.00250	0.00616	-3.08151
D7	-3.14042	0.00001	0.00114	-0.00522	-0.00406	3.13870
D8	0.06218	0.00009	0.00063	0.00716	0.00775	0.06993

D9	-0.00208	-0.00001	0.00185	-0.00303	-0.00115	-0.00324
D10	-3.13905	-0.00010	-0.00084	-0.00066	-0.00150	-3.14055
D11	3.13185	0.00003	0.00138	-0.00008	0.00131	3.13316
D12	-0.00512	-0.00005	-0.00131	0.00229	0.00097	-0.00415
D13	-0.00233	0.00004	0.00075	-0.00311	-0.00237	-0.00470
D14	3.13159	-0.00019	-0.00274	-0.00226	-0.00494	3.12665
D15	3.13507	0.00011	0.00324	-0.00528	-0.00207	3.13299
D16	-0.01420	-0.00011	-0.00025	-0.00442	-0.00464	-0.01884
D17	-0.00057	0.00008	0.00001	0.00805	0.00806	0.00749
D18	-3.14071	0.00018	0.00369	0.00795	0.01162	-3.12909
D19	-3.13701	-0.00001	-0.00303	0.01070	0.00769	-3.12932
D20	0.00603	0.00009	0.00066	0.01059	0.01125	0.01728
D21	0.00580	-0.00005	-0.00304	0.00799	0.00494	0.01074
D22	3.08898	-0.00011	-0.00261	-0.00383	-0.00650	3.08247
D23	-3.12777	0.00019	0.00052	0.00719	0.00778	-3.11999
D24	-0.04460	0.00012	0.00095	-0.00463	-0.00366	-0.04825
D25	1.45462	0.00027	0.00152	0.01405	0.01556	1.47018
D26	-2.72381	0.00012	0.00184	0.01716	0.01900	-2.70481
D27	-0.68530	-0.00002	0.00121	0.01583	0.01701	-0.66829
D28	-1.61763	0.00036	0.00104	0.02810	0.02916	-1.58847
D29	0.48713	0.00021	0.00136	0.03122	0.03260	0.51973
D30	2.52564	0.00007	0.00072	0.02988	0.03061	2.55625
D31	-1.12252	-0.00023	-0.01109	0.00488	-0.00622	-1.12874
D32	0.91523	-0.00031	-0.01408	0.00418	-0.00991	0.90533
D33	3.08900	-0.00055	-0.01294	0.00573	-0.00721	3.08179
D34	3.08732	-0.00006	-0.01236	0.00129	-0.01106	3.07626
D35	-1.15811	-0.00014	-0.01535	0.00059	-0.01475	-1.17286
D36	1.01566	-0.00039	-0.01420	0.00214	-0.01205	1.00360
D37	0.99571	0.00013	-0.00826	0.00111	-0.00716	0.98855
D38	3.03346	0.00005	-0.01125	0.00041	-0.01084	3.02262
D39	-1.07595	-0.00020	-0.01011	0.00196	-0.00815	-1.08411
D40	2.84093	0.00016	0.00157	-0.02035	-0.01858	2.82235
D41	-1.35585	0.00022	0.00023	-0.01809	-0.01804	-1.37389
D42	0.76886	-0.00004	0.00112	-0.01931	-0.01800	0.75086
D43	2.85527	0.00002	-0.00022	-0.01705	-0.01747	2.83780
D44	-1.33335	-0.00016	0.00117	-0.01932	-0.01795	-1.35129
D45	0.75306	-0.00011	-0.00016	-0.01706	-0.01741	0.73565
D46	-3.14078	0.00007	0.00365	-0.00109	0.00257	-3.13821
D47	0.00081	0.00005	0.00126	0.00126	0.00252	0.00333
D48	-0.00081	-0.00004	-0.00047	-0.00097	-0.00145	-0.00227
D49	3.14078	-0.00006	-0.00286	0.00137	-0.00150	3.13927
D50	1.20731	0.00029	0.01911	0.00423	0.02283	1.23015
D51	-0.54621	0.00019	-0.00581	-0.01062	-0.01689	-0.56310
D52	-2.97691	-0.00002	0.01447	-0.01511	-0.00018	-2.97710

D53	1.55275	-0.00012	-0.01045	-0.02996	-0.03990	1.51285
D54	-2.70008	0.00012	0.00096	-0.00321	-0.00224	-2.70232
D55	-0.01624	0.00005	0.00001	0.00016	0.00017	-0.01607
D56	-0.02338	-0.00004	-0.00031	-0.00003	-0.00034	-0.02373
D57	2.66045	-0.00012	-0.00127	0.00335	0.00207	2.66252
D58	1.97794	-0.00035	0.00005	-0.02381	-0.02384	1.95410
D59	-0.44375	-0.00008	-0.00024	-0.02037	-0.02067	-0.46442
D60	0.48148	0.00031	0.00092	0.02040	0.02137	0.50285
D61	-1.94391	0.00035	0.00039	0.02371	0.02416	-1.91975
D62	2.55250	-0.00001	0.00028	-0.00147	-0.00119	2.55132
D63	-1.65350	-0.00006	0.00009	-0.00204	-0.00195	-1.65545
D64	0.44747	-0.00003	0.00010	-0.00215	-0.00204	0.44543
D65	1.34868	0.00008	0.00059	-0.00088	-0.00030	1.34838
D66	-2.85732	0.00003	0.00040	-0.00145	-0.00107	-2.85839
D67	-0.75635	0.00005	0.00041	-0.00155	-0.00115	-0.75751
D68	-1.05092	0.00000	-0.00051	0.00272	0.00221	-1.04872
D69	1.02626	-0.00004	-0.00071	0.00214	0.00144	1.02770
D70	3.12723	-0.00002	-0.00069	0.00204	0.00136	3.12858

Item	Value	Threshold	Converged?
Maximum Force	0.001815	0.000450	NO
RMS Force	0.000322	0.000300	NO
Maximum Displacement	0.157367	0.001800	NO
RMS Displacement	0.052647	0.001200	NO

Predicted change in Energy=-8.567497D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.894055	2.146127	-0.234463
2	6	0	-3.771144	1.162411	0.092645
3	7	0	-3.052658	-0.027452	0.106603
4	6	0	-1.771730	0.238149	-0.209950
5	7	0	-1.656851	1.547692	-0.428402
6	6	0	-0.379900	2.220342	-0.729443
7	6	0	0.328723	2.721212	0.537569
8	1	0	-3.043410	3.205420	-0.353253
9	1	0	-4.823307	1.209765	0.306811
10	1	0	0.249027	1.494622	-1.245707
11	1	0	-0.578253	3.048324	-1.410325
12	1	0	-0.283671	3.496961	1.009010
13	1	0	0.400141	1.883445	1.247908

14	35	0	0.276285	-2.311798	-0.046889
15	1	0	-0.975742	-0.540746	-0.257281
16	6	0	-3.500192	-1.352087	0.388535
17	6	0	-4.753187	-1.663851	0.691486
18	1	0	-2.686133	-2.069969	0.328728
19	1	0	-5.001006	-2.696714	0.893766
20	1	0	-5.557386	-0.940494	0.750612
21	7	0	1.608135	3.292448	0.144259
22	1	0	1.978854	3.893828	0.870204
23	1	0	2.290920	2.553624	-0.026789
24	6	0	3.710124	-0.247536	-1.051815
25	6	0	3.664925	-0.432197	0.400506
26	8	0	3.477336	0.884527	-0.183711
27	1	0	4.671820	-0.229410	-1.559020
28	1	0	2.856684	-0.557627	-1.647220
29	1	0	2.745722	-0.858272	0.796575
30	6	0	4.905964	-0.620159	1.228548
31	1	0	4.786588	-0.164749	2.216068
32	1	0	5.096685	-1.687820	1.373245
33	1	0	5.775806	-0.170648	0.743410

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357933	0.000000			
3	N	2.205885	1.390033	0.000000		
4	C	2.213729	2.223394	1.345929	0.000000	
5	N	1.387952	2.211372	2.171540	1.332600	0.000000
6	C	2.563492	3.646311	3.590987	2.477126	1.474343
7	C	3.363488	4.408710	4.378883	3.337108	2.500550
8	H	1.076345	2.214116	3.265427	3.231471	2.162465
9	H	2.211734	1.074782	2.169329	3.243948	3.268207
10	H	3.365418	4.250097	3.878991	2.595184	2.074410
11	H	2.749463	4.001267	4.228965	3.280605	2.092712
12	H	3.191408	4.295616	4.571992	3.784183	2.784138
13	H	3.621899	4.387954	4.108031	3.090206	2.674689
14	Br	5.473513	5.335849	4.040255	3.274627	4.333385
15	H	3.301474	3.292030	2.170129	1.114681	2.203353
16	C	3.604585	2.546305	1.426335	2.423761	3.531857
17	C	4.339319	3.051356	2.431396	3.649558	4.599505
18	H	4.258625	3.417786	2.086997	2.540416	3.836683
19	H	5.400487	4.128826	3.397153	4.501092	5.562956
20	H	4.194155	2.836510	2.742637	4.079591	4.774444
21	N	4.661244	5.785876	5.722425	4.569212	3.745964

22	H	5.293391	6.413089	6.424611	5.347673	4.517641
23	H	5.205108	6.220801	5.935787	4.679754	4.093665
24	C	7.071978	7.698514	6.864808	5.567347	5.693497
25	C	7.076098	7.611352	6.736180	5.511737	5.738323
26	O	6.495294	7.259068	6.599758	5.288780	5.182619
27	H	8.039906	8.714861	7.904597	6.599844	6.669968
28	H	6.509775	7.064968	6.186865	4.911336	5.127366
29	H	6.472753	6.859170	5.898095	4.756322	5.164482
30	C	8.404347	8.930848	8.059139	6.884590	7.107433
31	H	8.386748	8.916561	8.119265	7.004244	7.172418
32	H	9.007542	9.402242	8.412669	7.306914	7.702254
33	H	9.027191	9.661511	8.852559	7.618485	7.718175

		6	7	8	9	10
6	C	0.000000				
7	C	1.535687	0.000000			
8	H	2.864644	3.521263	0.000000		
9	H	4.673217	5.374117	2.754335	0.000000	
10	H	1.090297	2.165859	3.816208	5.312253	0.000000
11	H	1.090183	2.173453	2.686834	4.934505	1.767903
12	H	2.158989	1.095020	3.091426	5.131535	3.062169
13	H	2.152180	1.100698	4.021116	5.350132	2.528267
14	Br	4.629983	5.067102	6.446234	6.207443	3.990832
15	H	2.863838	3.601914	4.279979	4.264533	2.572891
16	C	4.873228	5.592367	4.640019	2.884510	4.983086
17	C	6.019272	6.714035	5.265417	2.900096	6.225015
18	H	4.984496	5.664661	5.331273	3.914670	4.878557
19	H	6.940236	7.608338	6.342116	3.954323	7.050354
20	H	6.244022	6.935398	4.972645	2.315047	6.605264
21	N	2.421786	1.455300	4.678884	6.762207	2.647897
22	H	3.305018	2.051489	5.214775	7.334235	3.636698
23	H	2.781740	2.048610	5.383910	7.247722	2.603185
24	C	4.787759	4.772157	7.617159	8.762935	3.879678
25	C	4.967228	4.592714	7.668257	8.646092	4.253353
26	O	4.118312	3.715834	6.923541	8.321483	3.452830
27	H	5.675328	5.653702	8.530926	9.783148	4.757263
28	H	4.362900	4.681311	7.116599	8.119370	3.342576
29	H	4.645008	4.326855	7.165873	7.861733	3.992556
30	C	6.312094	5.709059	8.962683	9.942683	5.681664
31	H	6.407596	5.569443	8.903276	9.893667	5.943640
32	H	7.048972	6.547624	9.653276	10.389395	6.362911
33	H	6.766006	6.170570	9.506791	10.697540	6.105325

		11	12	13	14	15
11	H	0.000000				
12	H	2.478152	0.000000			

13	H	3.062744	1.768644	0.000000		
14	Br	5.596436	5.930442	4.392255	0.000000	
15	H	3.790637	4.287835	3.167862	2.179097	0.000000
16	C	5.580076	5.851860	5.140019	3.920768	2.729140
17	C	6.637188	6.834572	6.280899	5.124512	4.053469
18	H	5.802101	6.101255	5.098967	2.995913	2.367988
19	H	7.607564	7.786407	7.090533	5.374272	4.709125
20	H	6.735880	6.897090	6.611661	6.045511	4.708196
21	N	2.693812	2.090107	2.159301	5.763500	4.640154
22	H	3.529092	2.301258	2.583918	6.499968	5.446678
23	H	3.223516	2.931089	2.376771	5.266069	4.505478
24	C	5.420461	5.849671	4.559145	4.130654	4.761785
25	C	5.779074	5.603567	4.091345	3.900762	4.688311
26	O	4.757563	4.732079	3.537867	4.525698	4.676187
27	H	6.191035	6.710999	5.530845	5.093487	5.804000
28	H	4.985759	5.775558	4.513891	3.506655	4.076727
29	H	5.583968	5.309463	3.636271	2.987019	3.880815
30	C	7.106199	6.628060	5.154693	5.091395	6.066998
31	H	7.228837	6.369665	4.936938	5.483943	6.281981
32	H	7.898370	7.480832	5.901456	5.063831	6.391304
33	H	7.441399	7.087958	5.776816	5.954311	6.835332

		16	17	18	19	20
16	C	0.000000				
17	C	1.326262	0.000000			
18	H	1.087025	2.137577	0.000000		
19	H	2.077431	1.081267	2.463882	0.000000	
20	H	2.128979	1.083271	3.114127	1.847799	0.000000
21	N	6.908429	8.082745	6.872429	8.950562	8.344468
22	H	7.600762	8.731558	7.590927	9.599700	8.954321
23	H	6.997432	8.241508	6.802577	9.032478	8.626072
24	C	7.435275	8.756294	6.792589	9.255676	9.466556
25	C	7.223936	8.512711	6.559222	8.970491	9.242941
26	O	7.349545	8.660353	6.854196	9.266528	9.264441
27	H	8.475563	9.795568	7.816056	10.279461	10.510789
28	H	6.722004	8.037625	6.075720	8.530861	8.757440
29	H	6.278678	7.542787	5.584992	7.962481	8.303642
30	C	8.479670	9.730207	7.781489	10.127794	10.479157
31	H	8.568570	9.776450	7.939363	10.195898	10.476027
32	H	8.659600	9.873467	7.861890	10.159288	10.698383
33	H	9.357665	10.634474	8.682385	11.069927	11.359311

		21	22	23	24	25
21	N	0.000000				
22	H	1.012959	0.000000			
23	H	1.020449	1.642599	0.000000		

24	C	4.287242	4.882863	3.303227	0.000000	
25	C	4.262515	4.666684	3.314452	1.464712	0.000000
26	O	3.065871	3.523078	2.053799	1.445462	1.452674
27	H	4.968985	5.491292	3.970099	1.087403	2.212397
28	H	4.426212	5.188783	3.553275	1.085829	2.205033
29	H	4.352941	4.814142	3.539181	2.172468	1.087817
30	C	5.230665	5.391889	4.299677	2.601718	1.503716
31	H	5.132950	5.115346	4.318370	3.441611	2.150795
32	H	6.203504	6.413168	5.274681	3.142911	2.138398
33	H	5.451743	5.563532	4.489910	2.737843	2.154486

		26	27	28	29	30
26	O	0.000000				
27	H	2.135209	0.000000			
28	H	2.146364	1.846680	0.000000		
29	H	2.129218	3.107113	2.464718	0.000000	
30	C	2.509887	2.824543	3.531785	2.215840	0.000000
31	H	2.928150	3.777385	4.336344	2.580905	1.094004
32	H	3.415168	3.302370	3.926595	2.558853	1.094172
33	H	2.693680	2.554098	3.792906	3.107582	1.092724

		31	32	33
31	H	0.000000		
32	H	1.768123	0.000000	
33	H	1.774066	1.777557	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.857652	2.206329	-0.171571
2	6	0	-3.740525	1.215435	0.115914
3	7	0	-3.030601	0.021071	0.074736
4	6	0	-1.749048	0.291250	-0.235346
5	7	0	-1.625577	1.608261	-0.396776
6	6	0	-0.345000	2.284438	-0.673533
7	6	0	0.372216	2.724350	0.611151
8	1	0	-2.999821	3.270832	-0.243260
9	1	0	-4.791465	1.260774	0.336425
10	1	0	0.276627	1.577607	-1.223730

11	1	0	-0.540054	3.142814	-1.316684
12	1	0	-0.232693	3.483006	1.118688
13	1	0	0.440385	1.855803	1.283843
14	35	0	0.281127	-2.277749	-0.192737
15	1	0	-0.958898	-0.490411	-0.320102
16	6	0	-3.486574	-1.311453	0.300342
17	6	0	-4.740581	-1.627351	0.594695
18	1	0	-2.677962	-2.031743	0.205715
19	1	0	-4.995053	-2.666310	0.752642
20	1	0	-5.539296	-0.901631	0.688840
21	7	0	1.654158	3.303235	0.237767
22	1	0	2.032073	3.869627	0.987745
23	1	0	2.330910	2.567818	0.031649
24	6	0	3.725791	-0.195699	-1.120995
25	6	0	3.684992	-0.443449	0.322035
26	8	0	3.504613	0.898880	-0.203206
27	1	0	4.685584	-0.162156	-1.631012
28	1	0	2.867790	-0.473406	-1.725758
29	1	0	2.764306	-0.879974	0.702993
30	6	0	4.927899	-0.676221	1.135767
31	1	0	4.815714	-0.263656	2.142766
32	1	0	5.111475	-1.750511	1.232796
33	1	0	5.799044	-0.212036	0.667061

Rotational constants (GHZ): 0.4802847 0.2461298 0.1711182

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1292.7653214568 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 3.84D-06 NBF= 482

NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999987 0.000131 0.000170 -0.005077 Ang= 0.58 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes=

0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid=
0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0
NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3205.64680635 A.U. after 12 cycles
NFock= 12 Conv=0.65D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000076798	-0.000038435	-0.000480464
2	6	0.000067546	0.000154798	0.000445769
3	7	0.000656722	0.000507028	-0.000421119
4	6	-0.000922826	-0.001803173	-0.000895061
5	7	0.000194828	-0.000189817	0.000787288
6	6	0.000520939	0.000873096	0.000115772
7	6	-0.000773206	-0.000386617	0.000451243
8	1	0.000014710	0.000043799	-0.000124713
9	1	0.000099602	0.000109386	0.000065241
10	1	-0.000066169	-0.000063958	0.000021682
11	1	-0.000203750	-0.000013459	-0.000038344
12	1	0.000082508	0.000010932	0.000020604
13	1	0.000275212	0.000102928	-0.000174210
14	35	-0.000198700	-0.000000953	-0.000069106
15	1	0.000310849	0.000964175	0.000406256
16	6	0.000276049	0.000015475	-0.000044943
17	6	-0.000046670	-0.000199293	-0.000030351
18	1	-0.000206295	0.000225708	0.000277810
19	1	-0.000071539	0.000012635	0.000011910
20	1	0.000117429	-0.000089214	0.000002060

21	7	0.000065567	-0.000117877	-0.000372558
22	1	-0.000062263	0.000006241	-0.000094868
23	1	0.000084076	0.000203658	0.000337891
24	6	0.000339055	0.000244937	0.000446751
25	6	0.000164492	0.000176631	-0.000004080
26	8	-0.000680754	-0.000269271	-0.000307466
27	1	-0.000036458	-0.000035508	-0.000121152
28	1	-0.000054121	-0.000203149	0.000172910
29	1	-0.000085773	-0.000208370	-0.000321698
30	6	0.000069759	0.000010632	-0.000087264
31	1	-0.000064525	-0.000012509	-0.000017849
32	1	0.000058613	-0.000021921	0.000050773
33	1	-0.000001706	-0.000008536	-0.000008715

Cartesian Forces: Max 0.001803173 RMS 0.000353443

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000868554 RMS 0.000205630
Search for a local minimum.
Step number 9 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 2 3 1 4 5
6 7 8 9
DE= -9.98D-05 DEPred=-8.57D-05 R= 1.16D+00
TightC=F SS= 1.41D+00 RLast= 1.46D-01 DXNew= 5.1608D-01 4.3848D-01
Trust test= 1.16D+00 RLast= 1.46D-01 DXMaxT set to 4.38D-01
ITU= 1 1 1 -1 1 0 0 -1 0

Eigenvalues ---	0.00079	0.00232	0.00310	0.00395	0.00721
Eigenvalues ---	0.00724	0.01060	0.01319	0.01455	0.01484
Eigenvalues ---	0.01697	0.01888	0.02105	0.02177	0.02330
Eigenvalues ---	0.02373	0.02390	0.02465	0.02677	0.03066
Eigenvalues ---	0.03075	0.03096	0.03202	0.03322	0.04008
Eigenvalues ---	0.04093	0.04382	0.04679	0.04864	0.05428
Eigenvalues ---	0.05756	0.05868	0.05921	0.07945	0.08720
Eigenvalues ---	0.09556	0.10768	0.12114	0.12388	0.12519
Eigenvalues ---	0.12799	0.13166	0.14690	0.15587	0.16000
Eigenvalues ---	0.16000	0.16000	0.16001	0.16005	0.16021
Eigenvalues ---	0.16047	0.16125	0.17367	0.21194	0.22040

Eigenvalues --- 0.22608 0.22977 0.23792 0.25206 0.27567
Eigenvalues --- 0.29042 0.30307 0.31952 0.32106 0.33346
Eigenvalues --- 0.33751 0.34284 0.34312 0.34341 0.34543
Eigenvalues --- 0.34662 0.34705 0.35053 0.35064 0.35272
Eigenvalues --- 0.35303 0.35593 0.35885 0.36117 0.36428
Eigenvalues --- 0.36631 0.37989 0.39785 0.41826 0.42691
Eigenvalues --- 0.44637 0.45487 0.45564 0.49059 0.56412
Eigenvalues --- 0.57184 0.60617 0.98567
En-DIIS/RFO-DIIS IScMMF= 0 using points: 9 8 7 6 5
RFO step: Lambda=-2.63933681D-05.
DidBck=F Rises=F RFO-DIIS coefs: 1.19682 0.79565 -0.16673 -0.29816 -0.52757
Iteration 1 RMS(Cart)= 0.10636688 RMS(Int)= 0.00362709
Iteration 2 RMS(Cart)= 0.00722812 RMS(Int)= 0.00029969
Iteration 3 RMS(Cart)= 0.00003541 RMS(Int)= 0.00029914
Iteration 4 RMS(Cart)= 0.00000002 RMS(Int)= 0.00029914

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56612	-0.00020	0.00098	-0.00059	0.00036	2.56649
R2	2.62285	-0.00033	0.00129	-0.00004	0.00126	2.62411
R3	2.03400	0.00006	-0.00019	0.00003	-0.00016	2.03384
R4	2.62678	0.00018	-0.00155	-0.00060	-0.00218	2.62460
R5	2.03104	-0.00008	0.00003	0.00005	0.00008	2.03113
R6	2.54344	-0.00070	0.00045	0.00053	0.00098	2.54442
R7	2.69538	0.00005	0.00255	0.00191	0.00446	2.69984
R8	2.51825	0.00013	-0.00155	0.00191	0.00039	2.51864
R9	2.10644	-0.00061	-0.00289	-0.00385	-0.00675	2.09970
R10	2.78611	-0.00022	-0.00204	-0.00066	-0.00270	2.78341
R11	2.90203	-0.00044	0.00315	0.00026	0.00341	2.90544
R12	2.06036	0.00000	-0.00067	0.00025	-0.00042	2.05994
R13	2.06015	0.00005	-0.00049	0.00044	-0.00005	2.06009
R14	2.06929	-0.00003	0.00000	-0.00014	-0.00014	2.06915
R15	2.08002	-0.00018	0.00025	-0.00025	0.00000	2.08002
R16	2.75012	-0.00020	-0.00194	-0.00050	-0.00244	2.74768
R17	4.11790	-0.00012	0.02496	0.02522	0.05018	4.16808
R18	2.50627	0.00006	-0.00010	-0.00028	-0.00038	2.50589
R19	2.05418	-0.00032	0.00264	0.00123	0.00387	2.05805
R20	2.04330	0.00001	0.00014	0.00007	0.00020	2.04350
R21	2.04709	-0.00014	0.00047	-0.00002	0.00044	2.04753
R22	1.91422	-0.00009	-0.00006	-0.00029	-0.00035	1.91387
R23	1.92837	-0.00008	-0.00019	-0.00133	-0.00153	1.92684
R24	3.88112	0.00011	0.01377	0.01513	0.02890	3.91002
R25	2.76790	-0.00057	0.00046	-0.00082	-0.00102	2.76689
R26	2.73153	0.00003	0.00076	-0.00037	0.00068	2.73220

R27	2.05489	0.00002	-0.00020	0.00030	0.00011	2.05500
R28	2.05192	0.00000	-0.00013	0.00002	-0.00011	2.05180
R29	2.74516	0.00020	0.00158	0.00077	0.00274	2.74789
R30	2.05568	0.00004	-0.00003	-0.00004	-0.00007	2.05560
R31	2.84161	0.00003	-0.00013	-0.00005	-0.00018	2.84143
R32	2.06737	-0.00001	-0.00011	-0.00005	-0.00016	2.06720
R33	2.06768	0.00004	-0.00024	0.00008	-0.00016	2.06753
R34	2.06495	0.00000	0.00015	-0.00012	0.00003	2.06498
A1	1.87241	-0.00014	-0.00065	-0.00008	-0.00070	1.87171
A2	2.27826	0.00012	0.00053	0.00082	0.00131	2.27957
A3	2.13247	0.00002	0.00015	-0.00069	-0.00057	2.13190
A4	1.86363	-0.00006	0.00147	0.00064	0.00210	1.86573
A5	2.27626	-0.00007	-0.00020	-0.00119	-0.00139	2.27487
A6	2.14328	0.00013	-0.00126	0.00057	-0.00070	2.14258
A7	1.89720	0.00017	-0.00201	0.00032	-0.00167	1.89553
A8	2.25850	0.00017	0.00235	-0.00079	0.00154	2.26005
A9	2.12747	-0.00034	-0.00034	0.00048	0.00013	2.12760
A10	1.89075	-0.00019	0.00262	-0.00095	0.00167	1.89242
A11	2.15520	0.00049	-0.02290	-0.00683	-0.02982	2.12539
A12	2.23718	-0.00030	0.02025	0.00762	0.02774	2.26492
A13	1.90070	0.00022	-0.00146	0.00015	-0.00135	1.89935
A14	2.21913	-0.00047	0.00524	-0.00136	0.00365	2.22279
A15	2.16094	0.00025	-0.00448	0.00066	-0.00397	2.15697
A16	1.96059	-0.00020	-0.00101	0.00110	0.00010	1.96069
A17	1.86776	-0.00002	0.00344	-0.00041	0.00302	1.87078
A18	1.89278	-0.00003	0.00470	-0.00120	0.00350	1.89628
A19	1.91940	-0.00002	-0.00101	-0.00100	-0.00202	1.91738
A20	1.93001	0.00027	-0.00219	0.00212	-0.00008	1.92993
A21	1.89099	0.00000	-0.00381	-0.00076	-0.00460	1.88639
A22	1.90520	0.00030	-0.00350	0.00096	-0.00256	1.90264
A23	1.89035	0.00035	-0.00208	-0.00061	-0.00271	1.88764
A24	1.88674	-0.00087	0.00582	-0.00183	0.00398	1.89072
A25	1.87302	-0.00006	-0.00221	0.00110	-0.00114	1.87188
A26	1.90704	0.00031	0.00169	0.00222	0.00393	1.91096
A27	1.99998	0.00000	-0.00002	-0.00172	-0.00173	1.99825
A28	2.16505	0.00029	-0.00333	-0.00305	-0.00639	2.15866
A29	1.94708	-0.00012	-0.00187	-0.00120	-0.00308	1.94401
A30	2.17104	-0.00018	0.00520	0.00423	0.00942	2.18046
A31	2.07580	0.00011	-0.00166	-0.00050	-0.00217	2.07363
A32	2.16141	-0.00007	0.00158	0.00069	0.00227	2.16368
A33	2.04598	-0.00004	0.00008	-0.00019	-0.00011	2.04587
A34	1.94024	0.00010	0.00074	-0.00001	0.00155	1.94179
A35	1.92767	-0.00054	-0.00086	-0.00394	-0.00460	1.92306
A36	1.88083	0.00019	0.00049	0.00248	0.00274	1.88357

A37	2.08505	0.00006	-0.00178	0.00005	-0.00242	2.08262
A38	2.07538	-0.00019	0.00404	0.00030	0.00498	2.08036
A39	1.99271	-0.00005	-0.00056	0.00009	-0.00031	1.99239
A40	2.01131	0.00003	0.00102	0.00166	0.00238	2.01369
A41	2.03098	0.00004	-0.00199	-0.00127	-0.00325	2.02773
A42	2.02247	-0.00013	0.00354	-0.00026	0.00387	2.02634
A43	2.13684	-0.00006	-0.00155	-0.00051	-0.00278	2.13406
A44	1.97396	0.00004	0.00118	0.00242	0.00336	1.97732
A45	2.02788	-0.00014	0.00072	-0.00061	0.00029	2.02817
A46	2.03525	0.00015	-0.00228	-0.00020	-0.00244	2.03282
A47	2.45815	0.00029	0.01326	0.01622	0.02768	2.48582
A48	2.46626	0.00017	0.01320	0.01486	0.02624	2.49250
A49	1.93368	-0.00011	0.00051	-0.00049	0.00002	1.93370
A50	1.91628	0.00012	-0.00165	-0.00040	-0.00205	1.91422
A51	1.94022	0.00000	0.00065	0.00060	0.00125	1.94147
A52	1.88162	-0.00002	0.00030	-0.00023	0.00007	1.88169
A53	1.89270	0.00005	-0.00007	0.00029	0.00021	1.89292
A54	1.89796	-0.00004	0.00027	0.00023	0.00050	1.89846
A55	3.27923	0.00071	0.07652	0.04351	0.12003	3.39926
A56	3.01520	-0.00014	-0.05874	-0.01136	-0.06963	2.94557
A57	2.93805	0.00000	-0.06430	-0.05573	-0.12003	2.81802
A58	3.23706	-0.00021	-0.01742	0.01391	-0.00379	3.23327
D1	0.00956	-0.00019	0.00127	-0.00297	-0.00178	0.00778
D2	-3.12630	-0.00020	-0.00003	-0.00458	-0.00462	-3.13091
D3	3.14018	0.00000	0.00458	0.00122	0.00583	-3.13717
D4	0.00433	-0.00001	0.00327	-0.00039	0.00299	0.00732
D5	-0.01274	0.00031	-0.00149	0.00543	0.00401	-0.00873
D6	-3.08151	0.00024	0.01219	0.01372	0.02618	-3.05533
D7	3.13870	0.00013	-0.00447	0.00165	-0.00283	3.13587
D8	0.06993	0.00007	0.00922	0.00995	0.01934	0.08927
D9	-0.00324	0.00001	-0.00063	-0.00045	-0.00099	-0.00423
D10	-3.14055	-0.00010	0.00416	-0.00460	-0.00027	-3.14081
D11	3.13316	0.00002	0.00056	0.00100	0.00157	3.13473
D12	-0.00415	-0.00009	0.00535	-0.00315	0.00230	-0.00185
D13	-0.00470	0.00018	-0.00031	0.00385	0.00350	-0.00120
D14	3.12665	-0.00021	-0.00524	-0.01115	-0.01577	3.11088
D15	3.13299	0.00029	-0.00468	0.00763	0.00284	3.13584
D16	-0.01884	-0.00010	-0.00961	-0.00737	-0.01643	-0.03526
D17	0.00749	0.00017	0.00638	0.01711	0.02346	0.03095
D18	-3.12909	0.00026	0.00869	0.02130	0.02991	-3.09918
D19	-3.12932	0.00004	0.01172	0.01248	0.02427	-3.10505
D20	0.01728	0.00013	0.01403	0.01666	0.03073	0.04801
D21	0.01074	-0.00030	0.00111	-0.00572	-0.00463	0.00611
D22	3.08247	-0.00027	-0.01169	-0.01378	-0.02540	3.05707

D23	-3.11999	0.00011	0.00635	0.01031	0.01714	-3.10285
D24	-0.04825	0.00014	-0.00645	0.00225	-0.00363	-0.05188
D25	1.47018	0.00024	0.01779	0.03601	0.05376	1.52394
D26	-2.70481	0.00008	0.01821	0.03517	0.05332	-2.65149
D27	-0.66829	0.00005	0.01793	0.03345	0.05133	-0.61696
D28	-1.58847	0.00017	0.03324	0.04550	0.07879	-1.50968
D29	0.51973	0.00002	0.03365	0.04465	0.07836	0.59808
D30	2.55625	-0.00001	0.03338	0.04293	0.07636	2.63261
D31	-1.12874	-0.00018	-0.01361	-0.02005	-0.03367	-1.16241
D32	0.90533	0.00011	-0.01936	-0.01856	-0.03790	0.86743
D33	3.08179	-0.00021	-0.01703	-0.02220	-0.03922	3.04257
D34	3.07626	-0.00001	-0.01661	-0.01957	-0.03618	3.04008
D35	-1.17286	0.00027	-0.02236	-0.01807	-0.04041	-1.21327
D36	1.00360	-0.00005	-0.02003	-0.02172	-0.04174	0.96186
D37	0.98855	-0.00017	-0.00981	-0.01932	-0.02916	0.95939
D38	3.02262	0.00011	-0.01556	-0.01783	-0.03339	2.98923
D39	-1.08411	-0.00020	-0.01324	-0.02147	-0.03471	-1.11882
D40	2.82235	0.00008	-0.01964	-0.01577	-0.03559	2.78675
D41	-1.37389	0.00003	-0.01912	-0.01526	-0.03419	-1.40808
D42	0.75086	0.00005	-0.01973	-0.01713	-0.03705	0.71380
D43	2.83780	0.00000	-0.01920	-0.01661	-0.03565	2.80215
D44	-1.35129	-0.00010	-0.01810	-0.01902	-0.03730	-1.38859
D45	0.73565	-0.00014	-0.01758	-0.01851	-0.03590	0.69976
D46	-3.13821	0.00005	0.00267	0.00213	0.00482	-3.13339
D47	0.00333	0.00004	0.00132	0.00300	0.00434	0.00767
D48	-0.00227	-0.00005	0.00007	-0.00261	-0.00255	-0.00482
D49	3.13927	-0.00006	-0.00128	-0.00173	-0.00303	3.13624
D50	1.23015	-0.00001	-0.01041	0.02580	0.01562	1.24577
D51	-0.56310	0.00005	-0.01273	-0.01573	-0.02771	-0.59080
D52	-2.97710	-0.00002	-0.01076	0.01874	0.00724	-2.96985
D53	1.51285	0.00004	-0.01308	-0.02279	-0.03608	1.47676
D54	-2.70232	0.00014	-0.00003	0.00336	0.00344	-2.69887
D55	-0.01607	0.00010	-0.00125	0.00096	-0.00030	-0.01637
D56	-0.02373	-0.00007	0.00008	0.00087	0.00097	-0.02276
D57	2.66252	-0.00010	-0.00114	-0.00154	-0.00278	2.65974
D58	1.95410	-0.00022	-0.02428	-0.03218	-0.05709	1.89701
D59	-0.46442	-0.00025	-0.02155	-0.03222	-0.05427	-0.51869
D60	0.50285	0.00036	0.02275	0.03545	0.05873	0.56158
D61	-1.91975	0.00023	0.02417	0.03354	0.05824	-1.86151
D62	2.55132	0.00004	-0.00082	0.00076	-0.00004	2.55128
D63	-1.65545	0.00003	-0.00118	-0.00009	-0.00124	-1.65669
D64	0.44543	0.00006	-0.00151	0.00032	-0.00116	0.44427
D65	1.34838	0.00002	-0.00062	0.00137	0.00068	1.34906
D66	-2.85839	0.00000	-0.00097	0.00053	-0.00052	-2.85890

D67	-0.75751	0.00004	-0.00131	0.00094	-0.00044	-0.75795
D68	-1.04872	-0.00006	-0.00065	-0.00168	-0.00227	-1.05099
D69	1.02770	-0.00008	-0.00100	-0.00252	-0.00347	1.02423
D70	3.12858	-0.00004	-0.00133	-0.00211	-0.00340	3.12518

Item	Value	Threshold	Converged?
Maximum Force	0.000869	0.000450	NO
RMS Force	0.000206	0.000300	YES
Maximum Displacement	0.412620	0.001800	NO
RMS Displacement	0.111644	0.001200	NO

Predicted change in Energy=-1.602675D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.890011	2.148626	-0.267105
2	6	0	-3.719217	1.130383	0.079460
3	7	0	-2.950704	-0.026279	0.101927
4	6	0	-1.685360	0.292154	-0.230382
5	7	0	-1.627964	1.603341	-0.462470
6	6	0	-0.377301	2.325626	-0.751647
7	6	0	0.346998	2.775434	0.527787
8	1	0	-3.085586	3.199470	-0.392858
9	1	0	-4.770239	1.134824	0.304367
10	1	0	0.261133	1.649378	-1.320291
11	1	0	-0.608350	3.183803	-1.382983
12	1	0	-0.260932	3.532047	1.034605
13	1	0	0.419959	1.909311	1.203101
14	35	0	0.133432	-2.395587	0.115177
15	1	0	-0.876793	-0.469628	-0.252273
16	6	0	-3.337015	-1.368079	0.404423
17	6	0	-4.579561	-1.727535	0.696491
18	1	0	-2.483175	-2.043460	0.374458
19	1	0	-4.782657	-2.765710	0.920806
20	1	0	-5.417248	-1.040970	0.726423
21	7	0	1.626059	3.354374	0.149666
22	1	0	1.989594	3.951808	0.882215
23	1	0	2.309103	2.616969	-0.021661
24	6	0	3.598431	-0.278845	-1.053890
25	6	0	3.538763	-0.465544	0.397105
26	8	0	3.385829	0.857760	-0.185947
27	1	0	4.564988	-0.283601	-1.552199

28	1	0	2.745307	-0.567090	-1.660509
29	1	0	2.609490	-0.872737	0.789414
30	6	0	4.771352	-0.685930	1.229587
31	1	0	4.659179	-0.230218	2.217717
32	1	0	4.932708	-1.758629	1.372094
33	1	0	5.654900	-0.258100	0.749607

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.358126	0.000000			
3	N	2.206825	1.388879	0.000000		
4	C	2.213373	2.221532	1.346449	0.000000	
5	N	1.388620	2.211496	2.173440	1.332805	0.000000
6	C	2.565116	3.645236	3.589213	2.473408	1.472915
7	C	3.391602	4.409228	4.348078	3.297268	2.500977
8	H	1.076261	2.214880	3.266261	3.231025	2.162669
9	H	2.211251	1.074826	2.167914	3.242303	3.268247
10	H	3.359785	4.251099	3.891841	2.611282	2.075250
11	H	2.742763	4.004093	4.242193	3.293945	2.093996
12	H	3.243510	4.317410	4.557021	3.758470	2.798199
13	H	3.629694	4.359137	4.039859	3.017025	2.657392
14	Br	5.471491	5.222705	3.889176	3.263643	4.407677
15	H	3.302804	3.278636	2.150144	1.111112	2.214867
16	C	3.608043	2.548332	1.428695	2.426379	3.535773
17	C	4.336787	3.047724	2.429189	3.648923	4.598897
18	H	4.260364	3.418787	2.088511	2.541148	3.838097
19	H	5.398512	4.125325	3.395747	4.502112	5.563644
20	H	4.188979	2.831368	2.739239	4.076724	4.771217
21	N	4.692805	5.789908	5.690154	4.526270	3.745597
22	H	5.327564	6.418362	6.390662	5.304359	4.517765
23	H	5.225933	6.209735	5.887920	4.626453	4.089286
24	C	6.972196	7.537797	6.655139	5.377978	5.586377
25	C	6.971670	7.438155	6.511011	5.315948	5.631538
26	O	6.407737	7.115226	6.404377	5.102827	5.076463
27	H	7.946333	8.560941	7.699869	6.414479	6.565113
28	H	6.408860	6.906444	5.986919	4.734382	5.027083
29	H	6.363127	6.676006	5.666118	4.565379	5.064997
30	C	8.304894	8.758512	7.831788	6.691582	7.003931
31	H	8.295993	8.753336	7.901169	6.820500	7.076263
32	H	8.896547	9.212660	8.170835	7.111432	7.596768
33	H	8.935409	9.500056	8.633056	7.425805	7.614079

		6	7	8	9	10
6	C	0.000000				

7	C	1.537493	0.000000			
8	H	2.868300	3.579110	0.000000		
9	H	4.672374	5.378441	2.754440	0.000000	
10	H	1.090076	2.165817	3.803084	5.312154	0.000000
11	H	1.090154	2.174971	2.667825	4.936272	1.764764
12	H	2.158631	1.094946	3.182284	5.158854	3.059825
13	H	2.151739	1.100700	4.062074	5.324069	2.541711
14	Br	4.827224	5.191851	6.474940	6.045294	4.294022
15	H	2.883108	3.554797	4.284952	4.247709	2.631677
16	C	4.872357	5.545797	4.643423	2.885943	5.002635
17	C	6.015332	6.676539	5.262511	2.895379	6.237249
18	H	4.979130	5.590628	5.332916	3.916257	4.903106
19	H	6.937288	7.561223	6.339490	3.948964	7.067909
20	H	6.238568	6.915990	4.966967	2.308859	6.608405
21	N	2.425724	1.454010	4.745307	6.772220	2.632643
22	H	3.303961	2.051243	5.286708	7.346063	3.624885
23	H	2.799022	2.043737	5.438729	7.240175	2.610911
24	C	4.762464	4.733090	7.563844	8.595229	3.863492
25	C	4.944271	4.550646	7.611726	8.462227	4.262065
26	O	4.078700	3.663521	6.885175	8.175489	3.417180
27	H	5.645810	5.610301	8.485702	9.623161	4.723702
28	H	4.352530	4.659720	7.056432	7.952401	3.346580
29	H	4.639539	4.300753	7.100320	7.663287	4.040632
30	C	6.285171	5.661136	8.914042	9.757721	5.683099
31	H	6.380877	5.521296	8.863366	9.717930	5.949217
32	H	7.027632	6.503792	9.591186	10.181321	6.378641
33	H	6.731779	6.117627	9.468692	10.527203	6.084051

		11	12	13	14	15
11	H	0.000000				
12	H	2.467125	0.000000			
13	H	3.060977	1.767845	0.000000		
14	Br	5.824459	6.011466	4.449475	0.000000	
15	H	3.833813	4.248381	3.075554	2.205651	0.000000
16	C	5.600006	5.819850	5.049161	3.630900	2.700214
17	C	6.649510	6.813816	6.203105	4.795469	4.024050
18	H	5.824761	6.038248	4.973855	2.652894	2.334566
19	H	7.624237	7.753753	7.000195	4.995393	4.680158
20	H	6.739718	6.898917	6.557771	5.746186	4.679744
21	N	2.714902	2.091750	2.156991	5.940638	4.587899
22	H	3.531326	2.294403	2.595865	6.657561	5.390022
23	H	3.268950	2.925431	2.360019	5.466077	4.441869
24	C	5.458502	5.812004	4.470427	4.225345	4.550453
25	C	5.803877	5.552010	4.002062	3.924389	4.463053
26	O	4.774604	4.684061	3.439709	4.610101	4.465009

27	H	6.230165	6.673846	5.438916	5.184528	5.597982
28	H	5.039170	5.753610	4.442979	3.649433	3.887446
29	H	5.615098	5.263228	3.564404	2.984047	3.660845
30	C	7.123310	6.569111	5.066616	5.067064	5.843307
31	H	7.236535	6.305702	4.855720	5.439842	6.066725
32	H	7.919685	7.421526	5.817839	5.001861	6.168501
33	H	7.458079	7.031608	5.684007	5.954660	6.611470

		16	17	18	19	20
16	C	0.000000				
17	C	1.326060	0.000000			
18	H	1.089073	2.144377	0.000000		
19	H	2.076031	1.081375	2.471388	0.000000	
20	H	2.130271	1.083506	3.120521	1.848031	0.000000
21	N	6.855550	8.039561	6.787706	8.895039	8.322251
22	H	7.543358	8.685806	7.497114	9.538863	8.933834
23	H	6.923930	8.175828	6.696450	8.952907	8.581180
24	C	7.170322	8.487762	6.491531	8.962508	9.221324
25	C	6.934763	8.221280	6.225276	8.649338	8.980517
26	O	7.106302	8.420801	6.570870	9.004365	9.051616
27	H	8.212558	9.527032	7.515698	9.982740	10.266974
28	H	6.473034	7.781760	5.801532	8.256353	8.517588
29	H	5.979507	7.240289	5.241948	7.631805	8.028748
30	C	8.178743	9.423837	7.429824	9.782633	10.207193
31	H	8.277794	9.482110	7.595963	9.861995	10.218397
32	H	8.335301	9.536282	7.488106	9.777842	10.394879
33	H	9.066739	10.339549	8.340055	10.735922	11.099815

		21	22	23	24	25
21	N	0.000000				
22	H	1.012775	0.000000			
23	H	1.019641	1.643433	0.000000		
24	C	4.305703	4.922935	3.333708	0.000000	
25	C	4.279186	4.706193	3.345043	1.464173	0.000000
26	O	3.072867	3.558593	2.069093	1.445820	1.454122
27	H	4.976797	5.522474	3.980562	1.087459	2.210436
28	H	4.461763	5.239941	3.607538	1.085768	2.207636
29	H	4.386899	4.865092	3.595293	2.174507	1.087778
30	C	5.232891	5.419175	4.305512	2.599178	1.503620
31	H	5.130882	5.138054	4.317887	3.439616	2.150660
32	H	6.210560	6.442903	5.288829	3.139340	2.136763
33	H	5.444397	5.583492	4.478307	2.735342	2.155303

		26	27	28	29	30
26	O	0.000000				
27	H	2.135360	0.000000			
28	H	2.148208	1.844814	0.000000		

29	H	2.132757	3.107122	2.472648	0.000000	
30	C	2.511252	2.818295	3.531520	2.214113	0.000000
31	H	2.929627	3.771470	4.337859	2.579555	1.093918
32	H	3.415526	3.295818	3.924433	2.553754	1.094088
33	H	2.696125	2.546934	3.790761	3.107070	1.092739

		31	32	33
31	H	0.000000		
32	H	1.768031	0.000000	
33	H	1.774144	1.777818	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.792872	2.277000	-0.156081
2	6	0	-3.642274	1.253793	0.119728
3	7	0	-2.899663	0.082279	0.048541
4	6	0	-1.629782	0.397268	-0.269434
5	7	0	-1.544665	1.720674	-0.402551
6	6	0	-0.280148	2.435330	-0.646970
7	6	0	0.462604	2.771370	0.656595
8	1	0	-2.965759	3.338348	-0.200662
9	1	0	-4.691399	1.264122	0.353139
10	1	0	0.339180	1.790209	-1.270282
11	1	0	-0.496203	3.343554	-1.209897
12	1	0	-0.124848	3.500612	1.224057
13	1	0	0.520732	1.855347	1.264101
14	35	0	0.130782	-2.347855	-0.142620
15	1	0	-0.838604	-0.378110	-0.355437
16	6	0	-3.313817	-1.269802	0.252316
17	6	0	-4.562093	-1.623145	0.526885
18	1	0	-2.475501	-1.959422	0.164392
19	1	0	-4.786822	-2.670624	0.674042
20	1	0	-5.384010	-0.922724	0.615483
21	7	0	1.751711	3.349222	0.312451
22	1	0	2.133420	3.881581	1.084853
23	1	0	2.416942	2.612162	0.080331
24	6	0	3.634276	-0.224830	-1.177913

25	6	0	3.580206	-0.519212	0.255341
26	8	0	3.452962	0.847354	-0.225052
27	1	0	4.597115	-0.212990	-1.683254
28	1	0	2.770866	-0.447804	-1.797347
29	1	0	2.644725	-0.934535	0.623639
30	6	0	4.813131	-0.828611	1.058485
31	1	0	4.717812	-0.446477	2.079046
32	1	0	4.951433	-1.912266	1.118412
33	1	0	5.702772	-0.385100	0.604708

Rotational constants (GHZ): 0.4566519 0.2609154 0.1744770

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1298.4420681616 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 3.87D-06 NBF= 482

NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999924 -0.004216 -0.001559 0.011446 Ang= -1.41 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3205.64656377 A.U. after 11 cycles

NFock= 11 Conv=0.75D-08 -V/T= 2.0018

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000721879	-0.000066901	-0.000021336
2	6	-0.000214349	0.000268962	0.000312615
3	7	0.000917832	0.001143361	-0.001325738
4	6	-0.002277820	-0.003653364	0.001030649
5	7	0.000226795	-0.000063820	0.000689042
6	6	0.001261704	0.001512800	-0.000308636
7	6	-0.002071632	-0.000947951	0.000689229
8	1	0.000018941	0.000059393	-0.000215517
9	1	0.000107027	0.000081099	-0.000022646
10	1	0.000055139	-0.000172164	-0.000021945
11	1	-0.000541889	-0.000174707	-0.000035535
12	1	0.000284478	0.000033013	0.000035726
13	1	0.000529604	0.000293783	-0.000026656
14	35	0.001905207	-0.000683723	-0.000011794
15	1	0.000597599	0.001949642	-0.000544944
16	6	-0.000933194	0.000791551	0.000395732
17	6	-0.000285534	-0.000065599	-0.000010523
18	1	-0.000264930	-0.000070006	0.000126953
19	1	-0.000107422	-0.000011448	-0.000007047
20	1	-0.000016843	-0.000113735	-0.000024560
21	7	0.000218063	0.000088606	-0.000537231
22	1	-0.000033850	0.000001801	-0.000065949
23	1	0.000326727	0.000215763	0.000090775
24	6	0.000835502	0.000558218	0.000410481
25	6	0.000403500	0.000311331	0.000114492
26	8	-0.001018909	-0.000965993	-0.000388520
27	1	-0.000149049	-0.000012625	-0.000251577
28	1	-0.000192555	-0.000118906	0.000222607
29	1	-0.000275388	-0.000116184	-0.000362697
30	6	-0.000015364	-0.000008533	0.000012022
31	1	-0.000080198	-0.000031778	-0.000008423
32	1	0.000128844	-0.000030347	0.000113131
33	1	-0.000059917	-0.000001537	-0.000052182

Cartesian Forces: Max 0.003653364 RMS 0.000712389

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.006221746 RMS 0.000884202
Search for a local minimum.
Step number 10 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 6 7 8 9 10
DE= 2.43D-04 DEPred=-1.60D-04 R=-1.51D+00
Trust test=-1.51D+00 RLast= 3.29D-01 DXMaxT set to 2.19D-01
ITU= -1 1 1 1 -1 1 0 0 -1 0
Eigenvalues --- 0.00191 0.00246 0.00389 0.00523 0.00716
Eigenvalues --- 0.00723 0.01059 0.01148 0.01435 0.01521
Eigenvalues --- 0.01880 0.01980 0.02102 0.02191 0.02328
Eigenvalues --- 0.02352 0.02401 0.02468 0.02571 0.03070
Eigenvalues --- 0.03074 0.03114 0.03254 0.03507 0.04018
Eigenvalues --- 0.04058 0.04371 0.04999 0.05105 0.05432
Eigenvalues --- 0.05749 0.05871 0.05936 0.07812 0.08711
Eigenvalues --- 0.09521 0.10500 0.12135 0.12423 0.12511
Eigenvalues --- 0.12826 0.13102 0.15600 0.15858 0.15997
Eigenvalues --- 0.16000 0.16000 0.16002 0.16007 0.16026
Eigenvalues --- 0.16083 0.17212 0.17361 0.20382 0.22015
Eigenvalues --- 0.22206 0.22972 0.23643 0.25823 0.28387
Eigenvalues --- 0.29043 0.30473 0.31981 0.32105 0.33459
Eigenvalues --- 0.33793 0.34282 0.34303 0.34339 0.34541
Eigenvalues --- 0.34576 0.34670 0.34897 0.35058 0.35065
Eigenvalues --- 0.35277 0.35588 0.35885 0.36151 0.36429
Eigenvalues --- 0.36610 0.36765 0.38403 0.41817 0.42407
Eigenvalues --- 0.44298 0.45473 0.46016 0.49131 0.54885
Eigenvalues --- 0.56374 0.60533 0.96729
En-DIIS/RFO-DIIS IScMMF= 0 using points: 10 9 8 7 6
RFO step: Lambda=-2.83274762D-04.
EnCoef did 100 forward-backward iterations
DidBck=T Rises=T En-DIIS coefs: 0.51259 0.01646 0.00064 0.00658 0.46373
Iteration 1 RMS(Cart)= 0.07965536 RMS(Int)= 0.01300464
Iteration 2 RMS(Cart)= 0.04189335 RMS(Int)= 0.00280211
Iteration 3 RMS(Cart)= 0.00340811 RMS(Int)= 0.00028753

Iteration 4 RMS(Cart)= 0.00001836 RMS(Int)= 0.00028742
Iteration 5 RMS(Cart)= 0.00000000 RMS(Int)= 0.00028742

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56649	-0.00081	-0.00053	0.00029	-0.00022	2.56626
R2	2.62411	-0.00122	-0.00115	0.00037	-0.00080	2.62331
R3	2.03384	0.00008	0.00020	-0.00024	-0.00003	2.03380
R4	2.62460	0.00038	0.00213	-0.00282	-0.00066	2.62394
R5	2.03113	-0.00011	-0.00025	0.00042	0.00017	2.03130
R6	2.54442	0.00096	-0.00197	0.00459	0.00262	2.54704
R7	2.69984	0.00003	-0.00361	0.00371	0.00010	2.69994
R8	2.51864	0.00090	-0.00205	0.00663	0.00455	2.52318
R9	2.09970	0.00102	0.00517	-0.00521	-0.00004	2.09966
R10	2.78341	-0.00005	-0.00002	0.00513	0.00511	2.78852
R11	2.90544	-0.00084	-0.00339	0.00358	0.00019	2.90563
R12	2.05994	0.00015	0.00002	0.00084	0.00087	2.06081
R13	2.06009	0.00000	-0.00011	0.00050	0.00039	2.06048
R14	2.06915	-0.00012	0.00014	-0.00031	-0.00017	2.06898
R15	2.08002	-0.00021	-0.00010	-0.00024	-0.00034	2.07968
R16	2.74768	0.00020	0.00024	0.00373	0.00397	2.75165
R17	4.16808	0.00147	-0.04424	0.05836	0.01411	4.18219
R18	2.50589	0.00043	0.00063	-0.00111	-0.00048	2.50541
R19	2.05805	-0.00017	-0.00360	0.00373	0.00013	2.05818
R20	2.04350	0.00003	-0.00010	0.00000	-0.00010	2.04340
R21	2.04753	-0.00006	-0.00058	0.00071	0.00013	2.04766
R22	1.91387	-0.00006	0.00026	-0.00043	-0.00017	1.91370
R23	1.92684	0.00010	0.00209	-0.00420	-0.00208	1.92476
R24	3.91002	0.00015	-0.02322	0.02565	0.00242	3.91244
R25	2.76689	-0.00031	-0.00017	0.00116	0.00149	2.76837
R26	2.73220	-0.00030	-0.00011	-0.00108	-0.00140	2.73080
R27	2.05500	-0.00002	-0.00028	0.00081	0.00053	2.05553
R28	2.05180	0.00006	0.00005	0.00009	0.00013	2.05194
R29	2.74789	-0.00005	-0.00139	-0.00037	-0.00204	2.74586
R30	2.05560	0.00015	0.00007	0.00003	0.00010	2.05570
R31	2.84143	0.00003	0.00029	-0.00036	-0.00007	2.84136
R32	2.06720	-0.00001	0.00011	-0.00004	0.00007	2.06727
R33	2.06753	0.00006	0.00013	0.00002	0.00015	2.06768
R34	2.06498	-0.00003	0.00005	-0.00020	-0.00015	2.06482
A1	1.87171	-0.00006	-0.00031	0.00219	0.00185	1.87356
A2	2.27957	0.00011	-0.00088	0.00096	0.00011	2.27968
A3	2.13190	-0.00005	0.00116	-0.00314	-0.00196	2.12995
A4	1.86573	0.00032	-0.00216	0.00301	0.00086	1.86659
A5	2.27487	-0.00024	0.00120	-0.00182	-0.00062	2.27425
A6	2.14258	-0.00008	0.00094	-0.00118	-0.00024	2.14234

A7	1.89553	0.00003	0.00211	-0.00301	-0.00092	1.89461
A8	2.26005	-0.00256	-0.00070	-0.00300	-0.00369	2.25635
A9	2.12760	0.00254	-0.00141	0.00602	0.00462	2.13222
A10	1.89242	-0.00131	-0.00215	0.00239	0.00022	1.89264
A11	2.12539	0.00622	0.02601	-0.02063	0.00544	2.13083
A12	2.26492	-0.00491	-0.02363	0.01782	-0.00571	2.25921
A13	1.89935	0.00103	0.00252	-0.00459	-0.00202	1.89733
A14	2.22279	-0.00149	-0.00238	-0.00353	-0.00571	2.21708
A15	2.15697	0.00047	0.00124	0.00614	0.00754	2.16451
A16	1.96069	-0.00023	-0.00363	0.01033	0.00666	1.96736
A17	1.87078	0.00010	-0.00308	0.00560	0.00251	1.87329
A18	1.89628	-0.00034	-0.00170	-0.00375	-0.00544	1.89084
A19	1.91738	-0.00010	0.00166	-0.00112	0.00054	1.91792
A20	1.92993	0.00054	0.00278	-0.00757	-0.00476	1.92517
A21	1.88639	0.00003	0.00401	-0.00360	0.00043	1.88682
A22	1.90264	0.00068	0.00392	-0.00666	-0.00271	1.89992
A23	1.88764	0.00067	0.00401	-0.00593	-0.00192	1.88572
A24	1.89072	-0.00144	-0.00681	0.01152	0.00475	1.89546
A25	1.87188	-0.00017	0.00139	-0.00080	0.00063	1.87251
A26	1.91096	0.00034	-0.00219	-0.00046	-0.00268	1.90829
A27	1.99825	-0.00001	0.00007	0.00159	0.00163	1.99988
A28	2.15866	-0.00009	0.00649	-0.00839	-0.00189	2.15677
A29	1.94401	0.00030	0.00219	-0.00137	0.00082	1.94483
A30	2.18046	-0.00020	-0.00865	0.00963	0.00099	2.18144
A31	2.07363	0.00008	0.00204	-0.00203	0.00002	2.07365
A32	2.16368	0.00005	-0.00196	0.00195	-0.00001	2.16367
A33	2.04587	-0.00013	-0.00008	0.00007	-0.00001	2.04586
A34	1.94179	0.00001	-0.00137	0.00123	-0.00113	1.94066
A35	1.92306	-0.00060	0.00371	-0.00305	0.00037	1.92343
A36	1.88357	0.00035	-0.00186	0.00002	-0.00156	1.88200
A37	2.08262	0.00025	0.00155	-0.00105	0.00120	2.08382
A38	2.08036	-0.00029	-0.00502	0.00622	0.00053	2.08090
A39	1.99239	0.00012	0.00062	-0.00038	0.00005	1.99245
A40	2.01369	-0.00015	-0.00111	-0.00073	-0.00154	2.01215
A41	2.02773	0.00001	0.00293	-0.00318	-0.00026	2.02747
A42	2.02634	-0.00019	-0.00459	0.00656	0.00134	2.02768
A43	2.13406	0.00004	0.00200	-0.00235	0.00036	2.13442
A44	1.97732	-0.00011	-0.00131	-0.00183	-0.00290	1.97442
A45	2.02817	0.00004	0.00023	-0.00120	-0.00117	2.02700
A46	2.03282	0.00016	0.00226	-0.00142	0.00080	2.03362
A47	2.48582	0.00024	-0.02288	0.02691	0.00554	2.49136
A48	2.49250	-0.00003	-0.02171	0.02464	0.00448	2.49698
A49	1.93370	-0.00012	-0.00030	0.00031	0.00001	1.93371
A50	1.91422	0.00027	0.00218	-0.00235	-0.00017	1.91405

A51	1.94147	-0.00012	-0.00117	0.00150	0.00033	1.94180
A52	1.88169	-0.00008	-0.00005	-0.00031	-0.00036	1.88133
A53	1.89292	0.00010	-0.00020	0.00035	0.00015	1.89307
A54	1.89846	-0.00005	-0.00048	0.00049	0.00002	1.89848
A55	3.39926	-0.00477	-0.09803	0.04879	-0.04924	3.35002
A56	2.94557	-0.00045	0.07632	-0.08666	-0.01103	2.93455
A57	2.81802	0.00265	0.06909	0.28265	0.35175	3.16977
A58	3.23327	-0.00028	-0.03484	-0.04935	-0.08383	3.14944
D1	0.00778	-0.00002	-0.00157	0.00046	-0.00103	0.00675
D2	-3.13091	0.00006	0.00192	-0.00353	-0.00161	-3.13252
D3	-3.13717	-0.00020	-0.00543	0.00441	-0.00103	-3.13820
D4	0.00732	-0.00013	-0.00194	0.00042	-0.00160	0.00572
D5	-0.00873	-0.00008	0.00138	-0.00154	-0.00024	-0.00897
D6	-3.05533	-0.00027	-0.01947	0.02109	0.00146	-3.05388
D7	3.13587	0.00008	0.00485	-0.00509	-0.00024	3.13563
D8	0.08927	-0.00011	-0.01600	0.01754	0.00145	0.09072
D9	-0.00423	0.00011	0.00122	0.00081	0.00196	-0.00227
D10	-3.14081	-0.00004	0.00048	-0.00301	-0.00266	3.13971
D11	3.13473	0.00004	-0.00194	0.00443	0.00248	3.13721
D12	-0.00185	-0.00010	-0.00268	0.00061	-0.00214	-0.00399
D13	-0.00120	-0.00016	-0.00036	-0.00180	-0.00213	-0.00333
D14	3.11088	-0.00022	0.01200	-0.01512	-0.00363	3.10726
D15	3.13584	-0.00004	0.00032	0.00164	0.00207	3.13791
D16	-0.03526	-0.00010	0.01267	-0.01167	0.00057	-0.03469
D17	0.03095	0.00024	-0.01763	0.02805	0.01044	0.04139
D18	-3.09918	0.00018	-0.02428	0.04006	0.01584	-3.08334
D19	-3.10505	0.00009	-0.01846	0.02381	0.00528	-3.09977
D20	0.04801	0.00003	-0.02511	0.03582	0.01069	0.05870
D21	0.00611	0.00015	-0.00063	0.00207	0.00146	0.00757
D22	3.05707	0.00020	0.01913	-0.02013	-0.00102	3.05605
D23	-3.10285	-0.00004	-0.01444	0.01770	0.00285	-3.10000
D24	-0.05188	0.00001	0.00531	-0.00451	0.00036	-0.05152
D25	1.52394	0.00038	-0.03654	0.03128	-0.00522	1.51872
D26	-2.65149	0.00019	-0.03868	0.03985	0.00121	-2.65028
D27	-0.61696	0.00010	-0.03648	0.03667	0.00025	-0.61672
D28	-1.50968	0.00016	-0.06025	0.05764	-0.00266	-1.51234
D29	0.59808	-0.00003	-0.06239	0.06621	0.00377	0.60185
D30	2.63261	-0.00012	-0.06019	0.06303	0.00281	2.63541
D31	-1.16241	-0.00017	0.02445	-0.00208	0.02240	-1.14001
D32	0.86743	0.00037	0.03050	-0.00983	0.02065	0.88808
D33	3.04257	-0.00013	0.02881	-0.00438	0.02443	3.06699
D34	3.04008	-0.00008	0.02954	-0.01501	0.01453	3.05461
D35	-1.21327	0.00046	0.03558	-0.02277	0.01278	-1.20049
D36	0.96186	-0.00004	0.03389	-0.01732	0.01656	0.97842

D37	0.95939	-0.00038	0.02173	-0.00513	0.01662	0.97601
D38	2.98923	0.00015	0.02777	-0.01289	0.01487	3.00410
D39	-1.11882	-0.00035	0.02608	-0.00744	0.01864	-1.10018
D40	2.78675	0.00022	0.03215	-0.04304	-0.01066	2.77610
D41	-1.40808	0.00027	0.03137	-0.04423	-0.01309	-1.42118
D42	0.71380	0.00004	0.03262	-0.04149	-0.00863	0.70518
D43	2.80215	0.00010	0.03184	-0.04268	-0.01106	2.79109
D44	-1.38859	0.00002	0.03239	-0.04120	-0.00857	-1.39716
D45	0.69976	0.00007	0.03161	-0.04239	-0.01101	0.68875
D46	-3.13339	-0.00006	-0.00527	0.00973	0.00444	-3.12895
D47	0.00767	0.00001	-0.00420	0.00719	0.00297	0.01064
D48	-0.00482	0.00001	0.00227	-0.00400	-0.00171	-0.00653
D49	3.13624	0.00008	0.00334	-0.00654	-0.00317	3.13307
D50	1.24577	0.00014	-0.00950	-0.00395	-0.01365	1.23212
D51	-0.59080	0.00027	0.01584	-0.03842	-0.02354	-0.61434
D52	-2.96985	0.00003	0.01172	-0.00256	0.01011	-2.95974
D53	1.47676	0.00016	0.03707	-0.03704	0.00023	1.47699
D54	-2.69887	0.00002	0.00059	-0.00577	-0.00527	-2.70414
D55	-0.01637	0.00008	0.00028	0.00070	0.00100	-0.01537
D56	-0.02276	-0.00005	0.00008	-0.00190	-0.00185	-0.02460
D57	2.65974	0.00001	-0.00023	0.00457	0.00442	2.66416
D58	1.89701	-0.00029	0.04643	-0.06203	-0.01497	1.88204
D59	-0.51869	-0.00028	0.04221	-0.05547	-0.01274	-0.53143
D60	0.56158	0.00051	-0.04492	0.05768	0.01221	0.57379
D61	-1.86151	0.00034	-0.04732	0.06375	0.01588	-1.84563
D62	2.55128	-0.00001	0.00122	-0.00310	-0.00189	2.54938
D63	-1.65669	-0.00001	0.00236	-0.00479	-0.00244	-1.65913
D64	0.44427	0.00003	0.00245	-0.00476	-0.00232	0.44195
D65	1.34906	0.00002	0.00020	-0.00110	-0.00084	1.34822
D66	-2.85890	0.00002	0.00134	-0.00278	-0.00139	-2.86029
D67	-0.75795	0.00006	0.00144	-0.00275	-0.00126	-0.75921
D68	-1.05099	-0.00004	-0.00077	0.00533	0.00452	-1.04647
D69	1.02423	-0.00003	0.00037	0.00365	0.00397	1.02820
D70	3.12518	0.00000	0.00046	0.00368	0.00410	3.12928

Item	Value	Threshold	Converged?
Maximum Force	0.006222	0.000450	NO
RMS Force	0.000884	0.000300	NO
Maximum Displacement	0.633493	0.001800	NO
RMS Displacement	0.097590	0.001200	NO

Predicted change in Energy=-3.960116D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.885657	2.125923	-0.329860
2	6	0	-3.743778	1.135057	0.025103
3	7	0	-2.997721	-0.032277	0.118645
4	6	0	-1.714508	0.253926	-0.178189
5	7	0	-1.626301	1.556310	-0.458905
6	6	0	-0.356870	2.258409	-0.729191
7	6	0	0.329867	2.758353	0.552466
8	1	0	-3.058642	3.174004	-0.502778
9	1	0	-4.801783	1.165536	0.212573
10	1	0	0.296548	1.558733	-1.251460
11	1	0	-0.562823	3.094007	-1.398701
12	1	0	-0.300253	3.524516	1.015776
13	1	0	0.391365	1.915387	1.257287
14	35	0	0.347097	-2.332669	-0.220053
15	1	0	-0.914174	-0.515865	-0.140607
16	6	0	-3.422991	-1.352581	0.461087
17	6	0	-4.684226	-1.674401	0.713028
18	1	0	-2.581887	-2.043238	0.503091
19	1	0	-4.918537	-2.696574	0.976694
20	1	0	-5.507901	-0.971444	0.673661
21	7	0	1.614318	3.342807	0.193496
22	1	0	1.943313	3.974160	0.913696
23	1	0	2.313383	2.611279	0.076895
24	6	0	3.595928	-0.260219	-1.039779
25	6	0	3.593493	-0.463918	0.410949
26	8	0	3.396409	0.861534	-0.150896
27	1	0	4.542881	-0.241429	-1.574671
28	1	0	2.725187	-0.554474	-1.617937
29	1	0	2.685568	-0.887753	0.834520
30	6	0	4.859670	-0.669283	1.195413
31	1	0	4.775776	-0.224902	2.191515
32	1	0	5.045081	-1.740218	1.321608
33	1	0	5.717283	-0.221328	0.687738

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.358008	0.000000			
3	N	2.207157	1.388531	0.000000		
4	C	2.213361	2.221634	1.347834	0.000000	
5	N	1.388196	2.212561	2.176687	1.335211	0.000000

6	C	2.563548	3.647194	3.597244	2.482889	1.475619
7	C	3.393827	4.416762	4.364477	3.314436	2.508858
8	H	1.076243	2.214808	3.266514	3.230930	2.161125
9	H	2.210909	1.074918	2.167536	3.242683	3.269139
10	H	3.361172	4.258327	3.906496	2.626553	2.079783
11	H	2.734075	3.997897	4.243197	3.298802	2.092538
12	H	3.232818	4.306833	4.553235	3.757982	2.794086
13	H	3.647223	4.384815	4.071340	3.042326	2.673056
14	Br	5.508339	5.368471	4.073614	3.307936	4.367552
15	H	3.301758	3.280193	2.154586	1.111092	2.214125
16	C	3.607536	2.545845	1.428749	2.430730	3.540639
17	C	4.331851	3.041503	2.427790	3.651292	4.600199
18	H	4.262392	3.417605	2.089182	2.548225	3.846470
19	H	5.394086	4.119099	3.394740	4.506107	5.566577
20	H	4.180538	2.823137	2.736983	4.076396	4.768550
21	N	4.690893	5.797561	5.715566	4.556361	3.757500
22	H	5.318022	6.418186	6.410730	5.330292	4.524619
23	H	5.237464	6.234670	5.932786	4.673980	4.113532
24	C	6.943242	7.546659	6.698516	5.404389	5.559575
25	C	7.016798	7.519385	6.611797	5.388624	5.664293
26	O	6.410543	7.147592	6.461924	5.146981	5.079882
27	H	7.895383	8.551182	7.731219	6.430432	6.521933
28	H	6.350215	6.884882	6.003340	4.736801	4.973350
29	H	6.440230	6.788476	5.791726	4.657218	5.122363
30	C	8.374349	8.868178	7.956369	6.779301	7.053924
31	H	8.401265	8.895259	8.047431	6.925934	7.154301
32	H	8.976134	9.337675	8.309684	7.205418	7.651448
33	H	8.975281	9.580738	8.735612	7.497148	7.642187

		6	7	8	9	10
6	C	0.000000				
7	C	1.537595	0.000000			
8	H	2.861669	3.573276	0.000000		
9	H	4.673173	5.383904	2.753945	0.000000	
10	H	1.090535	2.166645	3.798279	5.318926	0.000000
11	H	1.090360	2.171776	2.652959	4.927879	1.765578
12	H	2.156651	1.094856	3.168213	5.145260	3.059548
13	H	2.150259	1.100521	4.072407	5.349999	2.535745
14	Br	4.672557	5.149329	6.480929	6.239837	4.026085
15	H	2.890262	3.570503	4.283112	4.250335	2.646469
16	C	4.884374	5.567052	4.642387	2.881620	5.024294
17	C	6.022707	6.694492	5.256209	2.886090	6.254637
18	H	4.997338	5.615695	5.334668	3.912616	4.933359
19	H	6.947712	7.581685	6.333382	3.938706	7.090092
20	H	6.239637	6.928608	4.956573	2.297365	6.618120

21	N	2.431636	1.456111	4.727563	6.775487	2.647138
22	H	3.306618	2.052287	5.259867	7.340045	3.637860
23	H	2.811501	2.045026	5.432433	7.261829	2.634389
24	C	4.697293	4.723789	7.507701	8.609455	3.773501
25	C	4.931161	4.588499	7.636772	8.554246	4.210056
26	O	4.046330	3.673734	6.865787	8.211874	3.362509
27	H	5.565212	5.592217	8.402220	9.617512	4.623461
28	H	4.266292	4.628502	6.971213	7.935016	3.240098
29	H	4.647575	4.350054	7.161158	7.788660	4.005499
30	C	6.283929	5.716746	8.964060	9.883127	5.636784
31	H	6.406357	5.599321	8.954880	9.878216	5.924434
32	H	7.026796	6.562161	9.651336	10.326378	6.328690
33	H	6.712088	6.158008	9.484855	10.620731	6.026067

		11	12	13	14	15
11	H	0.000000				
12	H	2.466572	0.000000			
13	H	3.058413	1.768038	0.000000		
14	Br	5.627254	6.021042	4.497830	0.000000	
15	H	3.838936	4.247210	3.093465	2.213118	0.000000
16	C	5.604598	5.817667	5.085554	3.954502	2.712249
17	C	6.647036	6.807321	6.240547	5.159280	4.035368
18	H	5.838213	6.038923	5.007969	3.030784	2.351273
19	H	7.625325	7.748034	7.038748	5.412164	4.694547
20	H	6.728772	6.888418	6.593615	6.077224	4.687527
21	N	2.708678	2.091588	2.159813	5.829914	4.625391
22	H	3.521728	2.290456	2.600989	6.603741	5.425598
23	H	3.268481	2.923455	2.360453	5.328891	4.499273
24	C	5.354892	5.807732	4.503221	3.939785	4.605962
25	C	5.762693	5.606664	4.078113	3.798616	4.541582
26	O	4.713435	4.702967	3.481935	4.416563	4.525313
27	H	6.101173	6.659482	5.468722	4.879844	5.649008
28	H	4.916349	5.720829	4.451275	3.281977	3.927969
29	H	5.603011	5.330674	3.646874	2.944207	3.747974
30	C	7.091912	6.651693	5.162373	5.013354	5.928385
31	H	7.239160	6.419233	4.967562	5.465487	6.156214
32	H	7.887864	7.508897	5.918163	4.979836	6.256982
33	H	7.401649	7.095752	5.766744	5.841297	6.689479

		16	17	18	19	20
16	C	0.000000				
17	C	1.325804	0.000000			
18	H	1.089141	2.144748	0.000000		
19	H	2.075771	1.081323	2.472059	0.000000	
20	H	2.130094	1.083576	3.120800	1.848040	0.000000
21	N	6.891499	8.069321	6.834725	8.931165	8.340823

22	H	7.574711	8.710384	7.540233	9.570143	8.946352
23	H	6.983249	8.230325	6.768297	9.015741	8.623486
24	C	7.260240	8.580979	6.612489	9.082847	9.290932
25	C	7.072714	8.371210	6.374799	8.818133	9.119319
26	O	7.195905	8.513167	6.678730	9.114270	9.128332
27	H	8.296631	9.613869	7.637141	10.102258	10.325024
28	H	6.539068	7.847741	5.905947	8.351480	8.556227
29	H	6.137590	7.412654	5.402876	7.817573	8.195475
30	C	8.343177	9.608794	7.598937	9.988547	10.385088
31	H	8.454929	9.683936	7.764814	10.077929	10.421862
32	H	8.520505	9.748545	7.676746	10.015351	10.600767
33	H	9.212802	10.502546	8.498805	10.923873	11.250228

		21	22	23	24	25
21	N	0.000000				
22	H	1.012686	0.000000			
23	H	1.018538	1.641534	0.000000		
24	C	4.292964	4.947441	3.337272	0.000000	
25	C	4.295996	4.761553	3.347703	1.464961	0.000000
26	O	3.074275	3.596288	2.070372	1.445078	1.453044
27	H	4.954760	5.542645	3.979482	1.087741	2.212131
28	H	4.438932	5.246810	3.614419	1.085838	2.208740
29	H	4.410910	4.918883	3.599408	2.176132	1.087831
30	C	5.256711	5.490543	4.300785	2.600088	1.503583
31	H	5.168698	5.223771	4.310327	3.440138	2.150660
32	H	6.235375	6.514712	5.286493	3.141112	2.136667
33	H	5.457257	5.647657	4.470272	2.736051	2.155446

		26	27	28	29	30
26	O	0.000000				
27	H	2.134961	0.000000			
28	H	2.146585	1.844961	0.000000		
29	H	2.129870	3.109911	2.475316	0.000000	
30	C	2.509399	2.820776	3.533290	2.214654	0.000000
31	H	2.927437	3.773416	4.338832	2.578716	1.093953
32	H	3.414015	3.299545	3.927954	2.555632	1.094168
33	H	2.694876	2.549141	3.792066	3.107566	1.092657

		31	32	33
31	H	0.000000		
32	H	1.767893	0.000000	
33	H	1.774203	1.777828	0.000000

Stoichiometry C10H18BrN3O

Framework group C1[X(C10H18BrN3O)]

Deg. of freedom 93

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.897872	2.147821	-0.283231
2	6	0	-3.747663	1.144985	0.057885
3	7	0	-2.993367	-0.018740	0.127177
4	6	0	-1.713502	0.281410	-0.170334
5	7	0	-1.635341	1.589160	-0.428151
6	6	0	-0.371922	2.304564	-0.691631
7	6	0	0.317424	2.786237	0.595611
8	1	0	-3.078686	3.197619	-0.436620
9	1	0	-4.804961	1.164935	0.250680
10	1	0	0.283727	1.618759	-1.229275
11	1	0	-0.586597	3.150545	-1.345172
12	1	0	-0.315649	3.539726	1.075387
13	1	0	0.387863	1.931280	1.284982
14	35	0	0.365183	-2.289975	-0.267748
15	1	0	-0.907856	-0.483478	-0.150142
16	6	0	-3.408170	-1.347794	0.447923
17	6	0	-4.666029	-1.682606	0.699813
18	1	0	-2.562267	-2.033365	0.473763
19	1	0	-4.892247	-2.710883	0.946250
20	1	0	-5.494574	-0.984667	0.676748
21	7	0	1.596237	3.385700	0.241294
22	1	0	1.924350	4.006336	0.971147
23	1	0	2.299639	2.661128	0.108473
24	6	0	3.596183	-0.181240	-1.065112
25	6	0	3.601887	-0.410774	0.381744
26	8	0	3.393298	0.923113	-0.155445
27	1	0	4.540480	-0.146493	-1.603885
28	1	0	2.724744	-0.471047	-1.644465
29	1	0	2.698811	-0.848244	0.801806
30	6	0	4.873061	-0.621488	1.156650
31	1	0	4.790840	-0.195510	2.160898
32	1	0	5.066236	-1.693219	1.262859
33	1	0	5.725272	-0.158746	0.653157

Rotational constants (GHZ): 0.4704799 0.2524722 0.1735773

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions
71 alpha electrons 71 beta electrons
nuclear repulsion energy 1296.0619349406 Hartrees.
NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 482 RedAO= T EigKep= 3.94D-06 NBF= 482
NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999786 0.005606 0.001482 -0.019880 Ang= 2.37 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3205.64611642 A.U. after 12 cycles
NFock= 12 Conv=0.84D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000593712	-0.000311148	-0.000174667
2	6	-0.001320365	0.000750939	-0.000111781
3	7	0.002228944	0.001814971	-0.001633949
4	6	-0.002799315	-0.002171635	0.004590348

5	7	0.000745426	-0.002489111	0.002041484
6	6	0.001997154	0.001201914	-0.001774701
7	6	-0.002283601	-0.000608627	0.001119355
8	1	-0.000134533	0.000051807	-0.000278551
9	1	0.000139979	0.000192450	-0.000242107
10	1	-0.000445354	-0.000425256	0.000286852
11	1	-0.000573749	-0.000325534	-0.000169372
12	1	0.000230928	0.000056974	0.000292368
13	1	0.000758294	0.000340817	0.000138625
14	35	-0.002114691	0.000827818	0.000873121
15	1	0.003019564	0.001239064	-0.003916653
16	6	0.002352641	0.002228650	0.000979116
17	6	-0.000092839	-0.001532574	0.000432282
18	1	-0.002075239	0.000283418	-0.001257007
19	1	-0.000294040	-0.000018099	-0.000094501
20	1	0.000475865	-0.000266554	-0.000263855
21	7	-0.001386273	-0.000505326	0.000146873
22	1	-0.000345850	0.000236813	0.000066537
23	1	0.000877451	-0.000826590	-0.001151460
24	6	0.000378783	0.000057124	-0.000259139
25	6	0.000536718	0.000794904	-0.000322085
26	8	-0.000775105	0.000617187	0.000480139
27	1	0.000133690	-0.000016884	0.000218603
28	1	-0.000160189	-0.000691430	0.000924585
29	1	0.000130921	-0.000280087	-0.001138772
30	6	-0.000005134	-0.000242819	0.000087729
31	1	0.000001463	0.000070916	0.000091156
32	1	0.000242967	-0.000046454	0.000067145
33	1	-0.000038225	-0.000007635	-0.000047716

Cartesian Forces: Max 0.004590348 RMS 0.001183250

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.006320774 RMS 0.001172322

Search for a local minimum.

Step number 11 out of a maximum of 172

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 2 3 1 4 5

6 7 8 10 11

DE= 6.90D-04 DEPred=-3.96D-04 R=-1.74D+00

Trust test=-1.74D+00 RLast= 3.98D-01 DXMaxT set to 1.10D-01

ITU= -1 -1 1 1 1 -1 1 0 0 -1 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.89542.

Iteration 1 RMS(Cart)= 0.07621021 RMS(Int)= 0.00276752

Iteration 2 RMS(Cart)= 0.00630514 RMS(Int)= 0.00004329

Iteration 3 RMS(Cart)= 0.00004934 RMS(Int)= 0.00002602

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00002602

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56626	-0.00125	-0.00013	0.00000	-0.00012	2.56614
R2	2.62331	-0.00003	-0.00041	0.00000	-0.00041	2.62290
R3	2.03380	0.00012	0.00017	0.00000	0.00017	2.03398
R4	2.62394	0.00018	0.00254	0.00000	0.00254	2.62649
R5	2.03130	-0.00017	-0.00023	0.00000	-0.00023	2.03107
R6	2.54704	-0.00209	-0.00322	0.00000	-0.00322	2.54381
R7	2.69994	-0.00079	-0.00408	0.00000	-0.00408	2.69586
R8	2.52318	-0.00173	-0.00442	0.00000	-0.00442	2.51876
R9	2.09966	-0.00087	0.00607	0.00000	0.00607	2.10573
R10	2.78852	-0.00067	-0.00216	0.00000	-0.00216	2.78636
R11	2.90563	-0.00064	-0.00323	0.00000	-0.00323	2.90241
R12	2.06081	-0.00013	-0.00040	0.00000	-0.00040	2.06041
R13	2.06048	-0.00004	-0.00030	0.00000	-0.00030	2.06018
R14	2.06898	0.00003	0.00028	0.00000	0.00028	2.06926
R15	2.07968	-0.00013	0.00030	0.00000	0.00030	2.07998
R16	2.75165	-0.00048	-0.00137	0.00000	-0.00137	2.75028
R17	4.18219	-0.00192	-0.05757	0.00000	-0.05757	4.12462
R18	2.50541	0.00037	0.00077	0.00000	0.00077	2.50618
R19	2.05818	-0.00183	-0.00358	0.00000	-0.00358	2.05460
R20	2.04340	0.00006	-0.00009	0.00000	-0.00009	2.04331
R21	2.04766	-0.00053	-0.00052	0.00000	-0.00052	2.04715
R22	1.91370	0.00008	0.00046	0.00000	0.00046	1.91416
R23	1.92476	0.00149	0.00323	0.00000	0.00323	1.92799
R24	3.91244	-0.00003	-0.02804	0.00000	-0.02804	3.88439
R25	2.76837	-0.00197	-0.00042	0.00000	-0.00036	2.76802
R26	2.73080	0.00078	0.00065	0.00000	0.00062	2.73142
R27	2.05553	0.00001	-0.00057	0.00000	-0.00057	2.05496
R28	2.05194	-0.00018	-0.00002	0.00000	-0.00002	2.05192
R29	2.74586	0.00058	-0.00063	0.00000	-0.00066	2.74519
R30	2.05570	-0.00044	-0.00002	0.00000	-0.00002	2.05568
R31	2.84136	0.00030	0.00022	0.00000	0.00022	2.84158

R32	2.06727	0.00011	0.00009	0.00000	0.00009	2.06736
R33	2.06768	0.00009	0.00001	0.00000	0.00001	2.06768
R34	2.06482	-0.00001	0.00011	0.00000	0.00011	2.06494
A1	1.87356	0.00027	-0.00103	0.00000	-0.00103	1.87253
A2	2.27968	-0.00020	-0.00127	0.00000	-0.00127	2.27841
A3	2.12995	-0.00007	0.00226	0.00000	0.00226	2.13221
A4	1.86659	-0.00145	-0.00265	0.00000	-0.00265	1.86394
A5	2.27425	0.00049	0.00181	0.00000	0.00181	2.27605
A6	2.14234	0.00096	0.00084	0.00000	0.00084	2.14318
A7	1.89461	0.00149	0.00232	0.00000	0.00232	1.89693
A8	2.25635	0.00044	0.00192	0.00000	0.00193	2.25828
A9	2.13222	-0.00193	-0.00425	0.00000	-0.00425	2.12797
A10	1.89264	-0.00073	-0.00170	0.00000	-0.00170	1.89095
A11	2.13083	0.00038	0.02182	0.00000	0.02183	2.15266
A12	2.25921	0.00039	-0.01973	0.00000	-0.01972	2.23950
A13	1.89733	0.00042	0.00302	0.00000	0.00302	1.90035
A14	2.21708	-0.00383	0.00184	0.00000	0.00185	2.21893
A15	2.16451	0.00345	-0.00320	0.00000	-0.00319	2.16132
A16	1.96736	-0.00110	-0.00606	0.00000	-0.00606	1.96130
A17	1.87329	0.00092	-0.00496	0.00000	-0.00495	1.86834
A18	1.89084	-0.00099	0.00174	0.00000	0.00174	1.89257
A19	1.91792	0.00066	0.00132	0.00000	0.00132	1.91925
A20	1.92517	0.00057	0.00433	0.00000	0.00433	1.92950
A21	1.88682	-0.00004	0.00373	0.00000	0.00373	1.89055
A22	1.89992	0.00034	0.00473	0.00000	0.00473	1.90465
A23	1.88572	0.00129	0.00415	0.00000	0.00415	1.88987
A24	1.89546	-0.00155	-0.00781	0.00000	-0.00781	1.88765
A25	1.87251	-0.00023	0.00046	0.00000	0.00046	1.87297
A26	1.90829	-0.00059	-0.00112	0.00000	-0.00112	1.90717
A27	1.99988	0.00079	0.00009	0.00000	0.00009	1.99997
A28	2.15677	0.00181	0.00741	0.00000	0.00741	2.16419
A29	1.94483	-0.00011	0.00202	0.00000	0.00202	1.94685
A30	2.18144	-0.00169	-0.00932	0.00000	-0.00932	2.17213
A31	2.07365	0.00049	0.00192	0.00000	0.00192	2.07558
A32	2.16367	-0.00042	-0.00203	0.00000	-0.00203	2.16164
A33	2.04586	-0.00007	0.00011	0.00000	0.00011	2.04597
A34	1.94066	-0.00226	-0.00038	0.00000	-0.00043	1.94023
A35	1.92343	0.00632	0.00379	0.00000	0.00378	1.92721
A36	1.88200	-0.00170	-0.00105	0.00000	-0.00103	1.88097
A37	2.08382	0.00029	0.00110	0.00000	0.00116	2.08499
A38	2.08090	-0.00117	-0.00494	0.00000	-0.00500	2.07590
A39	1.99245	-0.00061	0.00023	0.00000	0.00022	1.99266
A40	2.01215	0.00039	-0.00075	0.00000	-0.00072	2.01142
A41	2.02747	0.00058	0.00314	0.00000	0.00314	2.03061

A42	2.02768	-0.00115	-0.00466	0.00000	-0.00472	2.02296
A43	2.13442	0.00054	0.00217	0.00000	0.00223	2.13665
A44	1.97442	0.00021	-0.00041	0.00000	-0.00039	1.97403
A45	2.02700	-0.00077	0.00079	0.00000	0.00077	2.02777
A46	2.03362	0.00051	0.00146	0.00000	0.00146	2.03508
A47	2.49136	0.00015	-0.02974	0.00000	-0.02957	2.46179
A48	2.49698	0.00036	-0.02751	0.00000	-0.02733	2.46965
A49	1.93371	-0.00003	-0.00002	0.00000	-0.00002	1.93369
A50	1.91405	0.00036	0.00199	0.00000	0.00199	1.91604
A51	1.94180	-0.00016	-0.00142	0.00000	-0.00142	1.94038
A52	1.88133	-0.00009	0.00026	0.00000	0.00026	1.88159
A53	1.89307	0.00004	-0.00033	0.00000	-0.00033	1.89274
A54	1.89848	-0.00012	-0.00046	0.00000	-0.00046	1.89802
A55	3.35002	0.00446	-0.06338	0.00000	-0.06338	3.28664
A56	2.93455	0.00539	0.07222	0.00000	0.07219	3.00673
A57	3.16977	-0.00365	-0.20748	0.00000	-0.20748	2.96229
A58	3.14944	0.00088	0.07845	0.00000	0.07847	3.22792
D1	0.00675	-0.00018	0.00252	0.00000	0.00252	0.00927
D2	-3.13252	0.00034	0.00557	0.00000	0.00557	-3.12695
D3	-3.13820	-0.00057	-0.00430	0.00000	-0.00430	3.14069
D4	0.00572	-0.00006	-0.00124	0.00000	-0.00125	0.00447
D5	-0.00897	-0.00010	-0.00338	0.00000	-0.00338	-0.01235
D6	-3.05388	-0.00081	-0.02474	0.00000	-0.02475	-3.07862
D7	3.13563	0.00025	0.00275	0.00000	0.00275	3.13838
D8	0.09072	-0.00045	-0.01862	0.00000	-0.01862	0.07210
D9	-0.00227	0.00039	-0.00086	0.00000	-0.00087	-0.00314
D10	3.13971	0.00056	0.00262	0.00000	0.00261	-3.14086
D11	3.13721	-0.00008	-0.00363	0.00000	-0.00363	3.13358
D12	-0.00399	0.00010	-0.00015	0.00000	-0.00015	-0.00414
D13	-0.00333	-0.00045	-0.00123	0.00000	-0.00123	-0.00455
D14	3.10726	0.00063	0.01737	0.00000	0.01734	3.12459
D15	3.13791	-0.00061	-0.00440	0.00000	-0.00439	3.13351
D16	-0.03469	0.00047	0.01420	0.00000	0.01417	-0.02053
D17	0.04139	-0.00013	-0.03035	0.00000	-0.03035	0.01104
D18	-3.08334	-0.00090	-0.04097	0.00000	-0.04096	-3.12430
D19	-3.09977	0.00007	-0.02647	0.00000	-0.02647	-3.12624
D20	0.05870	-0.00071	-0.03708	0.00000	-0.03708	0.02161
D21	0.00757	0.00034	0.00283	0.00000	0.00284	0.01041
D22	3.05605	0.00053	0.02366	0.00000	0.02367	3.07972
D23	-3.10000	-0.00084	-0.01790	0.00000	-0.01793	-3.11793
D24	-0.05152	-0.00066	0.00292	0.00000	0.00290	-0.04862
D25	1.51872	-0.00041	-0.04346	0.00000	-0.04346	1.47526
D26	-2.65028	0.00036	-0.04883	0.00000	-0.04883	-2.69911
D27	-0.61672	0.00028	-0.04618	0.00000	-0.04618	-0.66289

D28	-1.51234	-0.00097	-0.06817	0.00000	-0.06817	-1.58051
D29	0.60185	-0.00020	-0.07354	0.00000	-0.07354	0.52831
D30	2.63541	-0.00028	-0.07089	0.00000	-0.07089	2.56452
D31	-1.14001	0.00093	0.01009	0.00000	0.01009	-1.12992
D32	0.88808	0.00153	0.01544	0.00000	0.01544	0.90352
D33	3.06699	0.00234	0.01325	0.00000	0.01325	3.08024
D34	3.05461	0.00003	0.01939	0.00000	0.01939	3.07400
D35	-1.20049	0.00063	0.02474	0.00000	0.02474	-1.17575
D36	0.97842	0.00144	0.02255	0.00000	0.02254	1.00097
D37	0.97601	-0.00068	0.01123	0.00000	0.01123	0.98724
D38	3.00410	-0.00008	0.01658	0.00000	0.01658	3.02068
D39	-1.10018	0.00073	0.01439	0.00000	0.01439	-1.08579
D40	2.77610	-0.00115	0.04141	0.00000	0.04143	2.81752
D41	-1.42118	-0.00059	0.04234	0.00000	0.04233	-1.37885
D42	0.70518	-0.00031	0.04090	0.00000	0.04091	0.74609
D43	2.79109	0.00025	0.04183	0.00000	0.04181	2.83290
D44	-1.39716	-0.00010	0.04107	0.00000	0.04109	-1.35608
D45	0.68875	0.00045	0.04200	0.00000	0.04199	0.73073
D46	-3.12895	-0.00057	-0.00829	0.00000	-0.00829	-3.13725
D47	0.01064	-0.00024	-0.00655	0.00000	-0.00655	0.00409
D48	-0.00653	0.00033	0.00382	0.00000	0.00382	-0.00271
D49	3.13307	0.00066	0.00556	0.00000	0.00556	3.13863
D50	1.23212	0.00007	-0.00176	0.00000	-0.00178	1.23034
D51	-0.61434	-0.00142	0.04588	0.00000	0.04583	-0.56851
D52	-2.95974	0.00118	-0.01554	0.00000	-0.01549	-2.97523
D53	1.47699	-0.00031	0.03211	0.00000	0.03212	1.50911
D54	-2.70414	0.00040	0.00163	0.00000	0.00162	-2.70252
D55	-0.01537	0.00025	-0.00062	0.00000	-0.00062	-0.01600
D56	-0.02460	-0.00017	0.00079	0.00000	0.00079	-0.02382
D57	2.66416	-0.00032	-0.00147	0.00000	-0.00146	2.66270
D58	1.88204	0.00006	0.06452	0.00000	0.06459	1.94662
D59	-0.53143	-0.00061	0.06000	0.00000	0.06005	-0.47138
D60	0.57379	0.00026	-0.06352	0.00000	-0.06357	0.51022
D61	-1.84563	0.00009	-0.06637	0.00000	-0.06642	-1.91205
D62	2.54938	0.00031	0.00173	0.00000	0.00173	2.55111
D63	-1.65913	0.00040	0.00329	0.00000	0.00329	-1.65584
D64	0.44195	0.00039	0.00312	0.00000	0.00311	0.44507
D65	1.34822	-0.00022	0.00014	0.00000	0.00015	1.34837
D66	-2.86029	-0.00013	0.00170	0.00000	0.00171	-2.85858
D67	-0.75921	-0.00014	0.00153	0.00000	0.00154	-0.75768
D68	-1.04647	-0.00025	-0.00201	0.00000	-0.00201	-1.04849
D69	1.02820	-0.00015	-0.00045	0.00000	-0.00045	1.02775
D70	3.12928	-0.00017	-0.00063	0.00000	-0.00063	3.12865

Item	Value	Threshold	Converged?

Maximum Force	0.006321	0.000450	NO
RMS Force	0.001172	0.000300	NO
Maximum Displacement	0.293637	0.001800	NO
RMS Displacement	0.076928	0.001200	NO

Predicted change in Energy=-4.802810D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.893635	2.144460	-0.244677
2	6	0	-3.768619	1.160018	0.085901
3	7	0	-3.047103	-0.027695	0.108473
4	6	0	-1.765970	0.239904	-0.206410
5	7	0	-1.654035	1.548788	-0.431884
6	6	0	-0.377798	2.224286	-0.730221
7	6	0	0.328841	2.725484	0.538010
8	1	0	-3.045580	3.202681	-0.369488
9	1	0	-4.821387	1.205739	0.297504
10	1	0	0.253534	1.500985	-1.246996
11	1	0	-0.576961	3.052845	-1.410194
12	1	0	-0.285245	3.500486	1.008437
13	1	0	0.399256	1.887444	1.248098
14	35	0	0.286469	-2.314390	-0.064667
15	1	0	-0.969368	-0.538321	-0.244755
16	6	0	-3.492129	-1.351950	0.397354
17	6	0	-4.746055	-1.664417	0.695476
18	1	0	-2.674948	-2.067429	0.348270
19	1	0	-4.992246	-2.696295	0.904686
20	1	0	-5.552547	-0.942793	0.744223
21	7	0	1.608812	3.297821	0.147816
22	1	0	1.975330	3.902618	0.873015
23	1	0	2.293332	2.559549	-0.017399
24	6	0	3.698186	-0.250145	-1.050652
25	6	0	3.657503	-0.435906	0.401724
26	8	0	3.469001	0.881379	-0.180979
27	1	0	4.658330	-0.232307	-1.560875
28	1	0	2.842849	-0.558918	-1.644017
29	1	0	2.739398	-0.861438	0.800917
30	6	0	4.901204	-0.625263	1.225418
31	1	0	4.785517	-0.170377	2.213612
32	1	0	5.091338	-1.693201	1.368833

33 1 0 5.769843 -0.176275 0.737662

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357942	0.000000			
3	N	2.206020	1.389877	0.000000		
4	C	2.213691	2.223209	1.346128	0.000000	
5	N	1.387977	2.211495	2.172078	1.332872	0.000000
6	C	2.563505	3.646422	3.591658	2.477735	1.474477
7	C	3.366681	4.409565	4.377384	3.334742	2.501421
8	H	1.076334	2.214190	3.265544	3.231415	2.162326
9	H	2.211648	1.074796	2.169142	3.243816	3.268304
10	H	3.365023	4.250952	3.881799	2.598374	2.074973
11	H	2.747829	4.000971	4.230564	3.282602	2.092693
12	H	3.195748	4.296832	4.570105	3.781508	2.785182
13	H	3.624578	4.387600	4.104131	3.085156	2.674515
14	Br	5.479672	5.342090	4.046189	3.279788	4.338726
15	H	3.301532	3.290820	2.168522	1.114306	2.204497
16	C	3.604897	2.546259	1.426588	2.424490	3.532776
17	C	4.338536	3.050310	2.431023	3.649759	4.599589
18	H	4.259040	3.417802	2.087227	2.541200	3.837699
19	H	5.399825	4.127810	3.396905	4.501628	5.563344
20	H	4.192716	2.835066	2.742049	4.079294	4.773846
21	N	4.664367	5.787123	5.721725	4.567876	3.747177
22	H	5.295958	6.413607	6.423138	5.345836	4.518358
23	H	5.208510	6.222267	5.935479	4.679147	4.095746
24	C	7.059450	7.683326	6.847772	5.550666	5.680255
25	C	7.070610	7.602237	6.723419	5.499146	5.731173
26	O	6.487107	7.247897	6.585575	5.274188	5.172415
27	H	8.025806	8.698501	7.886842	6.582491	6.655288
28	H	6.494124	7.046905	6.168058	4.893469	5.112108
29	H	6.469911	6.852140	5.887121	4.746157	5.160546
30	C	8.401908	8.924772	8.048616	6.873853	7.102415
31	H	8.388745	8.914615	8.111837	6.996201	7.170914
32	H	9.005046	9.396042	8.402180	7.296640	7.697605
33	H	9.022563	9.653638	8.840615	7.606113	7.710878

		6	7	8	9	10
6	C	0.000000				
7	C	1.535887	0.000000			
8	H	2.864340	3.526753	0.000000		
9	H	4.673237	5.375158	2.754297	0.000000	
10	H	1.090321	2.165944	3.814439	5.312954	0.000000
11	H	1.090201	2.173278	2.683206	4.933881	1.767661

12	H	2.158747	1.095003	3.099486	5.133019	3.061906
13	H	2.151981	1.100679	4.026577	5.350090	2.529047
14	Br	4.635061	5.075958	6.452405	6.213909	3.994505
15	H	2.866640	3.598679	4.280339	4.263078	2.580455
16	C	4.874417	5.589728	4.640271	2.884210	4.987296
17	C	6.019659	6.711974	5.264447	2.898594	6.228071
18	H	4.985866	5.659573	5.331661	3.914512	4.884103
19	H	6.941049	7.605531	6.341210	3.952686	7.054439
20	H	6.243589	6.934660	4.970935	2.313080	6.606632
21	N	2.422818	1.455385	4.684017	6.763629	2.647810
22	H	3.305204	2.051535	5.219507	7.334830	3.636876
23	H	2.784861	2.048227	5.389022	7.249220	2.606385
24	C	4.779030	4.767672	7.606863	8.747586	3.869190
25	C	4.964028	4.592706	7.665859	8.636981	4.249333
26	O	4.111317	3.711909	6.918362	8.310517	3.443767
27	H	5.664576	5.647859	8.518730	9.766606	4.743948
28	H	4.353597	4.676406	7.102650	8.100866	3.332472
29	H	4.645749	4.329655	7.166092	7.854433	3.994309
30	C	6.309700	5.710213	8.963718	9.936919	5.677552
31	H	6.407838	5.572757	8.909321	9.892309	5.942065
32	H	7.047281	6.549536	9.654058	10.383338	6.360010
33	H	6.760981	6.169649	9.505514	10.690082	6.097682

		11	12	13	14	15
11	H	0.000000				
12	H	2.476945	0.000000			
13	H	3.062299	1.768582	0.000000		
14	Br	5.600282	5.940639	4.403576	0.000000	
15	H	3.795879	4.283745	3.160075	2.182654	0.000000
16	C	5.582799	5.848390	5.134230	3.926520	2.727383
17	C	6.638354	6.831764	6.276570	5.130944	4.051604
18	H	5.806113	6.094931	5.089346	3.000250	2.366190
19	H	7.609600	7.782462	7.084976	5.380551	4.707612
20	H	6.735212	6.896159	6.609697	6.052247	4.706082
21	N	2.695369	2.090261	2.159354	5.769805	4.638653
22	H	3.528363	2.300053	2.585657	6.510198	5.444501
23	H	3.228281	2.930317	2.375022	5.271149	4.504853
24	C	5.414416	5.845922	4.553732	4.107687	4.745375
25	C	5.777985	5.604332	4.090290	3.887171	4.672939
26	O	4.753529	4.729566	3.532388	4.511649	4.660336
27	H	6.182491	6.706268	5.524797	5.068222	5.787642
28	H	4.979418	5.770549	4.507789	3.480102	4.060955
29	H	5.586489	5.312053	3.637663	2.979457	3.866882
30	C	7.105295	6.630847	5.155749	5.080674	6.052485
31	H	7.230305	6.374975	4.940257	5.479853	6.268784

32	H	7.897946	7.484110	5.903493	5.052481	6.377270
33	H	7.437904	7.089145	5.776044	5.939921	6.820057

		16	17	18	19	20
16	C	0.000000				
17	C	1.326214	0.000000			
18	H	1.087246	2.138330	0.000000		
19	H	2.077258	1.081273	2.464739	0.000000	
20	H	2.129096	1.083303	3.114829	1.847824	0.000000
21	N	6.906680	8.081341	6.868529	8.948533	8.344074
22	H	7.598015	8.729284	7.585638	9.596549	8.953408
23	H	6.995956	8.240331	6.799004	9.030713	8.625792
24	C	7.416962	8.738097	6.773208	9.237457	9.448672
25	C	7.208078	8.497960	6.539470	8.954356	9.230344
26	O	7.333454	8.645021	6.835472	9.250465	9.250509
27	H	8.456846	9.776734	7.796761	10.260791	10.491915
28	H	6.702838	8.017906	6.057301	8.511931	8.736917
29	H	6.263816	7.529137	5.565469	7.947061	8.292538
30	C	8.465329	9.717525	7.761914	10.112981	10.469636
31	H	8.556538	9.766666	7.920660	10.183232	10.470497
32	H	8.645006	9.860453	7.841989	10.143978	10.688570
33	H	9.342491	10.620756	8.662712	11.054454	11.348308

		21	22	23	24	25
21	N	0.000000				
22	H	1.012931	0.000000			
23	H	1.020249	1.642496	0.000000		
24	C	4.288342	4.890211	3.306903	0.000000	
25	C	4.266418	4.677030	3.318038	1.464773	0.000000
26	O	3.067181	3.531266	2.055532	1.445407	1.452692
27	H	4.967996	5.497264	3.971145	1.087438	2.212443
28	H	4.428086	5.195511	3.559873	1.085830	2.205414
29	H	4.359381	4.825477	3.545669	2.172846	1.087818
30	C	5.233704	5.402465	4.299839	2.601626	1.503702
31	H	5.136864	5.126757	4.317510	3.441522	2.150781
32	H	6.207187	6.424059	5.276018	3.142799	2.138217
33	H	5.452655	5.572613	4.487870	2.737751	2.154586

		26	27	28	29	30
26	O	0.000000				
27	H	2.135161	0.000000			
28	H	2.146392	1.846499	0.000000		
29	H	2.129284	3.107437	2.465750	0.000000	
30	C	2.509806	2.824328	3.531981	2.215713	0.000000
31	H	2.928049	3.777137	4.336615	2.580674	1.093998
32	H	3.415019	3.302256	3.926776	2.558511	1.094171
33	H	2.693772	2.553795	3.792902	3.107579	1.092717

		31	32	33
31	H	0.000000		
32	H	1.768099	0.000000	
33	H	1.774080	1.777586	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.864100	2.199546	-0.183318
2	6	0	-3.742918	1.206718	0.109901
3	7	0	-3.027543	0.015448	0.080359
4	6	0	-1.746276	0.289348	-0.228498
5	7	0	-1.628379	1.605855	-0.400127
6	6	0	-0.349808	2.286641	-0.675568
7	6	0	0.364424	2.731365	0.609361
8	1	0	-3.010994	3.262780	-0.263641
9	1	0	-4.794592	1.248979	0.327574
10	1	0	0.275694	1.582147	-1.224417
11	1	0	-0.547304	3.143616	-1.319872
12	1	0	-0.243743	3.489346	1.113968
13	1	0	0.433243	1.864324	1.283896
14	35	0	0.293310	-2.278987	-0.200985
15	1	0	-0.953914	-0.490649	-0.302284
16	6	0	-3.478354	-1.317352	0.316086
17	6	0	-4.732717	-1.635526	0.606229
18	1	0	-2.665128	-2.034319	0.234077
19	1	0	-4.983480	-2.673914	0.773617
20	1	0	-5.535223	-0.912460	0.688110
21	7	0	1.645829	3.312861	0.237862
22	1	0	2.018354	3.885278	0.985920
23	1	0	2.325821	2.578597	0.039431
24	6	0	3.711881	-0.193034	-1.114914
25	6	0	3.675935	-0.438504	0.328696
26	8	0	3.492040	0.902694	-0.198262
27	1	0	4.670091	-0.158971	-1.627938
28	1	0	2.852613	-0.472661	-1.716989
29	1	0	2.757193	-0.875528	0.713755

30	6	0	4.921857	-0.668069	1.138696
31	1	0	4.812438	-0.253867	2.145323
32	1	0	5.106962	-1.741975	1.237047
33	1	0	5.790909	-0.203696	0.666324

Rotational constants (GHZ): 0.4792170 0.2467657 0.1713528

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1293.0551800220 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 3.84D-06 NBF= 482

NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482

Lowest energy guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999999 0.000172 -0.000018 -0.001168 Ang= 0.14 deg.

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999974 -0.001379 0.000289 0.007122 Ang= -0.83 deg.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3205.64681680 A.U. after 9 cycles

NFock= 9 Conv=0.88D-08 -V/T= 2.0018

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000136989	-0.000071462	-0.000458881
2	6	-0.000079897	0.000217773	0.000397395
3	7	0.000822460	0.000659401	-0.000548665
4	6	-0.001127963	-0.001847140	-0.000291320
5	7	0.000241683	-0.000443000	0.000901509

6	6	0.000680597	0.000909018	-0.000087726
7	6	-0.000929979	-0.000407590	0.000525725
8	1	-0.000001705	0.000044973	-0.000140450
9	1	0.000103383	0.000120212	0.000033025
10	1	-0.000105404	-0.000101662	0.000051651
11	1	-0.000243586	-0.000046446	-0.000050012
12	1	0.000099651	0.000015182	0.000049327
13	1	0.000324638	0.000125802	-0.000141382
14	35	-0.000457470	0.000139396	0.000014207
15	1	0.000647883	0.000951084	-0.000054278
16	6	0.000506216	0.000231353	0.000072049
17	6	-0.000051209	-0.000340895	0.000009890
18	1	-0.000391378	0.000240430	0.000122715
19	1	-0.000095129	0.000010400	0.000002103
20	1	0.000152800	-0.000106964	-0.000029887
21	7	-0.000090708	-0.000156674	-0.000307080
22	1	-0.000087155	0.000030052	-0.000077870
23	1	0.000164942	0.000084716	0.000171008
24	6	0.000340868	0.000212203	0.000394458
25	6	0.000210172	0.000235133	-0.000042216
26	8	-0.000704757	-0.000148627	-0.000229923
27	1	-0.000017781	-0.000035706	-0.000082577
28	1	-0.000071736	-0.000253039	0.000253391
29	1	-0.000059679	-0.000215318	-0.000412195
30	6	0.000066727	-0.000017128	-0.000079441
31	1	-0.000058703	-0.000002917	-0.000005802
32	1	0.000077688	-0.000024196	0.000053543
33	1	-0.000002458	-0.000008363	-0.000012290

Cartesian Forces: Max 0.001847140 RMS 0.000381798

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.001090201 RMS 0.000245517
Search for a local minimum.
Step number 12 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Update second derivatives using D2CorX and points 2 3 1 4 5
6 7 8 10 11
9 12

ITU= 0 -1 -1 1 1 1 -1 1 0 0 -1 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00225	0.00333	0.00397	0.00665	0.00723
Eigenvalues ---	0.00909	0.01108	0.01259	0.01458	0.01644
Eigenvalues ---	0.01886	0.02009	0.02108	0.02184	0.02347
Eigenvalues ---	0.02386	0.02421	0.02476	0.02950	0.03071
Eigenvalues ---	0.03076	0.03121	0.03335	0.03539	0.04003
Eigenvalues ---	0.04102	0.04365	0.04882	0.05243	0.05425
Eigenvalues ---	0.05755	0.05837	0.05923	0.07896	0.08720
Eigenvalues ---	0.09507	0.10731	0.12136	0.12422	0.12575
Eigenvalues ---	0.12795	0.13134	0.15579	0.15929	0.16000
Eigenvalues ---	0.16000	0.16002	0.16003	0.16008	0.16025
Eigenvalues ---	0.16082	0.17069	0.17456	0.21300	0.22139
Eigenvalues ---	0.23039	0.23094	0.24797	0.26061	0.27416
Eigenvalues ---	0.29086	0.30169	0.31823	0.32074	0.33005
Eigenvalues ---	0.33683	0.34282	0.34312	0.34341	0.34542
Eigenvalues ---	0.34658	0.34729	0.35053	0.35066	0.35276
Eigenvalues ---	0.35440	0.35585	0.35865	0.35913	0.36424
Eigenvalues ---	0.36626	0.38096	0.38815	0.41884	0.42481
Eigenvalues ---	0.44873	0.45471	0.46041	0.49358	0.55626
Eigenvalues ---	0.59271	0.60878	0.98028		

RFO step: Lambda=-1.05213909D-04 EMin= 2.24578765D-03

Quartic linear search produced a step of 0.06074.

Iteration 1 RMS(Cart)= 0.02916008 RMS(Int)= 0.00031663

Iteration 2 RMS(Cart)= 0.00050034 RMS(Int)= 0.00002519

Iteration 3 RMS(Cart)= 0.00000013 RMS(Int)= 0.00002519

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56614	-0.00030	0.00000	-0.00033	-0.00033	2.56581
R2	2.62290	-0.00030	0.00000	-0.00041	-0.00041	2.62249
R3	2.03398	0.00006	0.00000	0.00007	0.00007	2.03404
R4	2.62649	0.00018	-0.00002	-0.00025	-0.00027	2.62622
R5	2.03107	-0.00009	0.00000	-0.00015	-0.00014	2.03093
R6	2.54381	-0.00087	0.00002	-0.00019	-0.00017	2.54364
R7	2.69586	-0.00004	0.00003	0.00100	0.00103	2.69689
R8	2.51876	-0.00009	0.00003	0.00020	0.00023	2.51899
R9	2.10573	-0.00063	-0.00004	-0.00235	-0.00239	2.10334
R10	2.78636	-0.00026	0.00002	-0.00074	-0.00073	2.78563
R11	2.90241	-0.00045	0.00002	-0.00034	-0.00032	2.90209
R12	2.06041	-0.00002	0.00000	-0.00005	-0.00005	2.06036
R13	2.06018	0.00004	0.00000	0.00002	0.00002	2.06020
R14	2.06926	-0.00002	0.00000	-0.00012	-0.00012	2.06914
R15	2.07998	-0.00017	0.00000	-0.00039	-0.00039	2.07959
R16	2.75028	-0.00023	0.00001	-0.00058	-0.00057	2.74970

R17	4.12462	-0.00037	0.00041	0.01212	0.01253	4.13715
R18	2.50618	0.00009	-0.00001	0.00004	0.00004	2.50622
R19	2.05460	-0.00046	0.00003	-0.00001	0.00001	2.05461
R20	2.04331	0.00001	0.00000	0.00008	0.00008	2.04339
R21	2.04715	-0.00018	0.00000	-0.00022	-0.00022	2.04693
R22	1.91416	-0.00007	0.00000	-0.00017	-0.00017	1.91399
R23	1.92799	0.00008	-0.00002	-0.00033	-0.00035	1.92764
R24	3.88439	0.00010	0.00020	0.00875	0.00895	3.89334
R25	2.76802	-0.00074	0.00001	-0.00088	-0.00095	2.76707
R26	2.73142	0.00012	-0.00001	-0.00005	-0.00003	2.73140
R27	2.05496	0.00002	0.00000	0.00008	0.00009	2.05505
R28	2.05192	-0.00001	0.00000	-0.00002	-0.00002	2.05190
R29	2.74519	0.00026	0.00000	0.00061	0.00066	2.74585
R30	2.05568	-0.00002	0.00000	0.00005	0.00005	2.05573
R31	2.84158	0.00006	0.00000	0.00008	0.00008	2.84167
R32	2.06736	0.00000	0.00000	-0.00003	-0.00003	2.06733
R33	2.06768	0.00004	0.00000	0.00007	0.00007	2.06775
R34	2.06494	0.00000	0.00000	-0.00001	-0.00001	2.06493
A1	1.87253	-0.00010	0.00001	-0.00033	-0.00033	1.87220
A2	2.27841	0.00009	0.00001	0.00069	0.00070	2.27911
A3	2.13221	0.00001	-0.00002	-0.00033	-0.00035	2.13186
A4	1.86394	-0.00022	0.00002	0.00019	0.00020	1.86414
A5	2.27605	-0.00001	-0.00001	-0.00064	-0.00065	2.27540
A6	2.14318	0.00023	-0.00001	0.00044	0.00044	2.14362
A7	1.89693	0.00031	-0.00002	0.00028	0.00026	1.89719
A8	2.25828	0.00023	-0.00001	-0.00054	-0.00055	2.25773
A9	2.12797	-0.00054	0.00003	0.00026	0.00029	2.12826
A10	1.89095	-0.00023	0.00001	-0.00065	-0.00064	1.89030
A11	2.15266	0.00046	-0.00015	-0.00046	-0.00063	2.15204
A12	2.23950	-0.00023	0.00014	0.00101	0.00114	2.24064
A13	1.90035	0.00024	-0.00002	0.00059	0.00057	1.90092
A14	2.21893	-0.00079	-0.00001	-0.00146	-0.00147	2.21746
A15	2.16132	0.00055	0.00002	0.00082	0.00084	2.16217
A16	1.96130	-0.00030	0.00004	-0.00057	-0.00053	1.96077
A17	1.86834	0.00008	0.00004	0.00053	0.00057	1.86890
A18	1.89257	-0.00013	-0.00001	-0.00065	-0.00067	1.89191
A19	1.91925	0.00005	-0.00001	-0.00060	-0.00061	1.91863
A20	1.92950	0.00030	-0.00003	0.00148	0.00145	1.93096
A21	1.89055	-0.00001	-0.00003	-0.00022	-0.00025	1.89031
A22	1.90465	0.00031	-0.00003	0.00123	0.00119	1.90584
A23	1.88987	0.00046	-0.00003	0.00057	0.00054	1.89041
A24	1.88765	-0.00096	0.00006	-0.00237	-0.00231	1.88534
A25	1.87297	-0.00009	0.00000	0.00099	0.00099	1.87396
A26	1.90717	0.00022	0.00001	0.00155	0.00156	1.90872

A27	1.99997	0.00009	0.00000	-0.00180	-0.00180	1.99816
A28	2.16419	0.00046	-0.00005	-0.00029	-0.00034	2.16384
A29	1.94685	-0.00013	-0.00001	-0.00060	-0.00062	1.94623
A30	2.17213	-0.00033	0.00007	0.00090	0.00096	2.17309
A31	2.07558	0.00015	-0.00001	0.00012	0.00011	2.07568
A32	2.16164	-0.00010	0.00001	0.00015	0.00016	2.16181
A33	2.04597	-0.00005	0.00000	-0.00027	-0.00027	2.04570
A34	1.94023	-0.00010	0.00000	0.00052	0.00052	1.94075
A35	1.92721	0.00018	-0.00003	-0.00116	-0.00119	1.92602
A36	1.88097	-0.00002	0.00001	0.00137	0.00138	1.88234
A37	2.08499	0.00008	0.00000	-0.00013	-0.00020	2.08479
A38	2.07590	-0.00029	0.00003	-0.00076	-0.00067	2.07523
A39	1.99266	-0.00011	0.00000	0.00045	0.00045	1.99312
A40	2.01142	0.00006	0.00001	0.00141	0.00139	2.01281
A41	2.03061	0.00010	-0.00002	-0.00038	-0.00040	2.03021
A42	2.02296	-0.00023	0.00003	-0.00107	-0.00099	2.02197
A43	2.13665	0.00000	-0.00001	-0.00058	-0.00065	2.13600
A44	1.97403	0.00005	0.00000	0.00144	0.00142	1.97545
A45	2.02777	-0.00021	-0.00001	-0.00010	-0.00009	2.02768
A46	2.03508	0.00020	-0.00001	0.00058	0.00057	2.03565
A47	2.46179	0.00028	0.00022	0.01150	0.01154	2.47333
A48	2.46965	0.00020	0.00021	0.00962	0.00963	2.47928
A49	1.93369	-0.00011	0.00000	-0.00046	-0.00046	1.93322
A50	1.91604	0.00015	-0.00001	0.00028	0.00027	1.91631
A51	1.94038	-0.00001	0.00001	0.00015	0.00016	1.94054
A52	1.88159	-0.00003	0.00000	-0.00016	-0.00016	1.88143
A53	1.89274	0.00004	0.00000	0.00015	0.00015	1.89289
A54	1.89802	-0.00005	0.00000	0.00004	0.00004	1.89805
A55	3.28664	0.00109	0.00045	0.03332	0.03377	3.32041
A56	3.00673	0.00045	-0.00051	-0.01107	-0.01157	2.99516
A57	2.96229	-0.00048	0.00147	-0.01648	-0.01501	2.94728
A58	3.22792	-0.00010	-0.00056	-0.01820	-0.01876	3.20916
D1	0.00927	-0.00019	-0.00002	-0.00540	-0.00541	0.00386
D2	-3.12695	-0.00015	-0.00004	-0.00330	-0.00334	-3.13029
D3	3.14069	-0.00005	0.00003	-0.00195	-0.00192	3.13877
D4	0.00447	-0.00001	0.00001	0.00014	0.00015	0.00462
D5	-0.01235	0.00027	0.00002	0.00632	0.00635	-0.00601
D6	-3.07862	0.00015	0.00018	0.00700	0.00718	-3.07145
D7	3.13838	0.00014	-0.00002	0.00322	0.00321	3.14158
D8	0.07210	0.00002	0.00013	0.00390	0.00404	0.07614
D9	-0.00314	0.00005	0.00001	0.00268	0.00269	-0.00045
D10	-3.14086	-0.00004	-0.00002	0.00044	0.00042	-3.14044
D11	3.13358	0.00001	0.00003	0.00078	0.00081	3.13439
D12	-0.00414	-0.00008	0.00000	-0.00146	-0.00146	-0.00560

D13	-0.00455	0.00012	0.00001	0.00125	0.00126	-0.00330
D14	3.12459	-0.00012	-0.00013	-0.00634	-0.00646	3.11813
D15	3.13351	0.00020	0.00003	0.00329	0.00332	3.13683
D16	-0.02053	-0.00005	-0.00010	-0.00430	-0.00439	-0.02492
D17	0.01104	0.00014	0.00022	0.01199	0.01220	0.02324
D18	-3.12430	0.00013	0.00029	0.01183	0.01212	-3.11218
D19	-3.12624	0.00004	0.00019	0.00948	0.00967	-3.11657
D20	0.02161	0.00004	0.00026	0.00933	0.00959	0.03120
D21	0.01041	-0.00024	-0.00002	-0.00465	-0.00467	0.00574
D22	3.07972	-0.00019	-0.00017	-0.00542	-0.00559	3.07413
D23	-3.11793	0.00001	0.00013	0.00344	0.00357	-3.11436
D24	-0.04862	0.00006	-0.00002	0.00267	0.00265	-0.04597
D25	1.47526	0.00017	0.00031	0.02525	0.02556	1.50082
D26	-2.69911	0.00011	0.00035	0.02451	0.02486	-2.67425
D27	-0.66289	0.00008	0.00033	0.02420	0.02453	-0.63836
D28	-1.58051	0.00006	0.00048	0.02606	0.02654	-1.55397
D29	0.52831	-0.00001	0.00052	0.02532	0.02584	0.55415
D30	2.56452	-0.00004	0.00050	0.02501	0.02551	2.59003
D31	-1.12992	-0.00007	-0.00007	-0.00312	-0.00319	-1.13310
D32	0.90352	0.00025	-0.00011	-0.00096	-0.00107	0.90246
D33	3.08024	0.00005	-0.00009	-0.00430	-0.00439	3.07585
D34	3.07400	-0.00001	-0.00014	-0.00301	-0.00315	3.07085
D35	-1.17575	0.00031	-0.00018	-0.00085	-0.00103	-1.17678
D36	1.00097	0.00011	-0.00016	-0.00420	-0.00436	0.99661
D37	0.98724	-0.00023	-0.00008	-0.00329	-0.00337	0.98387
D38	3.02068	0.00009	-0.00012	-0.00113	-0.00125	3.01943
D39	-1.08579	-0.00011	-0.00010	-0.00447	-0.00458	-1.09036
D40	2.81752	-0.00006	-0.00029	-0.00817	-0.00847	2.80906
D41	-1.37885	-0.00003	-0.00030	-0.00689	-0.00719	-1.38604
D42	0.74609	0.00000	-0.00029	-0.00915	-0.00944	0.73665
D43	2.83290	0.00003	-0.00030	-0.00786	-0.00816	2.82474
D44	-1.35608	-0.00011	-0.00029	-0.01035	-0.01064	-1.36672
D45	0.73073	-0.00008	-0.00030	-0.00906	-0.00936	0.72137
D46	-3.13725	-0.00002	0.00006	0.00005	0.00011	-3.13714
D47	0.00409	0.00001	0.00005	0.00082	0.00087	0.00496
D48	-0.00271	-0.00001	-0.00003	0.00022	0.00019	-0.00252
D49	3.13863	0.00002	-0.00004	0.00099	0.00096	3.13958
D50	1.23034	-0.00001	0.00001	0.01968	0.01968	1.25002
D51	-0.56851	-0.00010	-0.00033	-0.00560	-0.00592	-0.57443
D52	-2.97523	0.00008	0.00011	0.02478	0.02488	-2.95035
D53	1.50911	-0.00002	-0.00023	-0.00050	-0.00072	1.50839
D54	-2.70252	0.00017	-0.00001	0.00311	0.00311	-2.69940
D55	-0.01600	0.00012	0.00000	0.00066	0.00066	-0.01533
D56	-0.02382	-0.00008	-0.00001	0.00002	0.00001	-0.02381

D57	2.66270	-0.00012	0.00001	-0.00244	-0.00244	2.66027
D58	1.94662	-0.00020	-0.00045	-0.02111	-0.02162	1.92500
D59	-0.47138	-0.00030	-0.00042	-0.02274	-0.02321	-0.49459
D60	0.51022	0.00035	0.00045	0.02570	0.02619	0.53641
D61	-1.91205	0.00021	0.00047	0.02310	0.02360	-1.88845
D62	2.55111	0.00007	-0.00001	0.00084	0.00083	2.55195
D63	-1.65584	0.00007	-0.00002	0.00053	0.00052	-1.65532
D64	0.44507	0.00010	-0.00002	0.00086	0.00085	0.44591
D65	1.34837	-0.00001	0.00000	0.00101	0.00100	1.34937
D66	-2.85858	-0.00001	-0.00001	0.00070	0.00068	-2.85790
D67	-0.75768	0.00002	-0.00001	0.00103	0.00101	-0.75667
D68	-1.04849	-0.00008	0.00001	-0.00203	-0.00201	-1.05050
D69	1.02775	-0.00009	0.00000	-0.00234	-0.00233	1.02542
D70	3.12865	-0.00006	0.00000	-0.00201	-0.00200	3.12665

Item	Value	Threshold	Converged?
Maximum Force	0.001090	0.000450	NO
RMS Force	0.000246	0.000300	YES
Maximum Displacement	0.185340	0.001800	NO
RMS Displacement	0.029361	0.001200	NO

Predicted change in Energy=-5.289023D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.895025	2.141153	-0.280286
2	6	0	-3.765152	1.155684	0.059215
3	7	0	-3.034758	-0.025568	0.109474
4	6	0	-1.752113	0.246827	-0.194572
5	7	0	-1.647931	1.553208	-0.438268
6	6	0	-0.373760	2.236586	-0.725379
7	6	0	0.324071	2.730764	0.550259
8	1	0	-3.053766	3.195630	-0.426751
9	1	0	-4.820466	1.196943	0.258289
10	1	0	0.263931	1.520394	-1.244190
11	1	0	-0.574122	3.068686	-1.400676
12	1	0	-0.293469	3.501568	1.022911
13	1	0	0.394019	1.888179	1.254668
14	35	0	0.255339	-2.336574	0.033411
15	1	0	-0.949477	-0.524229	-0.204887
16	6	0	-3.473227	-1.348366	0.417143
17	6	0	-4.730308	-1.666690	0.695193

18	1	0	-2.647902	-2.055952	0.400389
19	1	0	-4.971406	-2.696257	0.921257
20	1	0	-5.544504	-0.952448	0.710657
21	7	0	1.605089	3.305786	0.168678
22	1	0	1.964586	3.913477	0.894845
23	1	0	2.291739	2.568373	0.009725
24	6	0	3.693331	-0.240235	-1.065367
25	6	0	3.647664	-0.448133	0.383348
26	8	0	3.452442	0.876820	-0.180312
27	1	0	4.655635	-0.208895	-1.570947
28	1	0	2.843285	-0.548056	-1.666754
29	1	0	2.731255	-0.888045	0.770746
30	6	0	4.889647	-0.641497	1.208782
31	1	0	4.766452	-0.203042	2.203458
32	1	0	5.087114	-1.710138	1.336453
33	1	0	5.756901	-0.178587	0.731703

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357766	0.000000			
3	N	2.205928	1.389733	0.000000		
4	C	2.214061	2.223230	1.346039	0.000000	
5	N	1.387761	2.210913	2.171599	1.332993	0.000000
6	C	2.562029	3.644924	3.590992	2.478054	1.474093
7	C	3.376393	4.409506	4.367309	3.321936	2.500524
8	H	1.076370	2.214409	3.265580	3.231663	2.161956
9	H	2.211090	1.074719	2.169201	3.243855	3.267582
10	H	3.360574	4.250339	3.886354	2.605399	2.075044
11	H	2.739012	3.996690	4.231984	3.287132	2.091882
12	H	3.212032	4.299356	4.559575	3.768719	2.786704
13	H	3.638392	4.389118	4.090282	3.065977	2.673537
14	Br	5.483908	5.325494	4.021352	3.279604	4.356067
15	H	3.300774	3.289359	2.166998	1.113041	2.204098
16	C	3.605200	2.546292	1.427134	2.425092	3.533067
17	C	4.338144	3.049884	2.431304	3.650051	4.599295
18	H	4.259117	3.417492	2.087282	2.541497	3.837879
19	H	5.399592	4.127422	3.397378	4.502296	5.563429
20	H	4.191906	2.834554	2.742144	4.079207	4.773009
21	N	4.670007	5.785707	5.712232	4.556312	3.744603
22	H	5.304516	6.413547	6.412981	5.333385	4.516453
23	H	5.212403	6.219651	5.925373	4.667338	4.092952
24	C	7.049383	7.670870	6.833265	5.536097	5.669107
25	C	7.067645	7.591254	6.701368	5.474902	5.720468

26	O	6.472934	7.226949	6.556069	5.242565	5.151490
27	H	8.012553	8.684996	7.873980	6.569728	6.642509
28	H	6.487090	7.039398	6.162739	4.890484	5.108376
29	H	6.475781	6.847365	5.867542	4.724443	5.157393
30	C	8.400094	8.913860	8.023966	6.846276	7.090094
31	H	8.388234	8.901245	8.079303	6.960216	7.155937
32	H	9.008931	9.391852	8.384989	7.276591	7.691547
33	H	9.014496	9.638569	8.814978	7.577879	7.694120

		6	7	8	9	10
6	C	0.000000				
7	C	1.535719	0.000000			
8	H	2.862058	3.546891	0.000000		
9	H	4.671365	5.376255	2.754135	0.000000	
10	H	1.090297	2.165332	3.805488	5.311606	0.000000
11	H	1.090212	2.174187	2.667074	4.928187	1.767493
12	H	2.159431	1.094940	3.132788	5.137086	3.061943
13	H	2.152082	1.100470	4.052632	5.353638	2.529127
14	Br	4.678175	5.094092	6.462756	6.188708	4.063071
15	H	2.867832	3.575913	4.279557	4.261634	2.594801
16	C	4.874826	5.574630	4.640690	2.884248	4.995614
17	C	6.019393	6.701146	5.264190	2.898173	6.233870
18	H	4.986477	5.636288	5.331791	3.914275	4.896291
19	H	6.941375	7.591592	6.341040	3.952127	7.062440
20	H	6.242494	6.930509	4.970314	2.312736	6.608653
21	N	2.420407	1.455081	4.698042	6.763358	2.642447
22	H	3.302265	2.051545	5.238872	7.336327	3.632430
23	H	2.784842	2.047013	5.399851	7.247487	2.604336
24	C	4.774041	4.773782	7.598442	8.735118	3.859090
25	C	4.960731	4.602121	7.670883	8.627349	4.239532
26	O	4.097058	3.709117	6.911466	8.290709	3.422372
27	H	5.655987	5.648324	8.504990	9.752896	4.731203
28	H	4.357728	4.691721	7.094223	8.092211	3.333183
29	H	4.652185	4.351888	7.181704	7.851005	3.993524
30	C	6.302999	5.714042	8.971974	9.928222	5.664635
31	H	6.399348	5.574498	8.923272	9.881935	5.926989
32	H	7.046199	6.559443	9.666922	10.381411	6.352885
33	H	6.748419	6.165459	9.505536	10.676933	6.079754

		11	12	13	14	15
11	H	0.000000				
12	H	2.477887	0.000000			
13	H	3.062964	1.769004	0.000000		
14	Br	5.653446	5.946781	4.399914	0.000000	
15	H	3.805239	4.259681	3.123299	2.189283	0.000000
16	C	5.587453	5.830924	5.111973	3.876340	2.726800

17	C	6.640055	6.819372	6.261695	5.073793	4.050931
18	H	5.814320	6.067694	5.053636	2.939768	2.365836
19	H	7.613281	7.765723	7.065125	5.313804	4.707634
20	H	6.732900	6.892687	6.605389	6.001054	4.704877
21	N	2.695931	2.091068	2.157701	5.803133	4.618915
22	H	3.525354	2.298887	2.588047	6.536569	5.421662
23	H	3.233064	2.929282	2.369364	5.310932	4.485056
24	C	5.410411	5.852911	4.560501	4.173936	4.730406
25	C	5.777044	5.616200	4.099239	3.898274	4.635248
26	O	4.744131	4.729576	3.526466	4.537956	4.619571
27	H	6.174293	6.707404	5.526590	5.144277	5.777788
28	H	4.983000	5.785583	4.524251	3.575866	4.064808
29	H	5.594311	5.336782	3.661184	2.961766	3.825181
30	C	7.101232	6.638088	5.158685	5.072632	6.008958
31	H	7.226044	6.381271	4.938782	5.441617	6.210888
32	H	7.898014	7.497390	5.914364	5.043450	6.342124
33	H	7.427898	7.087687	5.771093	5.950773	6.780278

		16	17	18	19	20
16	C	0.000000				
17	C	1.326233	0.000000			
18	H	1.087253	2.138889	0.000000		
19	H	2.077373	1.081314	2.465758	0.000000	
20	H	2.129105	1.083188	3.115170	1.847609	0.000000
21	N	6.892906	8.070934	6.847616	8.935389	8.339243
22	H	7.581887	8.717782	7.560001	9.581089	8.949725
23	H	6.981523	8.228898	6.777688	9.016678	8.619408
24	C	7.401712	8.723075	6.756960	9.222602	9.433934
25	C	7.177650	8.471868	6.497656	8.923664	9.211809
26	O	7.298856	8.613556	6.793568	9.216374	9.224158
27	H	8.445667	9.765064	7.787133	10.250755	10.478618
28	H	6.699361	8.011831	6.058050	8.507759	8.727578
29	H	6.231575	7.502461	5.516929	7.913487	8.276228
30	C	8.429947	9.688050	7.711603	10.076957	10.450661
31	H	8.508525	9.726539	7.852195	10.133412	10.445375
32	H	8.617160	9.838438	7.799120	10.115268	10.676938
33	H	9.309274	10.592324	8.618293	11.021396	11.327888

		21	22	23	24	25
21	N	0.000000				
22	H	1.012840	0.000000			
23	H	1.020064	1.643098	0.000000		
24	C	4.296264	4.907577	3.317916	0.000000	
25	C	4.279031	4.702981	3.328279	1.464269	0.000000
26	O	3.071544	3.548375	2.060267	1.445393	1.453040
27	H	4.968411	5.505981	3.974890	1.087485	2.211902

28	H	4.444551	5.219116	3.581468	1.085817	2.204525
29	H	4.383943	4.863928	3.566392	2.171764	1.087844
30	C	5.239387	5.422391	4.300015	2.600757	1.503745
31	H	5.142608	5.148655	4.314790	3.440667	2.150478
32	H	6.216726	6.447499	5.280150	3.141971	2.138476
33	H	5.449348	5.581510	4.480446	2.737075	2.154735

		26	27	28	29	30
26	O	0.000000				
27	H	2.135490	0.000000			
28	H	2.147290	1.846300	0.000000		
29	H	2.130580	3.106124	2.463645	0.000000	
30	C	2.510065	2.822906	3.530586	2.216149	0.000000
31	H	2.928324	3.776036	4.335452	2.581457	1.093984
32	H	3.415418	3.300436	3.924851	2.558502	1.094206
33	H	2.693731	2.552626	3.791868	3.107956	1.092712

		31	32	33
31	H	0.000000		
32	H	1.768010	0.000000	
33	H	1.774162	1.777635	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.855173	2.212372	-0.200386
2	6	0	-3.730638	1.214569	0.085059
3	7	0	-3.008338	0.027504	0.062308
4	6	0	-1.725216	0.308616	-0.231622
5	7	0	-1.612976	1.626314	-0.398790
6	6	0	-0.335363	2.316755	-0.651667
7	6	0	0.371753	2.730502	0.647269
8	1	0	-3.007171	3.274674	-0.283958
9	1	0	-4.784715	1.251189	0.291464
10	1	0	0.294900	1.627960	-1.214762
11	1	0	-0.532963	3.188385	-1.275989
12	1	0	-0.238187	3.476386	1.167387
13	1	0	0.439003	1.847576	1.300687
14	35	0	0.265061	-2.297192	-0.165558

15	1	0	-0.928072	-0.465902	-0.291142
16	6	0	-3.454676	-1.308083	0.294041
17	6	0	-4.712677	-1.633691	0.559200
18	1	0	-2.634428	-2.019016	0.231704
19	1	0	-4.959965	-2.673100	0.725684
20	1	0	-5.521756	-0.916113	0.620585
21	7	0	1.655019	3.318273	0.293696
22	1	0	2.022096	3.879863	1.052456
23	1	0	2.335737	2.586846	0.088347
24	6	0	3.712630	-0.163218	-1.156596
25	6	0	3.672134	-0.455464	0.277640
26	8	0	3.483647	0.901571	-0.206357
27	1	0	4.672807	-0.108752	-1.664254
28	1	0	2.857699	-0.429474	-1.770761
29	1	0	2.754440	-0.911163	0.643128
30	6	0	4.916492	-0.705309	1.084115
31	1	0	4.800933	-0.325163	2.103397
32	1	0	5.107029	-1.780908	1.147903
33	1	0	5.784784	-0.221058	0.630696

Rotational constants (GHZ): 0.4750358 0.2485614 0.1714302

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1293.0179738655 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 3.87D-06 NBF= 482

NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999996 -0.001967 -0.000125 0.001766 Ang= -0.30 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3205.64690000 A.U. after 11 cycles
NFock= 11 Conv=0.36D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000359837	0.000029993	0.000113243
2	6	-0.000240144	0.000092618	-0.000065254
3	7	0.000618316	0.000310925	-0.000333269
4	6	-0.001095455	-0.001126418	0.000422975
5	7	0.000056724	-0.000270261	0.000204149
6	6	0.000441309	0.000593694	-0.000196837
7	6	-0.000813338	-0.000460361	0.000297197
8	1	0.000006241	0.000023776	-0.000037344
9	1	0.000040113	0.000016582	-0.000020110
10	1	-0.000008975	-0.000019832	0.000007323
11	1	-0.000141751	-0.000042824	0.000042843
12	1	0.000100485	-0.000001255	-0.000000967
13	1	0.000162451	0.000119042	-0.000038724
14	35	-0.000173833	0.000192609	0.000048083
15	1	0.000446229	0.000443615	-0.000267298
16	6	0.000349518	0.000308665	0.000118270
17	6	-0.000004440	-0.000247798	-0.000026071
18	1	-0.000210330	0.000055198	0.000018639
19	1	-0.000035478	0.000022417	0.000015581
20	1	0.000051643	-0.000031040	-0.000028612
21	7	0.000173571	0.000063954	-0.000137651
22	1	-0.000002404	0.000020274	-0.000036050
23	1	0.000276638	0.000155867	-0.000004304
24	6	0.000631409	0.000274035	0.000317366

25	6	0.000336508	-0.000003940	0.000205202
26	8	-0.000913929	-0.000502337	-0.000366789
27	1	-0.000124486	0.000009224	-0.000163275
28	1	-0.000130140	0.000006263	0.000074312
29	1	-0.000149116	-0.000041100	-0.000146123
30	6	-0.000003421	0.000018288	-0.000023115
31	1	-0.000043527	-0.000025301	-0.000014716
32	1	0.000031578	0.000005421	0.000044251
33	1	0.000008197	0.000010008	-0.000022926

Cartesian Forces: Max 0.001126418 RMS 0.000289681

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000737913 RMS 0.000155995

Search for a local minimum.

Step number 13 out of a maximum of 172

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 2 3 1 4 5
6 7 8 10 11
9 12 13

DE= -8.32D-05 DEPred=-5.29D-05 R= 1.57D+00

TightC=F SS= 1.41D+00 RLast= 1.05D-01 DXNew= 1.8436D-01 3.1404D-01

Trust test= 1.57D+00 RLast= 1.05D-01 DXMaxT set to 1.84D-01

ITU= 1 0 -1 -1 1 1 1 -1 1 0 0 -1 0

Eigenvalues ---	0.00162	0.00231	0.00376	0.00663	0.00723
Eigenvalues ---	0.00889	0.00989	0.01376	0.01454	0.01577
Eigenvalues ---	0.01873	0.01920	0.02109	0.02249	0.02346
Eigenvalues ---	0.02394	0.02425	0.02532	0.03018	0.03074
Eigenvalues ---	0.03080	0.03131	0.03331	0.03750	0.04037
Eigenvalues ---	0.04244	0.04417	0.04886	0.05016	0.05409
Eigenvalues ---	0.05753	0.05777	0.05922	0.07776	0.08662
Eigenvalues ---	0.09504	0.10722	0.12120	0.12393	0.12600
Eigenvalues ---	0.12776	0.13235	0.15560	0.15719	0.15996
Eigenvalues ---	0.16000	0.16000	0.16003	0.16007	0.16019
Eigenvalues ---	0.16046	0.16249	0.17499	0.21425	0.22126
Eigenvalues ---	0.22775	0.22993	0.23899	0.25532	0.26272
Eigenvalues ---	0.29193	0.30070	0.31425	0.32067	0.32586
Eigenvalues ---	0.33655	0.34273	0.34312	0.34341	0.34544
Eigenvalues ---	0.34656	0.34735	0.35045	0.35075	0.35270

Eigenvalues --- 0.35387 0.35561 0.35692 0.35890 0.36419
Eigenvalues --- 0.36620 0.38066 0.39184 0.41961 0.42420
Eigenvalues --- 0.44742 0.45473 0.45920 0.49279 0.54850
Eigenvalues --- 0.58620 0.60675 1.09145
En-DIIS/RFO-DIIS IScMMF= 0 using points: 13 12
RFO step: Lambda=-1.26837713D-05.
DidBck=F Rises=F RFO-DIIS coefs: 1.83487 -0.83487
Iteration 1 RMS(Cart)= 0.04536506 RMS(Int)= 0.00103379
Iteration 2 RMS(Cart)= 0.00181279 RMS(Int)= 0.00025057
Iteration 3 RMS(Cart)= 0.00000197 RMS(Int)= 0.00025057
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00025057

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56581	0.00001	-0.00028	0.00004	-0.00024	2.56557
R2	2.62249	-0.00028	-0.00034	-0.00079	-0.00113	2.62136
R3	2.03404	0.00003	0.00006	0.00002	0.00007	2.03412
R4	2.62622	0.00019	-0.00023	-0.00070	-0.00093	2.62529
R5	2.03093	-0.00004	-0.00012	-0.00013	-0.00025	2.03068
R6	2.54364	-0.00074	-0.00014	-0.00051	-0.00064	2.54300
R7	2.69689	-0.00013	0.00086	0.00141	0.00228	2.69917
R8	2.51899	-0.00004	0.00019	0.00120	0.00140	2.52039
R9	2.10334	-0.00025	-0.00200	-0.00373	-0.00573	2.09762
R10	2.78563	-0.00003	-0.00061	0.00070	0.00010	2.78573
R11	2.90209	-0.00032	-0.00026	0.00025	-0.00001	2.90207
R12	2.06036	0.00001	-0.00004	0.00018	0.00014	2.06050
R13	2.06020	-0.00003	0.00002	-0.00025	-0.00024	2.05996
R14	2.06914	-0.00006	-0.00010	-0.00041	-0.00051	2.06862
R15	2.07959	-0.00011	-0.00033	-0.00065	-0.00098	2.07861
R16	2.74970	0.00014	-0.00048	0.00124	0.00076	2.75046
R17	4.13715	-0.00025	0.01046	0.02145	0.03191	4.16905
R18	2.50622	0.00004	0.00003	-0.00009	-0.00006	2.50616
R19	2.05461	-0.00020	0.00001	0.00071	0.00072	2.05533
R20	2.04339	-0.00001	0.00007	0.00003	0.00010	2.04349
R21	2.04693	-0.00006	-0.00018	-0.00001	-0.00019	2.04674
R22	1.91399	-0.00002	-0.00014	-0.00027	-0.00041	1.91358
R23	1.92764	0.00003	-0.00029	-0.00099	-0.00127	1.92637
R24	3.89334	0.00001	0.00747	0.01386	0.02132	3.91466
R25	2.76707	-0.00016	-0.00079	0.00122	-0.00040	2.76667
R26	2.73140	-0.00018	-0.00002	-0.00213	-0.00182	2.72958
R27	2.05505	-0.00004	0.00007	0.00002	0.00009	2.05514
R28	2.05190	0.00006	-0.00002	0.00029	0.00027	2.05217
R29	2.74585	0.00012	0.00055	0.00026	0.00131	2.74716
R30	2.05573	0.00009	0.00004	0.00046	0.00050	2.05623
R31	2.84167	-0.00001	0.00007	0.00003	0.00010	2.84176

R32	2.06733	-0.00001	-0.00002	-0.00009	-0.00012	2.06721
R33	2.06775	0.00001	0.00005	0.00001	0.00007	2.06782
R34	2.06493	0.00002	-0.00001	0.00012	0.00011	2.06504
A1	1.87220	-0.00010	-0.00027	0.00035	0.00007	1.87227
A2	2.27911	0.00007	0.00059	0.00078	0.00136	2.28047
A3	2.13186	0.00003	-0.00029	-0.00117	-0.00146	2.13040
A4	1.86414	-0.00015	0.00017	0.00008	0.00024	1.86438
A5	2.27540	0.00005	-0.00054	-0.00030	-0.00084	2.27456
A6	2.14362	0.00010	0.00037	0.00025	0.00062	2.14424
A7	1.89719	0.00013	0.00022	0.00001	0.00024	1.89743
A8	2.25773	0.00018	-0.00046	-0.00084	-0.00131	2.25642
A9	2.12826	-0.00032	0.00025	0.00083	0.00107	2.12933
A10	1.89030	0.00000	-0.00054	0.00012	-0.00043	1.88987
A11	2.15204	0.00061	-0.00052	-0.00224	-0.00279	2.14924
A12	2.24064	-0.00061	0.00095	0.00205	0.00297	2.24361
A13	1.90092	0.00012	0.00047	-0.00062	-0.00015	1.90077
A14	2.21746	-0.00019	-0.00123	-0.00342	-0.00467	2.21279
A15	2.16217	0.00007	0.00070	0.00343	0.00411	2.16628
A16	1.96077	-0.00017	-0.00044	-0.00027	-0.00070	1.96007
A17	1.86890	0.00001	0.00047	0.00401	0.00449	1.87339
A18	1.89191	0.00000	-0.00056	-0.00277	-0.00333	1.88858
A19	1.91863	-0.00002	-0.00051	0.00003	-0.00048	1.91815
A20	1.93096	0.00018	0.00121	-0.00033	0.00088	1.93183
A21	1.89031	0.00000	-0.00021	-0.00059	-0.00079	1.88952
A22	1.90584	0.00023	0.00100	-0.00042	0.00058	1.90642
A23	1.89041	0.00027	0.00045	0.00174	0.00219	1.89259
A24	1.88534	-0.00060	-0.00193	-0.00048	-0.00243	1.88291
A25	1.87396	-0.00007	0.00082	0.00074	0.00157	1.87552
A26	1.90872	0.00020	0.00130	-0.00001	0.00129	1.91002
A27	1.99816	-0.00001	-0.00151	-0.00153	-0.00304	1.99512
A28	2.16384	0.00025	-0.00029	-0.00136	-0.00165	2.16219
A29	1.94623	-0.00002	-0.00052	-0.00052	-0.00104	1.94520
A30	2.17309	-0.00022	0.00081	0.00188	0.00269	2.17578
A31	2.07568	0.00007	0.00009	-0.00018	-0.00009	2.07559
A32	2.16181	-0.00005	0.00014	0.00046	0.00060	2.16240
A33	2.04570	-0.00002	-0.00022	-0.00028	-0.00050	2.04519
A34	1.94075	0.00016	0.00043	0.00089	0.00147	1.94222
A35	1.92602	-0.00048	-0.00099	-0.00119	-0.00215	1.92388
A36	1.88234	0.00016	0.00115	0.00042	0.00152	1.88387
A37	2.08479	0.00010	-0.00016	0.00177	0.00112	2.08591
A38	2.07523	-0.00008	-0.00056	0.00190	0.00175	2.07697
A39	1.99312	0.00010	0.00038	0.00071	0.00112	1.99423
A40	2.01281	-0.00018	0.00116	-0.00270	-0.00174	2.01107
A41	2.03021	-0.00002	-0.00033	-0.00181	-0.00212	2.02809

A42	2.02197	0.00000	-0.00083	0.00149	0.00098	2.02294
A43	2.13600	-0.00006	-0.00055	-0.00057	-0.00155	2.13445
A44	1.97545	-0.00010	0.00119	-0.00139	-0.00037	1.97509
A45	2.02768	0.00008	-0.00008	-0.00044	-0.00046	2.02722
A46	2.03565	0.00007	0.00048	0.00058	0.00111	2.03676
A47	2.47333	0.00021	0.00964	0.02388	0.03169	2.50502
A48	2.47928	0.00005	0.00804	0.02035	0.02629	2.50557
A49	1.93322	-0.00007	-0.00039	-0.00070	-0.00108	1.93214
A50	1.91631	0.00009	0.00022	0.00012	0.00034	1.91665
A51	1.94054	-0.00001	0.00013	0.00061	0.00075	1.94129
A52	1.88143	-0.00003	-0.00014	-0.00067	-0.00080	1.88062
A53	1.89289	0.00004	0.00013	0.00036	0.00049	1.89338
A54	1.89805	-0.00002	0.00003	0.00026	0.00029	1.89834
A55	3.32041	0.00005	0.02819	0.00964	0.03784	3.35824
A56	2.99516	-0.00038	-0.00966	-0.03148	-0.04117	2.95399
A57	2.94728	-0.00031	-0.01253	-0.04323	-0.05576	2.89152
A58	3.20916	0.00010	-0.01566	0.02112	0.00540	3.21456
D1	0.00386	0.00008	-0.00452	0.00835	0.00383	0.00768
D2	-3.13029	0.00002	-0.00279	0.00316	0.00037	-3.12992
D3	3.13877	0.00000	-0.00160	0.00147	-0.00015	3.13862
D4	0.00462	-0.00006	0.00012	-0.00372	-0.00360	0.00102
D5	-0.00601	-0.00006	0.00530	-0.00892	-0.00361	-0.00962
D6	-3.07145	-0.00007	0.00599	-0.00030	0.00567	-3.06578
D7	3.14158	0.00001	0.00268	-0.00275	-0.00007	3.14151
D8	0.07614	-0.00001	0.00337	0.00586	0.00921	0.08535
D9	-0.00045	-0.00007	0.00225	-0.00501	-0.00276	-0.00321
D10	-3.14044	-0.00010	0.00035	-0.00633	-0.00596	3.13678
D11	3.13439	-0.00002	0.00068	-0.00031	0.00037	3.13476
D12	-0.00560	-0.00005	-0.00122	-0.00162	-0.00283	-0.00843
D13	-0.00330	0.00003	0.00105	-0.00051	0.00053	-0.00277
D14	3.11813	-0.00003	-0.00539	-0.00401	-0.00938	3.10875
D15	3.13683	0.00006	0.00277	0.00068	0.00345	3.14028
D16	-0.02492	0.00000	-0.00367	-0.00281	-0.00646	-0.03138
D17	0.02324	0.00008	0.01019	0.02257	0.03275	0.05599
D18	-3.11218	0.00005	0.01012	0.02225	0.03237	-3.07981
D19	-3.11657	0.00005	0.00808	0.02110	0.02918	-3.08739
D20	0.03120	0.00002	0.00801	0.02079	0.02879	0.05999
D21	0.00574	0.00002	-0.00390	0.00579	0.00189	0.00762
D22	3.07413	0.00002	-0.00467	-0.00285	-0.00755	3.06657
D23	-3.11436	0.00006	0.00298	0.00958	0.01259	-3.10178
D24	-0.04597	0.00006	0.00221	0.00094	0.00315	-0.04282
D25	1.50082	0.00015	0.02134	0.03144	0.05278	1.55360
D26	-2.67425	0.00003	0.02075	0.03398	0.05473	-2.61951
D27	-0.63836	0.00004	0.02048	0.03398	0.05446	-0.58391

D28	-1.55397	0.00014	0.02216	0.04148	0.06364	-1.49033
D29	0.55415	0.00001	0.02157	0.04402	0.06559	0.61974
D30	2.59003	0.00002	0.02130	0.04402	0.06532	2.65535
D31	-1.13310	-0.00014	-0.00266	0.00188	-0.00079	-1.13389
D32	0.90246	0.00005	-0.00089	0.00350	0.00261	0.90507
D33	3.07585	-0.00017	-0.00367	0.00241	-0.00126	3.07459
D34	3.07085	-0.00003	-0.00263	-0.00302	-0.00566	3.06519
D35	-1.17678	0.00016	-0.00086	-0.00140	-0.00226	-1.17904
D36	0.99661	-0.00006	-0.00364	-0.00249	-0.00613	0.99048
D37	0.98387	-0.00013	-0.00281	-0.00210	-0.00492	0.97895
D38	3.01943	0.00006	-0.00104	-0.00048	-0.00152	3.01791
D39	-1.09036	-0.00016	-0.00382	-0.00157	-0.00539	-1.09576
D40	2.80906	0.00006	-0.00707	-0.02284	-0.02995	2.77910
D41	-1.38604	0.00006	-0.00600	-0.02253	-0.02850	-1.41454
D42	0.73665	0.00002	-0.00788	-0.02205	-0.02997	0.70669
D43	2.82474	0.00002	-0.00681	-0.02174	-0.02852	2.79623
D44	-1.36672	-0.00003	-0.00888	-0.02197	-0.03088	-1.39759
D45	0.72137	-0.00004	-0.00781	-0.02165	-0.02943	0.69194
D46	-3.13714	-0.00001	0.00009	0.00161	0.00170	-3.13543
D47	0.00496	0.00000	0.00073	0.00193	0.00266	0.00762
D48	-0.00252	0.00003	0.00016	0.00196	0.00212	-0.00039
D49	3.13958	0.00004	0.00080	0.00228	0.00308	-3.14053
D50	1.25002	0.00009	0.01643	0.03325	0.04981	1.29983
D51	-0.57443	0.00003	-0.00494	-0.02379	-0.02869	-0.60311
D52	-2.95035	0.00001	0.02077	0.02261	0.04334	-2.90701
D53	1.50839	-0.00005	-0.00060	-0.03443	-0.03516	1.47323
D54	-2.69940	0.00000	0.00260	-0.00269	0.00004	-2.69936
D55	-0.01533	0.00004	0.00055	0.00109	0.00167	-0.01366
D56	-0.02381	-0.00001	0.00001	0.00121	0.00124	-0.02257
D57	2.66027	0.00004	-0.00203	0.00498	0.00287	2.66314
D58	1.92500	-0.00025	-0.01805	-0.05185	-0.07037	1.85463
D59	-0.49459	-0.00012	-0.01938	-0.04645	-0.06614	-0.56073
D60	0.53641	0.00029	0.02186	0.05228	0.07439	0.61080
D61	-1.88845	0.00020	0.01971	0.05358	0.07357	-1.81487
D62	2.55195	-0.00002	0.00070	-0.00160	-0.00083	2.55111
D63	-1.65532	-0.00004	0.00043	-0.00278	-0.00228	-1.65760
D64	0.44591	-0.00002	0.00071	-0.00199	-0.00122	0.44470
D65	1.34937	0.00003	0.00083	0.00024	0.00098	1.35035
D66	-2.85790	0.00001	0.00057	-0.00094	-0.00047	-2.85837
D67	-0.75667	0.00004	0.00084	-0.00015	0.00059	-0.75607
D68	-1.05050	0.00001	-0.00168	0.00242	0.00077	-1.04973
D69	1.02542	-0.00001	-0.00195	0.00124	-0.00068	1.02474
D70	3.12665	0.00001	-0.00167	0.00203	0.00039	3.12704

Item	Value	Threshold	Converged?

Maximum Force	0.000738	0.000450	NO
RMS Force	0.000156	0.000300	YES
Maximum Displacement	0.313777	0.001800	NO
RMS Displacement	0.046265	0.001200	NO

Predicted change in Energy=-7.087784D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.899588	2.142011	-0.305886
2	6	0	-3.759855	1.149646	0.038116
3	7	0	-3.014596	-0.020372	0.113240
4	6	0	-1.733295	0.264009	-0.183917
5	7	0	-1.644382	1.568567	-0.446732
6	6	0	-0.378934	2.271597	-0.725103
7	6	0	0.333816	2.719351	0.559387
8	1	0	-3.069637	3.192231	-0.469526
9	1	0	-4.817150	1.180581	0.227622
10	1	0	0.258297	1.584963	-1.283115
11	1	0	-0.598315	3.128343	-1.362398
12	1	0	-0.280886	3.466829	1.070970
13	1	0	0.422654	1.851010	1.228704
14	35	0	0.205895	-2.354493	0.199454
15	1	0	-0.923336	-0.494782	-0.165909
16	6	0	-3.439630	-1.343815	0.441861
17	6	0	-4.700507	-1.677099	0.682544
18	1	0	-2.600210	-2.034666	0.474181
19	1	0	-4.931891	-2.704011	0.930066
20	1	0	-5.527454	-0.978603	0.645939
21	7	0	1.605966	3.316018	0.179846
22	1	0	1.961357	3.919849	0.910932
23	1	0	2.299353	2.588641	0.008693
24	6	0	3.693341	-0.247451	-1.088299
25	6	0	3.625266	-0.472521	0.356753
26	8	0	3.413917	0.854696	-0.197470
27	1	0	4.663414	-0.192304	-1.576814
28	1	0	2.860618	-0.562589	-1.710049
29	1	0	2.710572	-0.933878	0.723450
30	6	0	4.856902	-0.649733	1.201188
31	1	0	4.707081	-0.224149	2.197730
32	1	0	5.073223	-1.715482	1.322623

33 1 0 5.723107 -0.165027 0.744135

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357639	0.000000			
3	N	2.205627	1.389243	0.000000		
4	C	2.214047	2.222745	1.345699	0.000000	
5	N	1.387163	2.210385	2.171585	1.333735	0.000000
6	C	2.558561	3.643063	3.592026	2.481448	1.474144
7	C	3.396604	4.415183	4.349367	3.294564	2.499969
8	H	1.076409	2.215006	3.265495	3.231387	2.160592
9	H	2.210434	1.074589	2.169002	3.243397	3.266763
10	H	3.352241	4.252141	3.903683	2.630513	2.078459
11	H	2.717523	3.983971	4.234422	3.298698	2.089403
12	H	3.241679	4.305735	4.533320	3.733938	2.786744
13	H	3.671095	4.404860	4.069523	3.026910	2.675723
14	Br	5.487982	5.294544	3.978332	3.280852	4.385371
15	H	3.298157	3.285059	2.162489	1.110010	2.203673
16	C	3.605794	2.546155	1.428338	2.426577	3.534754
17	C	4.336577	3.048049	2.431285	3.650069	4.598860
18	H	4.259432	3.416837	2.087912	2.543333	3.839919
19	H	5.398311	4.125520	3.397815	4.503456	5.564011
20	H	4.189257	2.832542	2.741611	4.077792	4.770771
21	N	4.681265	5.788375	5.699607	4.538474	3.743119
22	H	5.316968	6.416237	6.397012	5.311715	4.513661
23	H	5.227565	6.227807	5.920805	4.658676	4.098903
24	C	7.056091	7.666213	6.818481	5.525204	5.674576
25	C	7.060353	7.567890	6.659692	5.435897	5.707960
26	O	6.444322	7.183697	6.495234	5.181012	5.114501
27	H	8.016439	8.681031	7.863694	6.562490	6.645753
28	H	6.516633	7.058221	6.175477	4.910843	5.141285
29	H	6.480319	6.832071	5.829615	4.691077	5.157245
30	C	8.380230	8.879133	7.971212	6.795892	7.064219
31	H	8.350343	8.845352	8.000683	6.883966	7.109718
32	H	9.005444	9.374550	8.351577	7.246844	7.683867
33	H	8.987538	9.599656	8.761644	7.526173	7.661814

		6	7	8	9	10
6	C	0.000000				
7	C	1.535712	0.000000			
8	H	2.855305	3.586888	0.000000		
9	H	4.668593	5.386124	2.754370	0.000000	
10	H	1.090370	2.165029	3.784228	5.310933	0.000000
11	H	1.090086	2.174719	2.628447	4.911264	1.766944

12	H	2.159646	1.094669	3.197759	5.149355	3.061675
13	H	2.153322	1.099951	4.108400	5.376540	2.531211
14	Br	4.753687	5.088203	6.476325	6.142355	4.209522
15	H	2.874356	3.526632	4.277014	4.257170	2.640028
16	C	4.878614	5.546353	4.641469	2.883754	5.022744
17	C	6.020769	6.684934	5.262829	2.896013	6.252568
18	H	4.991618	5.587168	5.332110	3.913237	4.935673
19	H	6.944471	7.568218	6.339757	3.949259	7.087420
20	H	6.241058	6.930861	4.967995	2.311189	6.615742
21	N	2.418589	1.455482	4.722104	6.768957	2.636857
22	H	3.297015	2.052723	5.267446	7.342933	3.628491
23	H	2.795030	2.045406	5.423935	7.257767	2.615731
24	C	4.802180	4.775269	7.612631	8.729225	3.898104
25	C	4.973349	4.589417	7.676904	8.603708	4.273041
26	O	4.083102	3.679238	6.897430	8.248476	3.416116
27	H	5.676398	5.637953	8.513591	9.747917	4.759201
28	H	4.415588	4.722943	7.127796	8.108102	3.400930
29	H	4.681711	4.361418	7.201304	7.834755	4.047779
30	C	6.297519	5.676349	8.965600	9.893693	5.684435
31	H	6.374892	5.520308	8.902990	9.826778	5.931344
32	H	7.058045	6.535461	9.674896	10.363671	6.392677
33	H	6.732807	6.115408	9.489809	10.638348	6.085749

		11	12	13	14	15
11	H	0.000000				
12	H	2.477219	0.000000			
13	H	3.063946	1.769384	0.000000		
14	Br	5.757398	5.906292	4.335042	0.000000	
15	H	3.829394	4.199640	3.042921	2.206169	0.000000
16	C	5.597199	5.789279	5.073782	3.790790	2.724331
17	C	6.640937	6.792932	6.244407	4.976447	4.047810
18	H	5.834148	6.000156	4.980511	2.837603	2.364924
19	H	7.619163	7.728582	7.036231	5.201231	4.706418
20	H	6.722859	6.889775	6.614386	5.913013	4.700115
21	N	2.696774	2.092141	2.155593	5.840828	4.586841
22	H	3.513749	2.293140	2.597823	6.554023	5.382379
23	H	3.250792	2.925283	2.356804	5.371548	4.463598
24	C	5.467122	5.852589	4.524316	4.273197	4.714412
25	C	5.810364	5.593443	4.051643	3.906233	4.578586
26	O	4.756525	4.699334	3.460385	4.554980	4.542449
27	H	6.225629	6.696724	5.479974	5.263047	5.770089
28	H	5.070311	5.817157	4.517233	3.728897	4.087453
29	H	5.639250	5.332525	3.639430	2.926794	3.766836
30	C	7.113735	6.584824	5.090877	5.053864	5.941727
31	H	7.215327	6.306562	4.858149	5.365831	6.112416

32	H	7.927063	7.455613	5.861440	5.035943	6.297980
33	H	7.432640	7.024608	5.691573	5.960710	6.716555

		16	17	18	19	20
16	C	0.000000				
17	C	1.326204	0.000000			
18	H	1.087633	2.140681	0.000000		
19	H	2.077335	1.081367	2.468317	0.000000	
20	H	2.129327	1.083087	3.116653	1.847284	0.000000
21	N	6.873190	8.059499	6.812369	8.918921	8.339465
22	H	7.556246	8.703932	7.513648	9.559956	8.952505
23	H	6.970493	8.224880	6.752582	9.008440	8.624976
24	C	7.377173	8.696923	6.726386	9.192558	9.410910
25	C	7.118929	8.418767	6.419551	8.861894	9.171260
26	O	7.225877	8.545659	6.705912	9.142661	9.166266
27	H	8.429731	9.746401	7.769242	10.230494	10.460052
28	H	6.703295	8.008573	6.062880	8.501711	8.722585
29	H	6.170278	7.448365	5.429390	7.847503	8.238512
30	C	8.360070	9.626450	7.619390	10.005700	10.404389
31	H	8.408664	9.638961	7.723024	10.033268	10.378967
32	H	8.566362	9.794742	7.726792	10.061491	10.647781
33	H	9.243195	10.532895	8.534988	10.954907	11.280366

		21	22	23	24	25
21	N	0.000000				
22	H	1.012622	0.000000			
23	H	1.019390	1.643287	0.000000		
24	C	4.320143	4.935898	3.345147	0.000000	
25	C	4.296730	4.729548	3.354087	1.464059	0.000000
26	O	3.077200	3.568424	2.071550	1.444431	1.453732
27	H	4.974150	5.513601	3.979481	1.087534	2.212455
28	H	4.493266	5.269769	3.633090	1.085962	2.205554
29	H	4.424622	4.914788	3.617751	2.172430	1.088109
30	C	5.228662	5.417519	4.295366	2.599511	1.503796
31	H	5.120698	5.134936	4.301258	3.438924	2.149700
32	H	6.216415	6.450594	5.286421	3.141932	2.138794
33	H	5.420972	5.555609	4.454845	2.735792	2.155355

		26	27	28	29	30
26	O	0.000000				
27	H	2.135426	0.000000			
28	H	2.145398	1.845247	0.000000		
29	H	2.131146	3.107208	2.466229	0.000000	
30	C	2.510331	2.822052	3.531012	2.217139	0.000000
31	H	2.927997	3.774931	4.335286	2.581330	1.093921
32	H	3.416109	3.300720	3.927071	2.559694	1.094241
33	H	2.694218	2.551567	3.791426	3.109168	1.092771

		31	32	33
31	H	0.000000		
32	H	1.767470	0.000000	
33	H	1.774470	1.777895	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.842353	2.235929	-0.194869
2	6	0	-3.710647	1.225183	0.065211
3	7	0	-2.976568	0.046174	0.032622
4	6	0	-1.693996	0.343653	-0.245626
5	7	0	-1.593544	1.665420	-0.392901
6	6	0	-0.322618	2.378388	-0.615434
7	6	0	0.400746	2.704388	0.699434
8	1	0	-3.002864	3.298036	-0.264301
9	1	0	-4.766651	1.249176	0.262749
10	1	0	0.305108	1.737724	-1.235447
11	1	0	-0.536667	3.290032	-1.173445
12	1	0	-0.204080	3.409542	1.278435
13	1	0	0.484303	1.779592	1.289065
14	35	0	0.221205	-2.316500	-0.105711
15	1	0	-0.891457	-0.421318	-0.299221
16	6	0	-3.412986	-1.297063	0.245703
17	6	0	-4.675890	-1.638461	0.463269
18	1	0	-2.580249	-1.995900	0.212186
19	1	0	-4.916150	-2.680994	0.620605
20	1	0	-5.496100	-0.931747	0.493121
21	7	0	1.676836	3.320275	0.366710
22	1	0	2.041702	3.853903	1.146144
23	1	0	2.362198	2.604373	0.128131
24	6	0	3.722882	-0.136811	-1.222595
25	6	0	3.659635	-0.487837	0.197351
26	8	0	3.458646	0.885018	-0.236478
27	1	0	4.691060	-0.047866	-1.709884
28	1	0	2.884083	-0.388060	-1.864937
29	1	0	2.742248	-0.971162	0.527167

30	6	0	4.893568	-0.750377	1.015817
31	1	0	4.752793	-0.412981	2.046841
32	1	0	5.099992	-1.824662	1.041575
33	1	0	5.762259	-0.235370	0.598333

Rotational constants (GHZ): 0.4699518 0.2516522 0.1719668

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1293.7998133377 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 3.93D-06 NBF= 482

NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999990 -0.003274 -0.000160 0.002953 Ang= -0.51 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3205.64698246 A.U. after 11 cycles

NFock= 11 Conv=0.56D-08 -V/T= 2.0018

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000193498	0.000028753	-0.000423597
2	6	-0.000283773	0.000281454	0.000181705
3	7	0.000200161	-0.000278546	-0.000299058
4	6	-0.001020442	-0.000024109	0.000388740
5	7	0.000188462	-0.000195001	0.000525098
6	6	0.000153683	0.000078399	-0.000145880
7	6	-0.000334466	-0.000196965	-0.000039920
8	1	-0.000075574	-0.000018020	0.000026746
9	1	-0.000019475	-0.000099276	0.000091635
10	1	-0.000085284	-0.000064456	0.000053618
11	1	0.000021919	-0.000028350	0.000068925
12	1	-0.000003680	0.000014955	-0.000019686
13	1	0.000014778	0.000092149	0.000038978
14	35	0.000186314	0.000171294	0.000074944
15	1	0.000565991	-0.000270669	-0.000358640
16	6	0.000189009	0.000583085	0.000074324
17	6	0.000016316	-0.000172008	-0.000027802
18	1	-0.000055074	-0.000138983	-0.000071152
19	1	0.000033706	0.000019679	0.000014488
20	1	-0.000061458	0.000063291	-0.000039226
21	7	0.000166229	0.000276042	-0.000061088
22	1	0.000052252	-0.000024036	0.000101868
23	1	0.000424560	0.000039931	-0.000059617
24	6	0.000553401	0.000481536	-0.000110295
25	6	0.000239570	-0.000069436	0.000332316
26	8	-0.000804824	-0.000581888	-0.000255943
27	1	-0.000115980	-0.000035077	-0.000151417
28	1	-0.000082780	-0.000018403	-0.000006482
29	1	-0.000119163	0.000063392	0.000049100
30	6	-0.000122239	0.000000243	0.000077113
31	1	-0.000001844	-0.000013588	-0.000008643
32	1	0.000004012	0.000027854	0.000002953
33	1	-0.000017803	0.000006755	-0.000024106

Cartesian Forces: Max 0.001020442 RMS 0.000238508

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.001083465 RMS 0.000234791
Search for a local minimum.
Step number 14 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 6 7 8 10 11
9 12 13 14
DE= -8.25D-05 DEPred=-7.09D-05 R= 1.16D+00
TightC=F SS= 1.41D+00 RLast= 2.60D-01 DXNew= 3.1006D-01 7.7949D-01
Trust test= 1.16D+00 RLast= 2.60D-01 DXMaxT set to 3.10D-01
ITU= 1 1 0 -1 -1 1 1 1 -1 1 0 0 -1 0
Eigenvalues --- 0.00117 0.00236 0.00394 0.00614 0.00723
Eigenvalues --- 0.00835 0.00894 0.01405 0.01440 0.01554
Eigenvalues --- 0.01809 0.01881 0.02117 0.02321 0.02351
Eigenvalues --- 0.02389 0.02438 0.02569 0.02994 0.03073
Eigenvalues --- 0.03083 0.03149 0.03350 0.03644 0.04045
Eigenvalues --- 0.04226 0.04413 0.04925 0.05323 0.05399
Eigenvalues --- 0.05752 0.05797 0.05924 0.07851 0.08609
Eigenvalues --- 0.09500 0.10561 0.12096 0.12365 0.12614
Eigenvalues --- 0.12845 0.13351 0.14476 0.15608 0.15998
Eigenvalues --- 0.16001 0.16001 0.16005 0.16012 0.16025
Eigenvalues --- 0.16104 0.16121 0.17580 0.20975 0.22123
Eigenvalues --- 0.22816 0.22899 0.23528 0.25531 0.26241
Eigenvalues --- 0.29164 0.30228 0.31942 0.32088 0.32498
Eigenvalues --- 0.33648 0.34275 0.34313 0.34341 0.34544
Eigenvalues --- 0.34662 0.34735 0.35030 0.35067 0.35258
Eigenvalues --- 0.35365 0.35574 0.35771 0.35891 0.36418
Eigenvalues --- 0.36620 0.38101 0.39459 0.41971 0.42564
Eigenvalues --- 0.44661 0.45481 0.45948 0.49191 0.54661
Eigenvalues --- 0.57691 0.60610 1.12005
En-DIIS/RFO-DIIS IScMMF= 0 using points: 14 13 12
RFO step: Lambda=-1.47560402D-05.
DidBck=F Rises=F RFO-DIIS coefs: 1.15149 -0.16356 0.01206
Iteration 1 RMS(Cart)= 0.02967456 RMS(Int)= 0.00046323
Iteration 2 RMS(Cart)= 0.00116837 RMS(Int)= 0.00014507
Iteration 3 RMS(Cart)= 0.00000091 RMS(Int)= 0.00014507

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56557	0.00019	-0.00003	0.00009	0.00005	2.56562
R2	2.62136	-0.00003	-0.00017	-0.00049	-0.00066	2.62070
R3	2.03412	-0.00001	0.00001	0.00002	0.00003	2.03414

R4	2.62529	0.00030	-0.00014	0.00024	0.00010	2.62539
R5	2.03068	0.00003	-0.00004	0.00002	-0.00002	2.03066
R6	2.54300	-0.00028	-0.00010	-0.00074	-0.00083	2.54218
R7	2.69917	-0.00038	0.00033	-0.00044	-0.00011	2.69906
R8	2.52039	-0.00023	0.00021	0.00095	0.00116	2.52155
R9	2.09762	0.00061	-0.00084	-0.00029	-0.00113	2.09649
R10	2.78573	0.00001	0.00002	0.00135	0.00138	2.78710
R11	2.90207	-0.00016	0.00000	-0.00040	-0.00040	2.90167
R12	2.06050	-0.00004	0.00002	0.00005	0.00007	2.06057
R13	2.05996	-0.00007	-0.00004	-0.00021	-0.00025	2.05972
R14	2.06862	0.00000	-0.00008	-0.00016	-0.00023	2.06839
R15	2.07861	-0.00005	-0.00014	-0.00066	-0.00080	2.07781
R16	2.75046	0.00023	0.00012	0.00201	0.00213	2.75259
R17	4.16905	-0.00004	0.00468	0.00786	0.01254	4.18160
R18	2.50616	0.00002	-0.00001	-0.00004	-0.00005	2.50611
R19	2.05533	0.00004	0.00011	0.00006	0.00017	2.05550
R20	2.04349	-0.00002	0.00001	-0.00006	-0.00004	2.04344
R21	2.04674	0.00009	-0.00003	0.00015	0.00013	2.04686
R22	1.91358	0.00008	-0.00006	0.00000	-0.00006	1.91352
R23	1.92637	0.00007	-0.00019	-0.00045	-0.00064	1.92573
R24	3.91466	-0.00012	0.00312	0.00457	0.00769	3.92235
R25	2.76667	0.00040	-0.00005	0.00164	0.00111	2.76778
R26	2.72958	-0.00021	-0.00028	-0.00189	-0.00197	2.72761
R27	2.05514	-0.00004	0.00001	0.00006	0.00007	2.05521
R28	2.05217	0.00007	0.00004	0.00030	0.00034	2.05251
R29	2.74716	-0.00013	0.00019	-0.00040	0.00008	2.74724
R30	2.05623	0.00009	0.00008	0.00030	0.00038	2.05661
R31	2.84176	-0.00009	0.00001	-0.00019	-0.00018	2.84159
R32	2.06721	-0.00001	-0.00002	-0.00005	-0.00006	2.06715
R33	2.06782	-0.00002	0.00001	-0.00001	0.00000	2.06782
R34	2.06504	0.00000	0.00002	0.00003	0.00004	2.06508
A1	1.87227	-0.00013	0.00001	0.00043	0.00043	1.87271
A2	2.28047	-0.00002	0.00020	-0.00017	0.00003	2.28050
A3	2.13040	0.00015	-0.00022	-0.00021	-0.00043	2.12997
A4	1.86438	-0.00010	0.00003	-0.00056	-0.00053	1.86385
A5	2.27456	0.00016	-0.00012	0.00073	0.00062	2.27518
A6	2.14424	-0.00006	0.00009	-0.00019	-0.00010	2.14413
A7	1.89743	0.00000	0.00003	0.00067	0.00069	1.89813
A8	2.25642	-0.00003	-0.00019	-0.00098	-0.00118	2.25524
A9	2.12933	0.00003	0.00016	0.00031	0.00047	2.12980
A10	1.88987	0.00008	-0.00006	-0.00039	-0.00045	1.88942
A11	2.14924	0.00096	-0.00042	0.00385	0.00343	2.15267
A12	2.24361	-0.00104	0.00044	-0.00355	-0.00312	2.24049
A13	1.90077	0.00015	-0.00003	-0.00006	-0.00010	1.90067

A14	2.21279	0.00050	-0.00069	-0.00325	-0.00395	2.20884
A15	2.16628	-0.00064	0.00061	0.00390	0.00451	2.17080
A16	1.96007	0.00008	-0.00010	0.00049	0.00039	1.96046
A17	1.87339	-0.00024	0.00067	0.00124	0.00191	1.87530
A18	1.88858	0.00014	-0.00050	-0.00273	-0.00323	1.88535
A19	1.91815	-0.00003	-0.00007	0.00112	0.00105	1.91920
A20	1.93183	-0.00001	0.00012	-0.00092	-0.00081	1.93102
A21	1.88952	0.00004	-0.00012	0.00084	0.00072	1.89024
A22	1.90642	0.00014	0.00007	-0.00028	-0.00020	1.90621
A23	1.89259	-0.00004	0.00032	0.00117	0.00150	1.89409
A24	1.88291	-0.00008	-0.00034	0.00073	0.00039	1.88330
A25	1.87552	-0.00003	0.00023	0.00052	0.00074	1.87627
A26	1.91002	0.00015	0.00018	-0.00099	-0.00081	1.90921
A27	1.99512	-0.00013	-0.00044	-0.00114	-0.00158	1.99355
A28	2.16219	0.00004	-0.00025	-0.00010	-0.00035	2.16184
A29	1.94520	0.00010	-0.00015	0.00056	0.00041	1.94561
A30	2.17578	-0.00014	0.00040	-0.00044	-0.00005	2.17573
A31	2.07559	-0.00002	-0.00002	0.00003	0.00001	2.07560
A32	2.16240	-0.00001	0.00009	-0.00006	0.00002	2.16243
A33	2.04519	0.00003	-0.00007	0.00003	-0.00004	2.04515
A34	1.94222	0.00025	0.00022	-0.00097	-0.00068	1.94154
A35	1.92388	-0.00104	-0.00031	-0.00042	-0.00071	1.92317
A36	1.88387	0.00040	0.00021	-0.00022	-0.00003	1.88384
A37	2.08591	0.00008	0.00017	0.00131	0.00122	2.08713
A38	2.07697	0.00002	0.00027	0.00000	0.00050	2.07747
A39	1.99423	0.00024	0.00016	0.00175	0.00191	1.99614
A40	2.01107	-0.00015	-0.00028	-0.00133	-0.00171	2.00936
A41	2.02809	-0.00008	-0.00032	-0.00111	-0.00142	2.02668
A42	2.02294	0.00018	0.00016	0.00130	0.00157	2.02452
A43	2.13445	-0.00008	-0.00023	-0.00018	-0.00059	2.13386
A44	1.97509	-0.00011	-0.00007	-0.00203	-0.00219	1.97289
A45	2.02722	0.00020	-0.00007	-0.00034	-0.00039	2.02683
A46	2.03676	-0.00007	0.00016	0.00063	0.00082	2.03758
A47	2.50502	0.00013	0.00466	0.01738	0.02103	2.52605
A48	2.50557	-0.00016	0.00387	0.01222	0.01479	2.52036
A49	1.93214	0.00000	-0.00016	-0.00045	-0.00061	1.93153
A50	1.91665	0.00002	0.00005	0.00037	0.00042	1.91708
A51	1.94129	-0.00004	0.00011	0.00012	0.00023	1.94152
A52	1.88062	-0.00001	-0.00012	-0.00044	-0.00056	1.88006
A53	1.89338	0.00002	0.00007	0.00031	0.00038	1.89376
A54	1.89834	0.00001	0.00004	0.00008	0.00012	1.89846
A55	3.35824	-0.00108	0.00532	-0.01280	-0.00747	3.35077
A56	2.95399	-0.00108	-0.00610	-0.02422	-0.03037	2.92363
A57	2.89152	0.00005	-0.00827	-0.02836	-0.03663	2.85490

A58	3.21456	-0.00003	0.00104	0.00819	0.00920	3.22376
D1	0.00768	-0.00010	0.00064	-0.00980	-0.00915	-0.00146
D2	-3.12992	-0.00005	0.00010	-0.00589	-0.00579	-3.13571
D3	3.13862	-0.00004	0.00000	-0.00402	-0.00402	3.13461
D4	0.00102	0.00001	-0.00055	-0.00012	-0.00066	0.00036
D5	-0.00962	0.00006	-0.00062	0.00930	0.00867	-0.00094
D6	-3.06578	-0.00001	0.00077	0.00155	0.00234	-3.06344
D7	3.14151	0.00001	-0.00005	0.00413	0.00408	-3.13760
D8	0.08535	-0.00006	0.00135	-0.00362	-0.00226	0.08309
D9	-0.00321	0.00010	-0.00045	0.00703	0.00658	0.00336
D10	3.13678	0.00006	-0.00091	0.00245	0.00154	3.13832
D11	3.13476	0.00006	0.00005	0.00349	0.00354	3.13830
D12	-0.00843	0.00001	-0.00041	-0.00109	-0.00150	-0.00993
D13	-0.00277	-0.00007	0.00007	-0.00128	-0.00122	-0.00398
D14	3.10875	-0.00007	-0.00134	-0.00418	-0.00553	3.10323
D15	3.14028	-0.00002	0.00048	0.00290	0.00339	-3.13951
D16	-0.03138	-0.00002	-0.00093	0.00000	-0.00092	-0.03230
D17	0.05599	0.00007	0.00481	0.01889	0.02371	0.07969
D18	-3.07981	0.00000	0.00476	0.01624	0.02099	-3.05882
D19	-3.08739	0.00002	0.00430	0.01377	0.01808	-3.06931
D20	0.05999	-0.00005	0.00425	0.01112	0.01536	0.07536
D21	0.00762	0.00001	0.00034	-0.00491	-0.00456	0.00306
D22	3.06657	0.00014	-0.00108	0.00216	0.00110	3.06768
D23	-3.10178	-0.00004	0.00186	-0.00197	-0.00012	-3.10189
D24	-0.04282	0.00009	0.00045	0.00510	0.00555	-0.03728
D25	1.55360	0.00019	0.00769	0.01553	0.02322	1.57683
D26	-2.61951	0.00005	0.00799	0.01805	0.02604	-2.59347
D27	-0.58391	0.00005	0.00795	0.01828	0.02623	-0.55768
D28	-1.49033	0.00007	0.00932	0.00694	0.01626	-1.47407
D29	0.61974	-0.00007	0.00962	0.00945	0.01908	0.63881
D30	2.65535	-0.00008	0.00959	0.00968	0.01926	2.67461
D31	-1.13389	-0.00021	-0.00008	0.01196	0.01188	-1.12201
D32	0.90507	-0.00019	0.00041	0.01309	0.01350	0.91857
D33	3.07459	-0.00042	-0.00014	0.01288	0.01274	3.08733
D34	3.06519	0.00005	-0.00082	0.00933	0.00851	3.07370
D35	-1.17904	0.00008	-0.00033	0.01045	0.01012	-1.16891
D36	0.99048	-0.00016	-0.00088	0.01024	0.00936	0.99985
D37	0.97895	0.00003	-0.00070	0.00815	0.00745	0.98640
D38	3.01791	0.00005	-0.00022	0.00928	0.00906	3.02697
D39	-1.09576	-0.00019	-0.00076	0.00906	0.00830	-1.08745
D40	2.77910	0.00028	-0.00444	-0.00678	-0.01123	2.76787
D41	-1.41454	0.00025	-0.00423	-0.00796	-0.01217	-1.42672
D42	0.70669	0.00007	-0.00443	-0.00632	-0.01076	0.69593
D43	2.79623	0.00005	-0.00422	-0.00749	-0.01170	2.78453

D44	-1.39759	0.00008	-0.00455	-0.00549	-0.01006	-1.40765
D45	0.69194	0.00006	-0.00435	-0.00667	-0.01100	0.68094
D46	-3.13543	-0.00003	0.00026	-0.00006	0.00020	-3.13524
D47	0.00762	-0.00001	0.00039	0.00068	0.00107	0.00869
D48	-0.00039	0.00006	0.00032	0.00295	0.00327	0.00287
D49	-3.14053	0.00007	0.00045	0.00369	0.00414	-3.13639
D50	1.29983	0.00015	0.00731	0.04756	0.05495	1.35478
D51	-0.60311	0.00030	-0.00427	0.00121	-0.00307	-0.60619
D52	-2.90701	-0.00012	0.00627	0.03979	0.04606	-2.86095
D53	1.47323	0.00003	-0.00532	-0.00656	-0.01196	1.46127
D54	-2.69936	-0.00006	-0.00003	-0.00200	-0.00195	-2.70132
D55	-0.01366	0.00000	0.00025	0.00238	0.00265	-0.01100
D56	-0.02257	-0.00004	0.00019	-0.00181	-0.00160	-0.02417
D57	2.66314	0.00002	0.00046	0.00258	0.00301	2.66615
D58	1.85463	-0.00013	-0.01040	-0.04000	-0.05067	1.80396
D59	-0.56073	-0.00011	-0.00974	-0.03870	-0.04861	-0.60934
D60	0.61080	0.00025	0.01095	0.04241	0.05344	0.66423
D61	-1.81487	0.00025	0.01086	0.04431	0.05527	-1.75961
D62	2.55111	-0.00007	-0.00014	-0.00149	-0.00158	2.54953
D63	-1.65760	-0.00007	-0.00035	-0.00208	-0.00238	-1.65999
D64	0.44470	-0.00007	-0.00019	-0.00165	-0.00180	0.44289
D65	1.35035	0.00003	0.00014	0.00000	0.00008	1.35042
D66	-2.85837	0.00003	-0.00008	-0.00059	-0.00073	-2.85910
D67	-0.75607	0.00003	0.00008	-0.00016	-0.00015	-0.75622
D68	-1.04973	0.00005	0.00014	0.00309	0.00324	-1.04649
D69	1.02474	0.00005	-0.00007	0.00250	0.00244	1.02718
D70	3.12704	0.00005	0.00008	0.00292	0.00302	3.13006

Item	Value	Threshold	Converged?
Maximum Force	0.001083	0.000450	NO
RMS Force	0.000235	0.000300	YES
Maximum Displacement	0.175911	0.001800	NO
RMS Displacement	0.030336	0.001200	NO

Predicted change in Energy=-3.700924D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.895756	2.138621	-0.308066
2	6	0	-3.755881	1.149129	0.044569
3	7	0	-3.011583	-0.021525	0.120322
4	6	0	-1.730199	0.260656	-0.176591

5	7	0	-1.640084	1.565302	-0.441658
6	6	0	-0.376820	2.272648	-0.722855
7	6	0	0.348067	2.704298	0.560100
8	1	0	-3.065459	3.187868	-0.478265
9	1	0	-4.812588	1.181494	0.237040
10	1	0	0.255734	1.595942	-1.298124
11	1	0	-0.606103	3.138202	-1.344346
12	1	0	-0.267472	3.435877	1.092955
13	1	0	0.456656	1.825831	1.212378
14	35	0	0.203708	-2.349339	0.292542
15	1	0	-0.918414	-0.495184	-0.154071
16	6	0	-3.438278	-1.342838	0.455065
17	6	0	-4.702340	-1.677372	0.676384
18	1	0	-2.597910	-2.031467	0.507181
19	1	0	-4.935262	-2.702265	0.930640
20	1	0	-5.530631	-0.981975	0.616548
21	7	0	1.609599	3.322502	0.175299
22	1	0	1.962087	3.924479	0.909273
23	1	0	2.311097	2.606174	-0.007036
24	6	0	3.719331	-0.236416	-1.111678
25	6	0	3.612063	-0.479907	0.328596
26	8	0	3.397397	0.850109	-0.217702
27	1	0	4.701897	-0.162672	-1.572047
28	1	0	2.909331	-0.554269	-1.761735
29	1	0	2.692830	-0.955727	0.664783
30	6	0	4.821284	-0.648000	1.206465
31	1	0	4.635810	-0.235188	2.202344
32	1	0	5.049856	-1.711617	1.324108
33	1	0	5.693149	-0.146003	0.779794

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357668	0.000000			
3	N	2.205258	1.389298	0.000000		
4	C	2.214173	2.222989	1.345261	0.000000	
5	N	1.386814	2.210478	2.171371	1.334347	0.000000
6	C	2.556375	3.642704	3.593906	2.485589	1.474872
7	C	3.405303	4.418904	4.348651	3.291397	2.500715
8	H	1.076423	2.215061	3.265182	3.231485	2.160036
9	H	2.210764	1.074579	2.168985	3.243478	3.266912
10	H	3.347627	4.253883	3.911975	2.642869	2.080529
11	H	2.704728	3.975752	4.232666	3.302653	2.087577
12	H	3.248631	4.300852	4.519933	3.719320	2.781753

13	H	3.694354	4.423479	4.078479	3.026771	2.683287
14	Br	5.487184	5.289529	3.973219	3.282096	4.388968
15	H	3.297048	3.285489	2.163562	1.109413	2.202071
16	C	3.605170	2.545442	1.428281	2.426461	3.534811
17	C	4.335285	3.046979	2.430986	3.649266	4.598083
18	H	4.259457	3.416299	2.088218	2.544463	3.841155
19	H	5.397050	4.124233	3.397576	4.503031	5.563589
20	H	4.187553	2.831696	2.741224	4.076332	4.769148
21	N	4.683315	5.790425	5.704460	4.544555	3.745508
22	H	5.316939	6.414471	6.397717	5.313725	4.512911
23	H	5.236463	6.239701	5.937335	4.675712	4.109032
24	C	7.074318	7.689957	6.846109	5.551473	5.693720
25	C	7.043702	7.551228	6.642754	5.416957	5.688693
26	O	6.424345	7.164328	6.476808	5.161530	5.092924
27	H	8.038528	8.710240	7.898216	6.595330	6.669663
28	H	6.562305	7.112619	6.235638	4.970113	5.189640
29	H	6.461711	6.811825	5.805988	4.663763	5.133609
30	C	8.343367	8.840104	7.932590	6.757250	7.025973
31	H	8.286230	8.774554	7.928625	6.814049	7.044101
32	H	8.978924	9.346769	8.324200	7.218802	7.655810
33	H	8.953895	9.565673	8.730565	7.495742	7.628684

		6	7	8	9	10
6	C	0.000000				
7	C	1.535499	0.000000			
8	H	2.850655	3.600584	0.000000		
9	H	4.667767	5.390330	2.754933	0.000000	
10	H	1.090408	2.165636	3.773158	5.311909	0.000000
11	H	1.089956	2.173852	2.607872	4.901429	1.767333
12	H	2.159219	1.094546	3.218535	5.145183	3.062085
13	H	2.153939	1.099528	4.137476	5.397349	2.529000
14	Br	4.767684	5.062774	6.476285	6.134581	4.254194
15	H	2.877105	3.514357	4.275486	4.257793	2.657120
16	C	4.881778	5.543171	4.640840	2.882449	5.035456
17	C	6.022513	6.687240	5.261479	2.894528	6.260652
18	H	4.997163	5.577549	5.332089	3.911636	4.955856
19	H	6.947172	7.568473	6.338363	3.947115	7.098479
20	H	6.240861	6.939084	4.966214	2.310890	6.617677
21	N	2.419656	1.456609	4.722440	6.769949	2.642903
22	H	3.295887	2.053246	5.267264	7.339760	3.634051
23	H	2.801524	2.045668	5.428423	7.268849	2.629068
24	C	4.819237	4.775779	7.626291	8.753465	3.922857
25	C	4.959163	4.565789	7.661130	8.587397	4.268526
26	O	4.064912	3.652589	6.877610	8.229244	3.404942
27	H	5.696076	5.632176	8.529613	9.777781	4.789167

28	H	4.457524	4.750710	7.165822	8.163088	3.446726
29	H	4.665908	4.347948	7.185668	7.815495	4.037754
30	C	6.266797	5.627198	8.930449	9.853848	5.670317
31	H	6.322380	5.451814	8.843784	9.754057	5.898422
32	H	7.036564	6.495447	9.649448	10.335357	6.387461
33	H	6.704651	6.061549	9.455719	10.603175	6.075985

		11	12	13	14	15
11	H	0.000000				
12	H	2.478653	0.000000			
13	H	3.064084	1.769427	0.000000		
14	Br	5.783451	5.859300	4.282771	0.000000	
15	H	3.836116	4.175170	3.024089	2.212807	0.000000
16	C	5.598108	5.770357	5.077843	3.781999	2.727504
17	C	6.637188	6.781364	6.258991	4.966707	4.050348
18	H	5.841312	5.972095	4.970556	2.827750	2.370258
19	H	7.617627	7.713066	7.046688	5.190447	4.709869
20	H	6.713564	6.888049	6.639759	5.904007	4.701421
21	N	2.693070	2.092449	2.155187	5.844661	4.590649
22	H	3.506085	2.289848	2.600484	6.544696	5.381580
23	H	3.252923	2.923595	2.352628	5.393324	4.479931
24	C	5.491044	5.851559	4.505458	4.335422	4.742642
25	C	5.803652	5.564927	4.006757	3.887540	4.556142
26	O	4.746863	4.672824	3.412495	4.549338	4.521072
27	H	6.254797	6.689277	5.452453	5.337782	5.805956
28	H	5.115352	5.844878	4.530545	3.842230	4.152073
29	H	5.628482	5.313465	3.610734	2.876882	3.731448
30	C	7.092143	6.525824	5.016957	5.005179	5.900724
31	H	7.171919	6.224921	4.763734	5.268824	6.039015
32	H	7.913992	7.404330	5.798578	4.995595	6.267773
33	H	7.414752	6.961102	5.612140	5.935156	6.686314

		16	17	18	19	20
16	C	0.000000				
17	C	1.326178	0.000000			
18	H	1.087725	2.140710	0.000000		
19	H	2.077300	1.081343	2.468300	0.000000	
20	H	2.129375	1.083154	3.116769	1.847299	0.000000
21	N	6.879297	8.067862	6.817497	8.927685	8.349019
22	H	7.557438	8.709165	7.511893	9.564915	8.961015
23	H	6.990246	8.246462	6.772775	9.031527	8.646177
24	C	7.410143	8.729151	6.763908	9.227863	9.439514
25	C	7.104080	8.407389	6.403358	8.852011	9.160996
26	O	7.210277	8.531899	6.691236	9.130787	9.152169
27	H	8.471389	9.787208	7.816826	10.275593	10.495992
28	H	6.769652	8.071141	6.136758	8.567404	8.779073

29	H	6.146895	7.430306	5.401294	7.829998	8.223644
30	C	8.322726	9.593748	7.579407	9.974281	10.374087
31	H	8.334913	9.571285	7.643749	9.965396	10.316442
32	H	8.540471	9.773743	7.697921	10.041851	10.629192
33	H	9.215249	10.508187	8.507112	10.932537	11.256053

		21	22	23	24	25
21	N	0.000000				
22	H	1.012591	0.000000			
23	H	1.019054	1.642972	0.000000		
24	C	4.332802	4.948252	3.359118	0.000000	
25	C	4.300195	4.739011	3.365867	1.464644	0.000000
26	O	3.076263	3.575183	2.075618	1.443389	1.453777
27	H	4.976139	5.510745	3.978906	1.087572	2.213779
28	H	4.524462	5.300069	3.664049	1.086142	2.206546
29	H	4.440295	4.940665	3.644749	2.174150	1.088309
30	C	5.209905	5.401009	4.285239	2.599517	1.503703
31	H	5.091563	5.111130	4.284738	3.438411	2.149157
32	H	6.204634	6.439874	5.283566	3.143178	2.139019
33	H	5.391782	5.523261	4.430785	2.735287	2.155456

		26	27	28	29	30
26	O	0.000000				
27	H	2.135813	0.000000			
28	H	2.143484	1.844620	0.000000		
29	H	2.129845	3.109453	2.469014	0.000000	
30	C	2.509987	2.823106	3.531934	2.217754	0.000000
31	H	2.927141	3.775666	4.335489	2.580396	1.093887
32	H	3.416174	3.302730	3.929851	2.561572	1.094242
33	H	2.694014	2.552256	3.791529	3.109790	1.092794

		31	32	33
31	H	0.000000		
32	H	1.767081	0.000000	
33	H	1.774702	1.777992	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.831356	2.245180	-0.186164

2	6	0	-3.702734	1.234590	0.064171
3	7	0	-2.972797	0.053570	0.013843
4	6	0	-1.688809	0.349885	-0.256892
5	7	0	-1.583242	1.673956	-0.384070
6	6	0	-0.312062	2.391630	-0.594531
7	6	0	0.421518	2.677581	0.723744
8	1	0	-2.988498	3.308459	-0.244752
9	1	0	-4.758445	1.259313	0.263134
10	1	0	0.310532	1.771423	-1.240062
11	1	0	-0.532253	3.320290	-1.120944
12	1	0	-0.183496	3.356597	1.332781
13	1	0	0.520945	1.734304	1.279896
14	35	0	0.213855	-2.318016	-0.071596
15	1	0	-0.886392	-0.413868	-0.316935
16	6	0	-3.414939	-1.290329	0.209892
17	6	0	-4.682457	-1.630985	0.399893
18	1	0	-2.583030	-1.990696	0.186215
19	1	0	-4.927382	-2.674012	0.546213
20	1	0	-5.502225	-0.923224	0.416555
21	7	0	1.689586	3.317497	0.400913
22	1	0	2.051450	3.834886	1.192561
23	1	0	2.381670	2.615849	0.141722
24	6	0	3.751646	-0.111958	-1.260388
25	6	0	3.645192	-0.503854	0.146832
26	8	0	3.445570	0.878612	-0.256166
27	1	0	4.733826	-0.002173	-1.714353
28	1	0	2.936049	-0.350101	-1.936992
29	1	0	2.721029	-1.001205	0.434898
30	6	0	4.854561	-0.777641	0.997472
31	1	0	4.676858	-0.469351	2.031865
32	1	0	5.070251	-1.850405	1.002056
33	1	0	5.731443	-0.244197	0.622352

Rotational constants (GHZ): 0.4698819 0.2524838 0.1723171

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1294.3305866551 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 482 RedAO= T EigKep= 4.04D-06 NBF= 482
NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999997 -0.001871 0.000640 0.001469 Ang= -0.28 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3205.64702174 A.U. after 11 cycles
NFock= 11 Conv=0.62D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Atomic Forces (Hartrees/Bohr)
Number Number X Y Z

Center Number	Atomic Number	X	Y	Z
1	6	0.000141261	0.000171038	0.000521061
2	6	-0.000227026	0.000142890	-0.000669805
3	7	0.000009743	-0.000453247	0.000415487
4	6	-0.000182992	0.000877019	-0.000006486
5	7	0.000078880	-0.000272939	-0.000203401
6	6	-0.000103206	-0.000296478	-0.000201761
7	6	0.000145782	0.000073051	-0.000052453
8	1	-0.000059129	0.000005445	0.000201086
9	1	-0.000023741	-0.000129799	0.000005079
10	1	-0.000070858	-0.000046129	0.000105133
11	1	0.000175314	0.000014004	-0.000027607

12	1	-0.000096167	0.000017465	-0.000031805
13	1	-0.000051298	0.000015788	0.000069100
14	35	0.000026061	0.000113153	0.000007170
15	1	0.000260671	-0.000495044	0.000035020
16	6	0.000176287	0.000379971	-0.000105194
17	6	-0.000059537	-0.000124032	-0.000018518
18	1	-0.000005766	-0.000076919	0.000034589
19	1	0.000036635	0.000003611	0.000029595
20	1	-0.000031944	0.000045581	-0.000013180
21	7	-0.000214721	0.000198800	-0.000068196
22	1	0.000051173	-0.000042697	0.000128354
23	1	0.000358137	-0.000097111	-0.000038032
24	6	0.000300214	0.000299369	-0.000011905
25	6	0.000073620	-0.000058875	0.000268362
26	8	-0.000569775	-0.000178043	-0.000339262
27	1	-0.000097752	0.000011794	-0.000102623
28	1	0.000050353	-0.000031015	-0.000096598
29	1	0.000020399	-0.000064228	0.000136339
30	6	-0.000102799	-0.000038374	0.000087275
31	1	0.000003908	-0.000005039	-0.000016136
32	1	-0.000023877	0.000032731	-0.000023236
33	1	0.000012149	0.000008259	-0.000017452

Cartesian Forces: Max 0.000877019 RMS 0.000202260

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000508378 RMS 0.000136007
Search for a local minimum.
Step number 15 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 10 11 9 12 13
14 15
DE= -3.93D-05 DEPred=-3.70D-05 R= 1.06D+00
TightC=F SS= 1.41D+00 RLast= 1.62D-01 DXNew= 5.2145D-01 4.8553D-01
Trust test= 1.06D+00 RLast= 1.62D-01 DXMaxT set to 4.86D-01
ITU= 1 1 1 0 -1 -1 1 1 1 -1 1 0 0 -1 0
Eigenvalues --- 0.00067 0.00256 0.00394 0.00604 0.00723
Eigenvalues --- 0.00809 0.00840 0.01408 0.01463 0.01537

Eigenvalues --- 0.01851 0.01896 0.02121 0.02336 0.02389
Eigenvalues --- 0.02400 0.02441 0.02938 0.03071 0.03086
Eigenvalues --- 0.03161 0.03289 0.03357 0.03728 0.04048
Eigenvalues --- 0.04297 0.04416 0.04907 0.05411 0.05598
Eigenvalues --- 0.05751 0.05827 0.05925 0.07892 0.08677
Eigenvalues --- 0.09549 0.10441 0.12156 0.12388 0.12639
Eigenvalues --- 0.12852 0.13440 0.15182 0.15772 0.16000
Eigenvalues --- 0.16001 0.16001 0.16005 0.16013 0.16032
Eigenvalues --- 0.16104 0.16630 0.18005 0.21348 0.22126
Eigenvalues --- 0.22881 0.22928 0.23939 0.25411 0.27079
Eigenvalues --- 0.29164 0.30413 0.32042 0.32434 0.32463
Eigenvalues --- 0.33659 0.34285 0.34319 0.34342 0.34546
Eigenvalues --- 0.34674 0.34736 0.35031 0.35069 0.35257
Eigenvalues --- 0.35374 0.35576 0.35843 0.35902 0.36421
Eigenvalues --- 0.36624 0.38196 0.39620 0.41942 0.42728
Eigenvalues --- 0.44653 0.45484 0.46372 0.49206 0.54768
Eigenvalues --- 0.57788 0.60628 1.09730
En-DIIS/RFO-DIIS IScMMF= 0 using points: 15 14 13 12
RFO step: Lambda=-7.81607635D-06.
DidBck=F Rises=F RFO-DIIS coefs: 1.23298 0.13394 -0.52728 0.16035
Iteration 1 RMS(Cart)= 0.05441108 RMS(Int)= 0.00120220
Iteration 2 RMS(Cart)= 0.00285264 RMS(Int)= 0.00039156
Iteration 3 RMS(Cart)= 0.00000563 RMS(Int)= 0.00039156
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00039156

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56562	0.00011	-0.00002	0.00003	0.00000	2.56562
R2	2.62070	0.00016	-0.00050	-0.00016	-0.00067	2.62003
R3	2.03414	-0.00002	0.00002	0.00002	0.00004	2.03419
R4	2.62539	0.00016	-0.00027	0.00053	0.00026	2.62565
R5	2.03066	0.00002	-0.00007	-0.00001	-0.00008	2.03058
R6	2.54218	-0.00004	-0.00040	-0.00071	-0.00111	2.54107
R7	2.69906	-0.00027	0.00064	-0.00085	-0.00020	2.69886
R8	2.52155	-0.00040	0.00075	0.00010	0.00085	2.52240
R9	2.09649	0.00047	-0.00198	0.00073	-0.00125	2.09523
R10	2.78710	-0.00017	0.00047	0.00032	0.00079	2.78790
R11	2.90167	-0.00010	-0.00005	-0.00103	-0.00107	2.90060
R12	2.06057	-0.00007	0.00008	-0.00019	-0.00012	2.06045
R13	2.05972	-0.00001	-0.00015	-0.00008	-0.00023	2.05949
R14	2.06839	0.00005	-0.00022	0.00004	-0.00019	2.06821
R15	2.07781	0.00003	-0.00048	-0.00049	-0.00097	2.07683
R16	2.75259	-0.00010	0.00087	0.00095	0.00182	2.75441
R17	4.18160	-0.00008	0.01262	0.00293	0.01555	4.19715
R18	2.50611	0.00007	-0.00004	0.00014	0.00010	2.50621

R19	2.05550	0.00004	0.00030	-0.00020	0.00011	2.05561
R20	2.04344	-0.00001	0.00001	-0.00004	-0.00002	2.04342
R21	2.04686	0.00006	-0.00001	0.00009	0.00009	2.04695
R22	1.91352	0.00009	-0.00014	0.00017	0.00003	1.91355
R23	1.92573	0.00014	-0.00056	0.00008	-0.00047	1.92526
R24	3.92235	-0.00013	0.00818	0.00099	0.00917	3.93152
R25	2.76778	0.00027	0.00026	0.00140	0.00040	2.76818
R26	2.72761	-0.00010	-0.00112	-0.00159	-0.00221	2.72540
R27	2.05521	-0.00004	0.00004	-0.00004	-0.00001	2.05521
R28	2.05251	0.00003	0.00018	0.00021	0.00040	2.05291
R29	2.74724	0.00009	0.00039	0.00024	0.00141	2.74865
R30	2.05661	0.00005	0.00026	0.00028	0.00054	2.05715
R31	2.84159	-0.00007	-0.00002	-0.00032	-0.00034	2.84125
R32	2.06715	-0.00002	-0.00005	-0.00009	-0.00014	2.06701
R33	2.06782	-0.00004	0.00001	-0.00007	-0.00005	2.06776
R34	2.06508	0.00002	0.00005	0.00006	0.00011	2.06519
A1	1.87271	-0.00009	0.00018	0.00002	0.00020	1.87291
A2	2.28050	-0.00006	0.00039	-0.00051	-0.00012	2.28038
A3	2.12997	0.00014	-0.00058	0.00048	-0.00010	2.12987
A4	1.86385	-0.00004	-0.00007	-0.00041	-0.00048	1.86337
A5	2.27518	0.00015	-0.00006	0.00105	0.00099	2.27617
A6	2.14413	-0.00011	0.00013	-0.00061	-0.00049	2.14365
A7	1.89813	-0.00008	0.00021	0.00040	0.00061	1.89874
A8	2.25524	0.00009	-0.00066	-0.00048	-0.00115	2.25409
A9	2.12980	-0.00001	0.00045	0.00008	0.00053	2.13032
A10	1.88942	0.00016	-0.00016	-0.00023	-0.00040	1.88903
A11	2.15267	-0.00002	-0.00013	0.00316	0.00302	2.15570
A12	2.24049	-0.00014	0.00018	-0.00297	-0.00280	2.23769
A13	1.90067	0.00005	-0.00017	0.00022	0.00005	1.90072
A14	2.20884	0.00046	-0.00240	-0.00195	-0.00435	2.20449
A15	2.17080	-0.00051	0.00243	0.00204	0.00447	2.17527
A16	1.96046	-0.00004	-0.00008	-0.00016	-0.00024	1.96022
A17	1.87530	-0.00011	0.00200	-0.00025	0.00175	1.87705
A18	1.88535	0.00020	-0.00187	-0.00055	-0.00243	1.88292
A19	1.91920	0.00002	0.00017	0.00058	0.00074	1.91994
A20	1.93102	-0.00007	-0.00010	-0.00046	-0.00057	1.93046
A21	1.89024	0.00000	-0.00008	0.00087	0.00080	1.89104
A22	1.90621	0.00007	-0.00003	0.00052	0.00050	1.90671
A23	1.89409	-0.00007	0.00107	0.00047	0.00154	1.89563
A24	1.88330	-0.00008	-0.00043	-0.00080	-0.00124	1.88206
A25	1.87627	-0.00002	0.00059	0.00062	0.00120	1.87747
A26	1.90921	0.00008	0.00004	-0.00003	0.00001	1.90922
A27	1.99355	0.00003	-0.00119	-0.00072	-0.00191	1.99164
A28	2.16184	0.00005	-0.00063	0.00058	-0.00005	2.16179

A29	1.94561	0.00004	-0.00019	0.00058	0.00040	1.94600
A30	2.17573	-0.00010	0.00082	-0.00116	-0.00034	2.17539
A31	2.07560	-0.00003	-0.00005	0.00008	0.00003	2.07563
A32	2.16243	0.00000	0.00020	-0.00021	-0.00001	2.16242
A33	2.04515	0.00003	-0.00015	0.00013	-0.00002	2.04513
A34	1.94154	0.00002	0.00030	-0.00199	-0.00146	1.94008
A35	1.92317	-0.00038	-0.00076	-0.00050	-0.00120	1.92197
A36	1.88384	0.00020	0.00033	0.00090	0.00116	1.88500
A37	2.08713	0.00002	0.00073	0.00085	0.00085	2.08798
A38	2.07747	0.00009	0.00087	0.00004	0.00153	2.07900
A39	1.99614	0.00007	0.00078	0.00129	0.00203	1.99817
A40	2.00936	-0.00001	-0.00126	0.00035	-0.00113	2.00824
A41	2.02668	-0.00011	-0.00104	-0.00146	-0.00248	2.02420
A42	2.02452	0.00023	0.00088	0.00120	0.00232	2.02683
A43	2.13386	-0.00007	-0.00060	-0.00049	-0.00148	2.13238
A44	1.97289	0.00006	-0.00087	-0.00018	-0.00128	1.97162
A45	2.02683	0.00011	-0.00024	0.00006	-0.00013	2.02670
A46	2.03758	-0.00016	0.00051	-0.00014	0.00046	2.03803
A47	2.52605	0.00014	0.01468	0.01554	0.02752	2.55357
A48	2.52036	-0.00011	0.01155	0.00912	0.01712	2.53748
A49	1.93153	0.00001	-0.00047	-0.00044	-0.00091	1.93062
A50	1.91708	-0.00004	0.00018	0.00019	0.00037	1.91745
A51	1.94152	0.00000	0.00030	0.00005	0.00035	1.94187
A52	1.88006	0.00001	-0.00040	-0.00022	-0.00062	1.87944
A53	1.89376	0.00001	0.00024	0.00036	0.00060	1.89436
A54	1.89846	0.00002	0.00013	0.00006	0.00019	1.89865
A55	3.35077	-0.00034	0.00673	0.00049	0.00722	3.35799
A56	2.92363	-0.00050	-0.02032	-0.01616	-0.03649	2.88714
A57	2.85490	0.00004	-0.02659	-0.00263	-0.02921	2.82568
A58	3.22376	-0.00017	0.00713	-0.01755	-0.01051	3.21325
D1	-0.00146	0.00031	0.00014	0.00484	0.00498	0.00352
D2	-3.13571	0.00011	-0.00068	-0.00063	-0.00131	-3.13702
D3	3.13461	0.00013	-0.00068	0.00270	0.00202	3.13663
D4	0.00036	-0.00006	-0.00150	-0.00277	-0.00427	-0.00391
D5	-0.00094	-0.00031	-0.00032	-0.00415	-0.00447	-0.00542
D6	-3.06344	-0.00024	0.00147	-0.00861	-0.00714	-3.07058
D7	-3.13760	-0.00015	0.00041	-0.00224	-0.00183	-3.13942
D8	0.08309	-0.00008	0.00221	-0.00669	-0.00449	0.07860
D9	0.00336	-0.00020	0.00009	-0.00391	-0.00382	-0.00046
D10	3.13832	-0.00013	-0.00190	-0.00409	-0.00599	3.13234
D11	3.13830	-0.00003	0.00083	0.00106	0.00188	3.14018
D12	-0.00993	0.00005	-0.00116	0.00088	-0.00028	-0.01021
D13	-0.00398	0.00001	-0.00029	0.00135	0.00106	-0.00292
D14	3.10323	0.00008	-0.00369	0.00009	-0.00362	3.09961

D15	-3.13951	-0.00006	0.00152	0.00152	0.00305	-3.13646
D16	-0.03230	0.00001	-0.00188	0.00026	-0.00163	-0.03393
D17	0.07969	-0.00001	0.01558	0.01464	0.03022	0.10992
D18	-3.05882	-0.00001	0.01482	0.01307	0.02790	-3.03093
D19	-3.06931	0.00007	0.01337	0.01444	0.02780	-3.04151
D20	0.07536	0.00007	0.01261	0.01287	0.02548	0.10084
D21	0.00306	0.00018	0.00038	0.00170	0.00208	0.00514
D22	3.06768	0.00017	-0.00162	0.00582	0.00420	3.07188
D23	-3.10189	0.00011	0.00402	0.00289	0.00690	-3.09500
D24	-0.03728	0.00009	0.00202	0.00700	0.00902	-0.02826
D25	1.57683	-0.00003	0.02068	0.00455	0.02523	1.60205
D26	-2.59347	-0.00009	0.02216	0.00501	0.02717	-2.56630
D27	-0.55768	-0.00005	0.02216	0.00561	0.02777	-0.52991
D28	-1.47407	0.00002	0.02288	-0.00044	0.02244	-1.45163
D29	0.63881	-0.00005	0.02437	0.00001	0.02438	0.66320
D30	2.67461	0.00000	0.02436	0.00062	0.02498	2.69959
D31	-1.12201	-0.00009	0.00299	0.01427	0.01726	-1.10474
D32	0.91857	-0.00012	0.00428	0.01557	0.01984	0.93841
D33	3.08733	-0.00017	0.00321	0.01448	0.01769	3.10501
D34	3.07370	0.00006	0.00041	0.01430	0.01471	3.08841
D35	-1.16891	0.00003	0.00170	0.01559	0.01729	-1.15162
D36	0.99985	-0.00003	0.00063	0.01450	0.01513	1.01498
D37	0.98640	0.00009	0.00047	0.01314	0.01361	1.00000
D38	3.02697	0.00006	0.00175	0.01443	0.01618	3.04316
D39	-1.08745	0.00000	0.00069	0.01334	0.01403	-1.07343
D40	2.76787	0.00019	-0.01225	0.00716	-0.00514	2.76273
D41	-1.42672	0.00021	-0.01214	0.00668	-0.00542	-1.43213
D42	0.69593	0.00011	-0.01199	0.00701	-0.00503	0.69090
D43	2.78453	0.00013	-0.01188	0.00653	-0.00530	2.77923
D44	-1.40765	0.00006	-0.01197	0.00672	-0.00530	-1.41295
D45	0.68094	0.00008	-0.01186	0.00624	-0.00557	0.67537
D46	-3.13524	0.00002	0.00065	0.00066	0.00132	-3.13392
D47	0.00869	0.00001	0.00108	0.00086	0.00195	0.01063
D48	0.00287	0.00003	0.00151	0.00244	0.00395	0.00682
D49	-3.13639	0.00001	0.00194	0.00263	0.00458	-3.13181
D50	1.35478	0.00015	0.02792	0.06597	0.09406	1.44884
D51	-0.60619	0.00012	-0.01029	0.01871	0.00851	-0.59768
D52	-2.86095	0.00001	0.02264	0.06651	0.08905	-2.77190
D53	1.46127	-0.00001	-0.01557	0.01924	0.00350	1.46476
D54	-2.70132	-0.00001	-0.00094	0.00008	-0.00064	-2.70196
D55	-0.01100	-0.00003	0.00113	0.00147	0.00269	-0.00831
D56	-0.02417	-0.00003	0.00008	-0.00166	-0.00152	-0.02569
D57	2.66615	-0.00005	0.00215	-0.00027	0.00181	2.66796
D58	1.80396	-0.00012	-0.03416	-0.03687	-0.07180	1.73216

D59	-0.60934	0.00000	-0.03187	-0.03647	-0.06885	-0.67819
D60	0.66423	0.00014	0.03555	0.04103	0.07670	0.74093
D61	-1.75961	0.00020	0.03609	0.04140	0.07768	-1.68193
D62	2.54953	-0.00006	-0.00081	-0.00053	-0.00121	2.54833
D63	-1.65999	-0.00006	-0.00148	-0.00095	-0.00230	-1.66229
D64	0.44289	-0.00007	-0.00100	-0.00072	-0.00159	0.44131
D65	1.35042	0.00005	0.00022	0.00079	0.00084	1.35126
D66	-2.85910	0.00005	-0.00045	0.00037	-0.00025	-2.85935
D67	-0.75622	0.00004	0.00002	0.00061	0.00046	-0.75576
D68	-1.04649	0.00002	0.00136	0.00119	0.00259	-1.04390
D69	1.02718	0.00001	0.00069	0.00077	0.00150	1.02868
D70	3.13006	0.00000	0.00117	0.00100	0.00221	3.13227

Item	Value	Threshold	Converged?
Maximum Force	0.000508	0.000450	NO
RMS Force	0.000136	0.000300	YES
Maximum Displacement	0.324546	0.001800	NO
RMS Displacement	0.056200	0.001200	NO

Predicted change in Energy=-3.710198D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.883358	2.128254	-0.327874
2	6	0	-3.748279	1.143276	0.025675
3	7	0	-3.002705	-0.023903	0.136790
4	6	0	-1.717649	0.254586	-0.144686
5	7	0	-1.625531	1.554600	-0.433066
6	6	0	-0.362620	2.263822	-0.713321
7	6	0	0.360953	2.694649	0.569973
8	1	0	-3.051602	3.174230	-0.518569
9	1	0	-4.807709	1.176665	0.202095
10	1	0	0.271349	1.590495	-1.290873
11	1	0	-0.595581	3.130464	-1.331710
12	1	0	-0.263033	3.411581	1.112621
13	1	0	0.489159	1.812846	1.213257
14	35	0	0.188397	-2.348398	0.464285
15	1	0	-0.902894	-0.495533	-0.091569
16	6	0	-3.433005	-1.338212	0.493320
17	6	0	-4.702790	-1.677262	0.671031
18	1	0	-2.590710	-2.018265	0.599785
19	1	0	-4.938389	-2.695740	0.947569

20	1	0	-5.533250	-0.991847	0.553279
21	7	0	1.611169	3.336594	0.183471
22	1	0	1.954618	3.940927	0.919814
23	1	0	2.323341	2.632558	-0.003891
24	6	0	3.760624	-0.197220	-1.156271
25	6	0	3.588648	-0.489883	0.268712
26	8	0	3.373423	0.853055	-0.246877
27	1	0	4.762323	-0.091737	-1.566492
28	1	0	2.989909	-0.507122	-1.856357
29	1	0	2.663372	-0.991417	0.546862
30	6	0	4.758335	-0.662836	1.197426
31	1	0	4.516985	-0.285279	2.195238
32	1	0	5.002423	-1.725094	1.294040
33	1	0	5.639189	-0.131483	0.828530

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357670	0.000000			
3	N	2.204980	1.389436	0.000000		
4	C	2.214287	2.223117	1.344676	0.000000	
5	N	1.386461	2.210359	2.170948	1.334798	0.000000
6	C	2.553638	3.642036	3.595334	2.489273	1.475291
7	C	3.413574	4.425925	4.346536	3.284088	2.500384
8	H	1.076446	2.215024	3.264956	3.231646	2.159673
9	H	2.211225	1.074537	2.168793	3.243294	3.266882
10	H	3.341965	4.253318	3.919686	2.656033	2.082132
11	H	2.691846	3.966221	4.230930	3.307376	2.086074
12	H	3.253930	4.298093	4.501178	3.696397	2.773793
13	H	3.721349	4.451354	4.089687	3.023605	2.692394
14	Br	5.486675	5.280301	3.961522	3.283197	4.396472
15	H	3.295806	3.285674	2.164206	1.108749	2.200425
16	C	3.604561	2.544774	1.428174	2.426212	3.534617
17	C	4.334755	3.046804	2.430905	3.648081	4.597117
18	H	4.259086	3.415393	2.088440	2.546041	3.842358
19	H	5.396372	4.123627	3.397491	4.502289	5.562964
20	H	4.187289	2.832532	2.741174	4.074256	4.767341
21	N	4.682129	5.793033	5.708148	4.548351	3.745911
22	H	5.314934	6.414777	6.395940	5.311103	4.510245
23	H	5.241087	6.251672	5.953431	4.690861	4.115795
24	C	7.087776	7.718650	6.888009	5.589178	5.709866
25	C	7.006956	7.520424	6.609121	5.374191	5.644473
26	O	6.385922	7.132822	6.447578	5.127146	5.051373
27	H	8.057231	8.745890	7.949932	6.643155	6.693262

28	H	6.616399	7.188118	6.333843	5.066668	5.251547
29	H	6.423685	6.777745	5.762697	4.606964	5.083026
30	C	8.277210	8.774823	7.859194	6.676923	6.951926
31	H	8.182684	8.663854	7.800722	6.681120	6.929909
32	H	8.925494	9.295756	8.265310	7.151813	7.594015
33	H	8.892553	9.507583	8.670203	7.430967	7.563773

		6	7	8	9	10
6	C	0.000000				
7	C	1.534931	0.000000			
8	H	2.845593	3.613925	0.000000		
9	H	4.666767	5.399507	2.755636	0.000000	
10	H	1.090345	2.165625	3.761206	5.310088	0.000000
11	H	1.089836	2.172852	2.587499	4.889980	1.767693
12	H	2.159012	1.094448	3.239327	5.145676	3.062466
13	H	2.154207	1.099013	4.170081	5.429915	2.523400
14	Br	4.791967	5.047105	6.477886	6.120121	4.313043
15	H	2.879672	3.494597	4.273925	4.257941	2.677441
16	C	4.884455	5.537506	4.640207	2.880838	5.048060
17	C	6.023757	6.690689	5.261040	2.894099	6.266527
18	H	5.002490	5.561004	5.331523	3.909068	4.978868
19	H	6.949351	7.568481	6.337671	3.945672	7.108010
20	H	6.240118	6.952134	4.966249	2.313479	6.615343
21	N	2.418867	1.457572	4.718120	6.772565	2.649089
22	H	3.293843	2.053135	5.264885	7.340662	3.639376
23	H	2.802434	2.045517	5.426630	7.281066	2.636833
24	C	4.822248	4.785456	7.627566	8.783453	3.922893
25	C	4.915262	4.544229	7.624858	8.560411	4.214826
26	O	4.020678	3.624043	6.836857	8.199830	3.355087
27	H	5.704524	5.630318	8.533587	9.814389	4.803615
28	H	4.497123	4.801023	7.200131	8.238641	3.479991
29	H	4.619662	4.346119	7.151831	7.786944	3.970557
30	C	6.200037	5.568067	8.869207	9.792019	5.603765
31	H	6.226409	5.366009	8.753083	9.646751	5.804905
32	H	6.980303	6.449934	9.599804	10.288403	6.329136
33	H	6.643531	5.992800	9.395332	10.547101	6.022523

		11	12	13	14	15
11	H	0.000000				
12	H	2.482814	0.000000			
13	H	3.064250	1.769710	0.000000		
14	Br	5.818775	5.813904	4.238792	0.000000	
15	H	3.844508	4.138240	2.994828	2.221035	0.000000
16	C	5.599176	5.743935	5.082405	3.759770	2.730140
17	C	6.632825	6.767774	6.279426	4.941343	4.051820
18	H	5.849839	5.929950	4.953721	2.801925	2.376006

19	H	7.615756	7.693216	7.060893	5.161215	4.712317
20	H	6.702776	6.890445	6.676173	5.880934	4.701314
21	N	2.684773	2.093221	2.154339	5.867049	4.591444
22	H	3.497102	2.288090	2.600463	6.548484	5.373122
23	H	3.245168	2.922807	2.348957	5.439402	4.494578
24	C	5.484595	5.861837	4.511930	4.473765	4.792806
25	C	5.759864	5.546986	3.975117	3.879953	4.505973
26	O	4.702813	4.649527	3.372264	4.571591	4.486613
27	H	6.256583	6.686185	5.441908	5.489751	5.867975
28	H	5.134494	5.895141	4.588957	4.077272	4.274170
29	H	5.580297	5.316984	3.610426	2.823778	3.656741
30	C	7.032074	6.467009	4.935090	4.925743	5.808530
31	H	7.088370	6.139006	4.646482	5.097974	5.886322
32	H	7.861848	7.358217	5.735250	4.924617	6.189063
33	H	7.360658	6.889864	5.518264	5.895636	6.616492

		16	17	18	19	20
16	C	0.000000				
17	C	1.326231	0.000000			
18	H	1.087781	2.140616	0.000000		
19	H	2.077355	1.081331	2.468100	0.000000	
20	H	2.129458	1.083201	3.116767	1.847316	0.000000
21	N	6.884295	8.077286	6.819357	8.936980	8.361512
22	H	7.554978	8.714759	7.501626	9.568681	8.974117
23	H	7.010688	8.270223	6.792826	9.056973	8.670223
24	C	7.468020	8.784016	6.836621	9.292017	9.483148
25	C	7.076279	8.385683	6.374170	8.833856	9.140130
26	O	7.188672	8.512947	6.673245	9.116296	9.130867
27	H	8.541658	9.854377	7.903882	10.353991	10.549997
28	H	6.889522	8.181353	6.281680	8.689646	8.870487
29	H	6.106468	7.399064	5.353747	7.800773	8.196625
30	C	8.249239	9.529902	7.496855	9.910680	10.316971
31	H	8.198020	9.448019	7.487860	9.837230	10.207962
32	H	8.482174	9.725306	7.630440	9.994095	10.587104
33	H	9.158235	10.458048	8.446509	10.884610	11.208897

		21	22	23	24	25
21	N	0.000000				
22	H	1.012608	0.000000			
23	H	1.018803	1.643476	0.000000		
24	C	4.347748	4.969512	3.376598	0.000000	
25	C	4.308088	4.767186	3.380083	1.464856	0.000000
26	O	3.075501	3.592927	2.080468	1.442221	1.454523
27	H	4.974494	5.507022	3.976448	1.087569	2.214499
28	H	4.564644	5.344538	3.705878	1.086352	2.207873
29	H	4.468878	4.996943	3.681325	2.176091	1.088595

30	C	5.189239	5.397456	4.269893	2.598483	1.503526
31	H	5.060527	5.104238	4.261692	3.436924	2.148296
32	H	6.193113	6.444606	5.277428	3.143324	2.139112
33	H	5.354307	5.492624	4.396328	2.733635	2.155589

		26	27	28	29	30
26	O	0.000000				
27	H	2.136132	0.000000			
28	H	2.141866	1.843371	0.000000		
29	H	2.129852	3.111476	2.473182	0.000000	
30	C	2.510362	2.822306	3.532303	2.218122	0.000000
31	H	2.927023	3.774687	4.335504	2.579080	1.093814
32	H	3.416858	3.302748	3.931751	2.562755	1.094214
33	H	2.694348	2.550805	3.790568	3.110355	1.092851

		31	32	33
31	H	0.000000		
32	H	1.766600	0.000000	
33	H	1.775073	1.778135	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.797845	2.269503	-0.187313
2	6	0	-3.682660	1.262978	0.030117
3	7	0	-2.960338	0.077037	-0.018124
4	6	0	-1.669466	0.365678	-0.259968
5	7	0	-1.551272	1.690688	-0.369804
6	6	0	-0.274104	2.406287	-0.552133
7	6	0	0.454985	2.645158	0.777296
8	1	0	-2.945151	3.334772	-0.234612
9	1	0	-4.741613	1.293055	0.209965
10	1	0	0.347803	1.804947	-1.215815
11	1	0	-0.488701	3.353057	-1.047429
12	1	0	-0.156011	3.294219	1.412291
13	1	0	0.564496	1.682063	1.295258
14	35	0	0.183896	-2.332815	-0.009831
15	1	0	-0.869679	-0.400636	-0.309266
16	6	0	-3.417075	-1.264693	0.157470

17	6	0	-4.693641	-1.599586	0.288300
18	1	0	-2.588498	-1.969360	0.170497
19	1	0	-4.949746	-2.641275	0.424576
20	1	0	-5.510257	-0.888312	0.264808
21	7	0	1.718372	3.308739	0.480599
22	1	0	2.071997	3.800987	1.291781
23	1	0	2.417019	2.622638	0.199322
24	6	0	3.801086	-0.052941	-1.326145
25	6	0	3.620320	-0.532292	0.046207
26	8	0	3.432563	0.872040	-0.282784
27	1	0	4.805546	0.087325	-1.718820
28	1	0	3.025968	-0.250011	-2.061343
29	1	0	2.684795	-1.048522	0.254389
30	6	0	4.784377	-0.852339	0.942382
31	1	0	4.548307	-0.608595	1.982232
32	1	0	5.007398	-1.922501	0.894224
33	1	0	5.676270	-0.293415	0.648348

Rotational constants (GHZ): 0.4670743 0.2541811 0.1727811

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1294.7259171817 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 4.11D-06 NBF= 482

NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999984 -0.003677 0.001307 0.004175 Ang= -0.65 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3205.64704663 A.U. after 11 cycles

NFock= 11 Conv=0.58D-08 -V/T= 2.0018

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000242758	-0.000014852	-0.000009166
2	6	0.000096447	0.000127414	-0.000185961
3	7	-0.000482882	-0.000686179	0.000415167
4	6	0.000797570	0.001646129	-0.000399995
5	7	0.000034671	0.000050909	-0.000031556
6	6	-0.000405815	-0.000706798	0.000037159
7	6	0.000719785	0.000313981	-0.000299448
8	1	-0.000054195	-0.000017093	0.000155580
9	1	-0.000030680	-0.000115319	0.000065619
10	1	0.000013982	-0.000035100	0.000083401
11	1	0.000257799	0.000038047	-0.000071640
12	1	-0.000144313	0.000030594	-0.000078153
13	1	-0.000213854	-0.000091218	0.000202398
14	35	0.000048439	0.000055748	-0.000013280
15	1	-0.000208381	-0.000787323	0.000198483
16	6	-0.000013334	0.000059687	-0.000141414
17	6	-0.000069294	0.000048072	0.000000620
18	1	0.000125030	-0.000092002	-0.000019349
19	1	0.000049445	-0.000013622	0.000020055
20	1	-0.000047812	0.000049127	-0.000008905
21	7	-0.000405525	0.000231803	0.000157304
22	1	0.000175229	-0.000089407	0.000103062
23	1	0.000294750	-0.000062777	-0.000080890
24	6	0.000253182	0.000280801	-0.000141468
25	6	-0.000063796	-0.000164955	0.000179588
26	8	-0.000434055	-0.000167683	-0.000357877

27	1	-0.000081659	0.000091531	-0.000140703
28	1	0.000160166	0.000032585	-0.000284364
29	1	0.000073353	-0.000021139	0.000576929
30	6	-0.000133335	0.000004164	0.000176891
31	1	0.000006700	-0.000046001	-0.000016842
32	1	-0.000075947	0.000035284	-0.000042952
33	1	0.000001086	0.000015592	-0.000048292

Cartesian Forces: Max 0.001646129 RMS 0.000291372

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000687435 RMS 0.000176275
Search for a local minimum.
Step number 16 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 10 14 15 16
DE= -2.49D-05 DEPred=-3.71D-05 R= 6.71D-01
TightC=F SS= 1.41D+00 RLast= 2.29D-01 DXNew= 8.1657D-01 6.8753D-01
Trust test= 6.71D-01 RLast= 2.29D-01 DXMaxT set to 6.88D-01
ITU= 1 1 1 1 0 -1 -1 1 1 1 -1 1 0 0 -1 0

Eigenvalues ---	0.00061	0.00258	0.00391	0.00557	0.00723
Eigenvalues ---	0.00780	0.00892	0.01402	0.01466	0.01542
Eigenvalues ---	0.01880	0.01985	0.02121	0.02350	0.02390
Eigenvalues ---	0.02434	0.02492	0.02967	0.03070	0.03100
Eigenvalues ---	0.03179	0.03282	0.03368	0.03900	0.04070
Eigenvalues ---	0.04326	0.04414	0.05147	0.05422	0.05749
Eigenvalues ---	0.05803	0.05928	0.06059	0.07766	0.08678
Eigenvalues ---	0.09540	0.10320	0.12228	0.12389	0.12691
Eigenvalues ---	0.12810	0.13521	0.15230	0.15961	0.16000
Eigenvalues ---	0.16001	0.16002	0.16010	0.16018	0.16054
Eigenvalues ---	0.16122	0.16909	0.18781	0.22088	0.22241
Eigenvalues ---	0.22875	0.22931	0.24282	0.25750	0.27713
Eigenvalues ---	0.29164	0.30775	0.31916	0.32137	0.32891
Eigenvalues ---	0.33767	0.34286	0.34323	0.34351	0.34550
Eigenvalues ---	0.34664	0.34734	0.35040	0.35068	0.35253
Eigenvalues ---	0.35417	0.35584	0.35856	0.35899	0.36425
Eigenvalues ---	0.36625	0.38377	0.39000	0.41854	0.42534
Eigenvalues ---	0.44633	0.45478	0.46286	0.49298	0.55305
Eigenvalues ---	0.57894	0.60613	1.03632		

En-DIIS/RFO-DIIS IScMMF= 0 using points: 16 15 14 13 12
RFO step: Lambda=-1.11067829D-05.
DidBck=F Rises=F RFO-DIIS coefs: 1.38287 -0.13115 -0.53933 0.25667 0.03094
Iteration 1 RMS(Cart)= 0.04404319 RMS(Int)= 0.00067192
Iteration 2 RMS(Cart)= 0.00202185 RMS(Int)= 0.00005605
Iteration 3 RMS(Cart)= 0.00000249 RMS(Int)= 0.00005604
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00005604

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56562	0.00010	0.00009	-0.00016	-0.00006	2.56556
R2	2.62003	0.00033	-0.00008	0.00004	-0.00004	2.61999
R3	2.03419	-0.00003	0.00000	-0.00001	-0.00001	2.03417
R4	2.62565	-0.00001	0.00040	-0.00001	0.00039	2.62604
R5	2.03058	0.00004	0.00004	-0.00003	0.00001	2.03059
R6	2.54107	0.00042	-0.00044	0.00012	-0.00033	2.54074
R7	2.69886	-0.00011	-0.00079	0.00010	-0.00069	2.69817
R8	2.52240	-0.00040	0.00021	-0.00008	0.00013	2.52253
R9	2.09523	0.00039	0.00096	-0.00065	0.00031	2.09554
R10	2.78790	-0.00015	0.00064	-0.00033	0.00031	2.78821
R11	2.90060	0.00011	-0.00050	-0.00039	-0.00089	2.89971
R12	2.06045	-0.00002	-0.00007	0.00003	-0.00004	2.06041
R13	2.05949	0.00002	-0.00008	0.00004	-0.00004	2.05945
R14	2.06821	0.00006	0.00002	0.00001	0.00003	2.06824
R15	2.07683	0.00017	-0.00028	0.00004	-0.00024	2.07659
R16	2.75441	-0.00017	0.00103	0.00002	0.00105	2.75546
R17	4.19715	-0.00003	-0.00045	0.00632	0.00586	4.20301
R18	2.50621	0.00005	0.00004	0.00014	0.00018	2.50639
R19	2.05561	0.00015	-0.00012	0.00014	0.00001	2.05562
R20	2.04342	0.00000	-0.00005	0.00004	-0.00001	2.04341
R21	2.04695	0.00007	0.00013	0.00001	0.00013	2.04709
R22	1.91355	0.00009	0.00012	0.00007	0.00019	1.91374
R23	1.92526	0.00006	0.00004	-0.00017	-0.00013	1.92513
R24	3.93152	-0.00018	-0.00097	0.00206	0.00109	3.93260
R25	2.76818	0.00067	0.00058	0.00179	0.00226	2.77043
R26	2.72540	-0.00009	-0.00082	-0.00142	-0.00221	2.72320
R27	2.05521	-0.00001	-0.00001	0.00002	0.00001	2.05521
R28	2.05291	0.00006	0.00016	0.00031	0.00047	2.05338
R29	2.74865	0.00001	0.00016	0.00069	0.00093	2.74958
R30	2.05715	0.00010	0.00016	0.00047	0.00063	2.05777
R31	2.84125	-0.00012	-0.00020	-0.00038	-0.00058	2.84067
R32	2.06701	-0.00003	-0.00003	-0.00015	-0.00019	2.06682
R33	2.06776	-0.00005	-0.00004	-0.00010	-0.00014	2.06762
R34	2.06519	0.00002	0.00002	0.00010	0.00012	2.06531

A1	1.87291	-0.00001	0.00018	0.00000	0.00018	1.87309
A2	2.28038	-0.00008	-0.00045	-0.00014	-0.00059	2.27979
A3	2.12987	0.00009	0.00028	0.00015	0.00043	2.13030
A4	1.86337	0.00007	-0.00039	0.00012	-0.00028	1.86309
A5	2.27617	0.00009	0.00080	0.00042	0.00122	2.27739
A6	2.14365	-0.00016	-0.00040	-0.00054	-0.00094	2.14271
A7	1.89874	-0.00020	0.00033	-0.00015	0.00018	1.89892
A8	2.25409	0.00007	-0.00034	-0.00043	-0.00078	2.25332
A9	2.13032	0.00013	0.00000	0.00058	0.00059	2.13091
A10	1.88903	0.00022	-0.00012	0.00007	-0.00004	1.88898
A11	2.15570	-0.00067	0.00284	-0.00192	0.00094	2.15663
A12	2.23769	0.00045	-0.00274	0.00187	-0.00087	2.23683
A13	1.90072	-0.00008	0.00002	-0.00004	-0.00003	1.90069
A14	2.20449	0.00069	-0.00127	-0.00048	-0.00177	2.20272
A15	2.17527	-0.00061	0.00164	0.00075	0.00237	2.17764
A16	1.96022	0.00021	0.00023	0.00066	0.00088	1.96110
A17	1.87705	-0.00014	-0.00016	0.00053	0.00037	1.87742
A18	1.88292	0.00017	-0.00076	-0.00018	-0.00094	1.88198
A19	1.91994	-0.00002	0.00071	-0.00003	0.00067	1.92062
A20	1.93046	-0.00023	-0.00072	-0.00079	-0.00151	1.92895
A21	1.89104	0.00001	0.00072	-0.00018	0.00054	1.89158
A22	1.90671	-0.00003	-0.00006	0.00010	0.00003	1.90674
A23	1.89563	-0.00018	0.00032	0.00051	0.00084	1.89647
A24	1.88206	0.00011	0.00039	-0.00163	-0.00124	1.88082
A25	1.87747	-0.00002	0.00017	0.00020	0.00037	1.87784
A26	1.90922	0.00000	-0.00062	0.00001	-0.00061	1.90861
A27	1.99164	0.00012	-0.00020	0.00082	0.00062	1.99225
A28	2.16179	-0.00011	0.00038	-0.00028	0.00010	2.16189
A29	1.94600	0.00004	0.00057	0.00002	0.00059	1.94660
A30	2.17539	0.00007	-0.00095	0.00026	-0.00069	2.17470
A31	2.07563	-0.00006	0.00004	-0.00006	-0.00002	2.07561
A32	2.16242	0.00002	-0.00017	0.00002	-0.00016	2.16226
A33	2.04513	0.00004	0.00014	0.00004	0.00017	2.04530
A34	1.94008	0.00012	-0.00117	0.00053	-0.00063	1.93944
A35	1.92197	-0.00027	0.00002	-0.00052	-0.00050	1.92147
A36	1.88500	0.00008	-0.00004	0.00081	0.00076	1.88576
A37	2.08798	-0.00001	0.00031	0.00077	0.00091	2.08889
A38	2.07900	0.00030	0.00023	0.00281	0.00321	2.08222
A39	1.99817	0.00008	0.00092	-0.00016	0.00072	1.99889
A40	2.00824	0.00005	-0.00040	-0.00012	-0.00051	2.00773
A41	2.02420	-0.00023	-0.00068	-0.00255	-0.00323	2.02098
A42	2.02683	0.00057	0.00103	0.00501	0.00593	2.03276
A43	2.13238	-0.00014	-0.00025	-0.00103	-0.00118	2.13119
A44	1.97162	0.00017	-0.00098	-0.00038	-0.00140	1.97022

A45	2.02670	0.00016	-0.00001	-0.00005	-0.00004	2.02666
A46	2.03803	-0.00041	0.00004	-0.00234	-0.00230	2.03574
A47	2.55357	0.00010	0.00636	0.01449	0.02081	2.57438
A48	2.53748	-0.00024	0.00242	0.00834	0.01023	2.54771
A49	1.93062	0.00005	-0.00017	-0.00023	-0.00040	1.93022
A50	1.91745	-0.00012	0.00014	-0.00046	-0.00032	1.91713
A51	1.94187	-0.00004	-0.00003	-0.00003	-0.00005	1.94182
A52	1.87944	0.00002	-0.00014	-0.00041	-0.00055	1.87889
A53	1.89436	0.00003	0.00018	0.00080	0.00098	1.89534
A54	1.89865	0.00006	0.00002	0.00034	0.00036	1.89901
A55	3.35799	-0.00024	-0.01104	0.00792	-0.00312	3.35486
A56	2.88714	-0.00054	-0.00942	-0.02161	-0.03104	2.85610
A57	2.82568	0.00014	-0.00390	0.00096	-0.00294	2.82274
A58	3.21325	-0.00011	-0.00268	-0.00934	-0.01203	3.20123
D1	0.00352	0.00002	-0.00133	-0.00127	-0.00260	0.00092
D2	-3.13702	0.00001	-0.00196	-0.00151	-0.00348	-3.14050
D3	3.13663	0.00005	-0.00014	0.00008	-0.00004	3.13658
D4	-0.00391	0.00004	-0.00077	-0.00016	-0.00093	-0.00484
D5	-0.00542	-0.00006	0.00131	0.00016	0.00147	-0.00395
D6	-3.07058	-0.00005	-0.00400	-0.00312	-0.00708	-3.07766
D7	-3.13942	-0.00008	0.00025	-0.00105	-0.00081	-3.14024
D8	0.07860	-0.00007	-0.00506	-0.00433	-0.00936	0.06924
D9	-0.00046	0.00002	0.00090	0.00196	0.00285	0.00240
D10	3.13234	0.00008	-0.00020	0.00225	0.00204	3.13438
D11	3.14018	0.00003	0.00148	0.00217	0.00365	-3.13935
D12	-0.01021	0.00008	0.00037	0.00247	0.00284	-0.00737
D13	-0.00292	-0.00006	-0.00009	-0.00187	-0.00196	-0.00488
D14	3.09961	0.00005	0.00012	-0.00141	-0.00128	3.09833
D15	-3.13646	-0.00011	0.00093	-0.00214	-0.00121	-3.13767
D16	-0.03393	0.00001	0.00114	-0.00167	-0.00053	-0.03447
D17	0.10992	-0.00004	0.00774	0.01085	0.01860	0.12851
D18	-3.03093	-0.00005	0.00628	0.00926	0.01554	-3.01539
D19	-3.04151	0.00001	0.00650	0.01118	0.01769	-3.02382
D20	0.10084	0.00000	0.00504	0.00959	0.01463	0.11547
D21	0.00514	0.00008	-0.00075	0.00107	0.00032	0.00546
D22	3.07188	0.00014	0.00423	0.00422	0.00849	3.08037
D23	-3.09500	-0.00001	-0.00112	0.00069	-0.00045	-3.09545
D24	-0.02826	0.00004	0.00386	0.00383	0.00772	-0.02054
D25	1.60205	-0.00011	-0.00047	0.00020	-0.00027	1.60179
D26	-2.56630	-0.00010	0.00045	0.00092	0.00136	-2.56494
D27	-0.52991	-0.00007	0.00081	0.00089	0.00170	-0.52821
D28	-1.45163	-0.00013	-0.00644	-0.00353	-0.00997	-1.46161
D29	0.66320	-0.00012	-0.00553	-0.00281	-0.00834	0.65486
D30	2.69959	-0.00009	-0.00516	-0.00284	-0.00800	2.69159

D31	-1.10474	-0.00004	0.00993	0.00836	0.01829	-1.08645
D32	0.93841	-0.00018	0.01028	0.00894	0.01922	0.95763
D33	3.10501	-0.00008	0.01048	0.00923	0.01971	3.12473
D34	3.08841	0.00002	0.00950	0.00729	0.01678	3.10519
D35	-1.15162	-0.00012	0.00985	0.00787	0.01771	-1.13391
D36	1.01498	-0.00002	0.01005	0.00816	0.01821	1.03319
D37	1.00000	0.00016	0.00860	0.00803	0.01663	1.01664
D38	3.04316	0.00001	0.00895	0.00861	0.01756	3.06072
D39	-1.07343	0.00012	0.00915	0.00890	0.01806	-1.05537
D40	2.76273	0.00018	0.00408	0.00752	0.01160	2.77432
D41	-1.43213	0.00018	0.00328	0.00853	0.01182	-1.42032
D42	0.69090	0.00015	0.00428	0.00834	0.01261	0.70351
D43	2.77923	0.00016	0.00348	0.00935	0.01283	2.79206
D44	-1.41295	0.00011	0.00465	0.00753	0.01217	-1.40078
D45	0.67537	0.00011	0.00385	0.00854	0.01239	0.68776
D46	-3.13392	0.00001	0.00006	-0.00003	0.00003	-3.13389
D47	0.01063	0.00000	0.00022	0.00065	0.00088	0.01151
D48	0.00682	0.00001	0.00172	0.00177	0.00348	0.01030
D49	-3.13181	0.00001	0.00188	0.00245	0.00433	-3.12748
D50	1.44884	0.00015	0.03491	0.04734	0.08227	1.53111
D51	-0.59768	-0.00004	0.01092	-0.00105	0.00986	-0.58782
D52	-2.77190	0.00011	0.03245	0.04708	0.07954	-2.69236
D53	1.46476	-0.00008	0.00846	-0.00131	0.00713	1.47189
D54	-2.70196	-0.00009	-0.00085	-0.00386	-0.00466	-2.70662
D55	-0.00831	-0.00013	0.00120	-0.00032	0.00093	-0.00738
D56	-0.02569	-0.00001	-0.00134	-0.00204	-0.00336	-0.02905
D57	2.66796	-0.00005	0.00070	0.00149	0.00223	2.67019
D58	1.73216	-0.00012	-0.01933	-0.04285	-0.06238	1.66978
D59	-0.67819	0.00011	-0.01885	-0.03836	-0.05738	-0.73557
D60	0.74093	-0.00007	0.02061	0.04017	0.06064	0.80157
D61	-1.68193	0.00019	0.02176	0.04452	0.06615	-1.61578
D62	2.54833	-0.00010	-0.00065	-0.00113	-0.00174	2.54658
D63	-1.66229	-0.00012	-0.00084	-0.00206	-0.00287	-1.66516
D64	0.44131	-0.00015	-0.00074	-0.00197	-0.00267	0.43863
D65	1.35126	0.00008	0.00003	0.00052	0.00052	1.35179
D66	-2.85935	0.00006	-0.00016	-0.00041	-0.00060	-2.85995
D67	-0.75576	0.00004	-0.00006	-0.00031	-0.00040	-0.75616
D68	-1.04390	0.00009	0.00165	0.00419	0.00583	-1.03807
D69	1.02868	0.00008	0.00145	0.00325	0.00470	1.03338
D70	3.13227	0.00005	0.00156	0.00335	0.00490	3.13717

Item	Value	Threshold	Converged?
Maximum Force	0.000687	0.000450	NO
RMS Force	0.000176	0.000300	YES
Maximum Displacement	0.209822	0.001800	NO

RMS Displacement 0.045366 0.001200 NO

Predicted change in Energy=-3.083209D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.861917	2.115617	-0.334795
2	6	0	-3.733579	1.137763	0.021839
3	7	0	-2.992705	-0.030488	0.153748
4	6	0	-1.703662	0.241254	-0.114977
5	7	0	-1.604486	1.537524	-0.417813
6	6	0	-0.338857	2.240915	-0.701361
7	6	0	0.374777	2.697262	0.578111
8	1	0	-3.025336	3.159750	-0.539250
9	1	0	-4.794434	1.175618	0.188553
10	1	0	0.299356	1.557071	-1.261583
11	1	0	-0.567542	3.096110	-1.337003
12	1	0	-0.261198	3.411022	1.110966
13	1	0	0.515813	1.825466	1.232041
14	35	0	0.195875	-2.354673	0.558145
15	1	0	-0.890954	-0.509807	-0.043566
16	6	0	-3.431879	-1.338995	0.519228
17	6	0	-4.706013	-1.676824	0.666168
18	1	0	-2.592980	-2.017431	0.657992
19	1	0	-4.948500	-2.690951	0.952536
20	1	0	-5.533349	-0.994581	0.512749
21	7	0	1.615345	3.355030	0.185080
22	1	0	1.953562	3.964903	0.919414
23	1	0	2.335380	2.659681	-0.004277
24	6	0	3.785544	-0.160936	-1.190478
25	6	0	3.558377	-0.490050	0.219976
26	8	0	3.348677	0.862198	-0.274520
27	1	0	4.801613	-0.034697	-1.557196
28	1	0	3.049105	-0.459586	-1.931536
29	1	0	2.627613	-1.004263	0.454552
30	6	0	4.691731	-0.671386	1.190690
31	1	0	4.405952	-0.319098	2.185896
32	1	0	4.943108	-1.732991	1.274029
33	1	0	5.580677	-0.123060	0.868859

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357638	0.000000			
3	N	2.204891	1.389641	0.000000		
4	C	2.214297	2.223288	1.344503	0.000000	
5	N	1.386440	2.210462	2.170828	1.334864	0.000000
6	C	2.552626	3.641991	3.596303	2.491021	1.475458
7	C	3.412901	4.429454	4.354381	3.291239	2.500868
8	H	1.076439	2.214692	3.264801	3.231787	2.159903
9	H	2.211812	1.074541	2.168439	3.243152	3.267173
10	H	3.341340	4.252946	3.919333	2.656720	2.082533
11	H	2.688856	3.963000	4.228400	3.306709	2.085510
12	H	3.245310	4.290843	4.496820	3.692028	2.766150
13	H	3.734732	4.471561	4.113026	3.041423	2.701962
14	Br	5.489164	5.284443	3.966411	3.286361	4.398067
15	H	3.295809	3.286226	2.164726	1.108912	2.200170
16	C	3.603963	2.544159	1.427809	2.426135	3.534369
17	C	4.334193	3.046750	2.430725	3.647372	4.596359
18	H	4.259112	3.414807	2.088537	2.547552	3.843459
19	H	5.395753	4.123261	3.397244	4.501820	5.562400
20	H	4.186671	2.833206	2.741027	4.072816	4.765865
21	N	4.674643	5.792574	5.718115	4.560860	3.746214
22	H	5.308647	6.414198	6.404291	5.320791	4.509995
23	H	5.236138	6.256930	5.970801	4.709024	4.117377
24	C	7.078391	7.726160	6.911485	5.608016	5.703876
25	C	6.951075	7.474065	6.567515	5.323162	5.583277
26	O	6.336101	7.093809	6.418211	5.092854	5.001042
27	H	8.052813	8.758854	7.979896	6.668939	6.693891
28	H	6.642397	7.236851	6.405936	5.136133	5.285425
29	H	6.363305	6.726089	5.711978	4.542644	5.013218
30	C	8.194638	8.696268	7.780524	6.590806	6.863593
31	H	8.068683	8.547371	7.678089	6.552511	6.808209
32	H	8.849774	9.224646	8.193331	7.071530	7.511962
33	H	8.816907	9.437292	8.603652	7.359501	7.485962

		6	7	8	9	10
6	C	0.000000				
7	C	1.534462	0.000000			
8	H	2.843889	3.608761	0.000000		
9	H	4.666794	5.402582	2.756117	0.000000	
10	H	1.090324	2.165686	3.760840	5.309905	0.000000
11	H	1.089814	2.171337	2.584804	4.886944	1.768005
12	H	2.158637	1.094465	3.229057	5.137908	3.062735
13	H	2.154322	1.098883	4.178220	5.450678	2.517350
14	Br	4.794969	5.055141	6.479918	6.123948	4.315537

15	H	2.881662	3.503405	4.273983	4.258132	2.678131
16	C	4.885936	5.548465	4.639434	2.879093	5.047830
17	C	6.024191	6.704835	5.260242	2.893503	6.263228
18	H	5.006239	5.571561	5.331371	3.906704	4.982714
19	H	6.950359	7.583555	6.336772	3.944333	7.105491
20	H	6.239010	6.967060	4.965410	2.315354	6.609056
21	N	2.417837	1.458129	4.700927	6.770163	2.656561
22	H	3.294576	2.053281	5.250276	7.338236	3.645655
23	H	2.795145	2.045617	5.410503	7.285181	2.634760
24	C	4.797792	4.788584	7.605205	8.792276	3.887173
25	C	4.847212	4.519129	7.565893	8.517328	4.123947
26	O	3.959920	3.597016	6.780625	8.162287	3.279559
27	H	5.686413	5.623167	8.514801	9.828357	4.784499
28	H	4.503813	4.839013	7.206726	8.287929	3.475179
29	H	4.546126	4.334954	7.091014	7.740117	3.863461
30	C	6.112951	5.509913	8.787686	9.716122	5.502056
31	H	6.115811	5.285242	8.645973	9.532610	5.680604
32	H	6.898786	6.401648	9.524862	10.220469	6.230431
33	H	6.564667	5.927912	9.317890	10.478182	5.937506

		11	12	13	14	15
11	H	0.000000				
12	H	2.487080	0.000000			
13	H	3.064014	1.769857	0.000000		
14	Br	5.821119	5.810144	4.246182	0.000000	
15	H	3.844504	4.135509	3.009928	2.224137	0.000000
16	C	5.596442	5.741605	5.109421	3.767455	2.731407
17	C	6.627257	6.770554	6.312980	4.949713	4.052201
18	H	5.850701	5.925411	4.976142	2.810946	2.379497
19	H	7.610838	7.696101	7.094707	5.170418	4.713098
20	H	6.694369	6.896577	6.712854	5.888626	4.700672
21	N	2.673719	2.093278	2.155148	5.895318	4.612025
22	H	3.493162	2.290991	2.596545	6.569400	5.389029
23	H	3.223908	2.924123	2.352704	5.480652	4.522878
24	C	5.438674	5.867849	4.528303	4.555863	4.827707
25	C	5.684007	5.531851	3.955134	3.859740	4.457173
26	O	4.632063	4.631120	3.350035	4.580585	4.462086
27	H	6.219185	6.680129	5.441335	5.574027	5.909495
28	H	5.106524	5.932667	4.652661	4.234476	4.369327
29	H	5.498340	5.317034	3.615460	2.783467	3.587886
30	C	6.945733	6.419028	4.865621	4.842137	5.719779
31	H	6.986423	6.070549	4.543366	4.951554	5.750138
32	H	7.778494	7.319307	5.680257	4.840991	6.104795
33	H	7.282134	6.831973	5.438888	5.837185	6.547068

		16	17	18	19	20

16	C	0.000000				
17	C	1.326326	0.000000			
18	H	1.087788	2.140325	0.000000		
19	H	2.077422	1.081324	2.467562	0.000000	
20	H	2.129516	1.083271	3.116582	1.847466	0.000000
21	N	6.900723	8.093860	6.840832	8.956949	8.374384
22	H	7.569310	8.731733	7.518491	9.588532	8.989755
23	H	7.037381	8.296746	6.826617	9.088435	8.691250
24	C	7.510133	8.823355	6.895577	9.342217	9.509874
25	C	7.047973	8.361080	6.353262	8.817458	9.110419
26	O	7.172951	8.497622	6.668219	9.108990	9.108118
27	H	8.590874	9.901257	7.969837	10.412452	10.583831
28	H	6.984465	8.268712	6.400443	8.789685	8.939758
29	H	6.069075	7.367442	5.321888	7.777557	8.161175
30	C	8.178606	9.465919	7.427154	9.852381	10.252625
31	H	8.077720	9.337072	7.362328	9.728959	10.101752
32	H	8.418156	9.668412	7.566573	9.943086	10.530002
33	H	9.100928	10.405347	8.392960	10.838110	11.153830

		21	22	23	24	25
21	N	0.000000				
22	H	1.012710	0.000000			
23	H	1.018733	1.643957	0.000000		
24	C	4.354761	4.983006	3.386138	0.000000	
25	C	4.308274	4.786569	3.386268	1.466050	0.000000
26	O	3.070811	3.605357	2.081045	1.441054	1.455017
27	H	4.967703	5.499253	3.969072	1.087573	2.216151
28	H	4.592062	5.376266	3.735446	1.086600	2.211174
29	H	4.483384	5.036174	3.704107	2.181313	1.088927
30	C	5.165987	5.391320	4.251628	2.598402	1.503216
31	H	5.028914	5.096161	4.237600	3.436543	2.147662
32	H	6.176388	6.444310	5.265917	3.144059	2.138553
33	H	5.318695	5.465341	4.363251	2.732180	2.155325

		26	27	28	29	30
26	O	0.000000				
27	H	2.135580	0.000000			
28	H	2.140691	1.841723	0.000000		
29	H	2.129591	3.116643	2.483494	0.000000	
30	C	2.510481	2.822822	3.534313	2.216594	0.000000
31	H	2.926934	3.774676	4.337513	2.574781	1.093715
32	H	3.416902	3.304552	3.935029	2.562051	1.094139
33	H	2.694415	2.549606	3.790028	3.109462	1.092914

		31	32	33
31	H	0.000000		
32	H	1.766106	0.000000	

33 H 1.775668 1.778352 0.000000

Stoichiometry C10H18BrN3O

Framework group C1[X(C10H18BrN3O)]

Deg. of freedom 93

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.759274	2.288893	-0.192400
2	6	0	-3.659888	1.293268	0.009607
3	7	0	-2.952125	0.098167	-0.034058
4	6	0	-1.654191	0.371068	-0.254469
5	7	0	-1.517478	1.694893	-0.357706
6	6	0	-0.231077	2.397224	-0.527646
7	6	0	0.485181	2.635065	0.808386
8	1	0	-2.892655	3.356091	-0.237322
9	1	0	-4.720529	1.335285	0.176682
10	1	0	0.392418	1.788113	-1.182660
11	1	0	-0.431636	3.344621	-1.027556
12	1	0	-0.135058	3.277805	1.440874
13	1	0	0.597538	1.670963	1.323583
14	35	0	0.168842	-2.348974	0.024975
15	1	0	-0.862804	-0.404673	-0.294689
16	6	0	-3.429499	-1.237663	0.128151
17	6	0	-4.713424	-1.557910	0.218242
18	1	0	-2.610454	-1.952540	0.165567
19	1	0	-4.985579	-2.596430	0.347352
20	1	0	-5.520697	-0.837386	0.166952
21	7	0	1.746103	3.309537	0.523248
22	1	0	2.095337	3.791881	1.342371
23	1	0	2.448313	2.630797	0.233369
24	6	0	3.829873	-0.018090	-1.360564
25	6	0	3.583328	-0.549768	-0.016750
26	8	0	3.414240	0.866961	-0.301993
27	1	0	4.851706	0.133481	-1.700707
28	1	0	3.091107	-0.180710	-2.140616
29	1	0	2.637178	-1.067168	0.134441
30	6	0	4.704062	-0.907240	0.919107
31	1	0	4.420587	-0.701285	1.955176
32	1	0	4.925791	-1.975895	0.841951

```
      33        1        0        5.609990     -0.341790      0.686680
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.4640402           0.2561703           0.1734129
 Standard basis: 6-311++G(d,p) (5D, 7F)
 There are     499 symmetry adapted cartesian basis functions of A      symmetry.
 There are     482 symmetry adapted basis functions of A      symmetry.
   482 basis functions,      760 primitive gaussians,      499 cartesian basis functions
    71 alpha electrons              71 beta electrons
         nuclear repulsion energy           1295.4284080454 Hartrees.
 NAtoms=       33 NActive=       33 NUniq=       33 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      482 RedAO= T EigKep=    4.19D-06    NBF=      482
 NBsUse=      482 1.00D-06 EigRej= -1.00D+00 NBFU=      482
 Initial                guess                from                the                checkpoint                file:
"/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"
 B after Tr=          0.000000        0.000000        0.000000
             Rot=        0.999990      -0.001799        0.001225        0.003798 Ang=    -0.50 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn=                5 AccDes=
0.00D+00
 Harris functional with IExCor=    402 and IRadAn=             5 diagonalized for initial guess.
 HarFok:    IExCor=    402 AccDes= 0.00D+00 IRadAn=                5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=    3500011 ScaDFX=    1.000000    1.000000    1.000000    1.000000
 FoFCou: FMM=F IPFlag=                  0 FMFlag=           100000 FMFlg1=                  0
             NFxFlg=                  0 DoJE=T BraDBF=F KetDBF=T FulRan=T
             wScrn=      0.000000  ICntrl=             500  IOpCl=      0  I1Cent=        200000004  NGrid=
0
             NMat0=         1 NMatS0=            1 NMatT0=         0 NMatD0=         1 NMtDS0=         0
NMtDT0=         0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                       energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3205.64708368          A.U. after      11 cycles
                  NFock= 11    Conv=0.61D-08         -V/T= 2.0018
 Calling FoFJK, ICntrl=             2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 ---------------------------------------------------------------------
 Center          Atomic                                Forces (Hartrees/Bohr)
```

Number	Number	X	Y	Z
1	6	-0.000345146	0.000005259	0.000236287
2	6	0.000198673	-0.000116309	-0.000388104
3	7	-0.000582484	-0.000449078	0.000743899
4	6	0.001221465	0.001611420	-0.000645314
5	7	-0.000052143	0.000044109	-0.000267454
6	6	-0.000533658	-0.000760469	0.000115674
7	6	0.000895556	0.000428441	-0.000441415
8	1	0.000005328	-0.000001371	0.000147110
9	1	-0.000038054	-0.000043549	0.000000082
10	1	0.000065390	-0.000013169	0.000095140
11	1	0.000257058	0.000058019	-0.000081440
12	1	-0.000118932	0.000063678	-0.000090672
13	1	-0.000235798	-0.000132229	0.000242272
14	35	-0.000221687	0.000057380	-0.000045044
15	1	-0.000365136	-0.000732123	0.000259738
16	6	-0.000045593	-0.000245281	-0.000122794
17	6	-0.000015621	0.000126020	0.000020566
18	1	0.000124521	-0.000040122	-0.000036231
19	1	0.000035491	-0.000015999	0.000011800
20	1	-0.000011533	0.000027625	0.000022410
21	7	-0.000449914	0.000212430	0.000312527
22	1	0.000182423	-0.000141625	0.000082715
23	1	0.000178643	-0.000018950	-0.000069457
24	6	0.000024714	0.000042666	0.000069623
25	6	-0.000154262	0.000009060	-0.000252927
26	8	-0.000390905	0.000160999	-0.000242846
27	1	0.000002875	0.000030774	-0.000030936
28	1	0.000155428	-0.000044832	-0.000200645
29	1	0.000273431	-0.000117018	0.000443151
30	6	-0.000011210	0.000013252	0.000130127
31	1	-0.000009093	-0.000048832	-0.000010325
32	1	-0.000067332	0.000013669	-0.000034938
33	1	0.000027505	0.000016153	0.000027421

Cartesian Forces: Max 0.001611420 RMS 0.000324840

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.001388982 RMS 0.000208372

Search for a local minimum.
Step number 17 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 14 15 16 17
DE= -3.71D-05 DEPred=-3.08D-05 R= 1.20D+00
TightC=F SS= 1.41D+00 RLast= 1.90D-01 DXNew= 1.1563D+00 5.6898D-01
Trust test= 1.20D+00 RLast= 1.90D-01 DXMaxT set to 6.88D-01
ITU= 1 1 1 1 1 0 -1 -1 1 1 1 -1 1 0 0 -1 0

Eigenvalues ---	0.00052	0.00256	0.00360	0.00463	0.00708
Eigenvalues ---	0.00725	0.00858	0.01412	0.01512	0.01554
Eigenvalues ---	0.01891	0.02107	0.02117	0.02355	0.02398
Eigenvalues ---	0.02438	0.02486	0.02986	0.03074	0.03104
Eigenvalues ---	0.03200	0.03361	0.03484	0.03980	0.04077
Eigenvalues ---	0.04338	0.04409	0.05112	0.05421	0.05750
Eigenvalues ---	0.05786	0.05940	0.06527	0.07734	0.08655
Eigenvalues ---	0.09543	0.10232	0.12266	0.12363	0.12593
Eigenvalues ---	0.12795	0.13512	0.15408	0.15994	0.16000
Eigenvalues ---	0.16001	0.16005	0.16015	0.16024	0.16089
Eigenvalues ---	0.16091	0.17294	0.18903	0.22114	0.22451
Eigenvalues ---	0.22887	0.22988	0.24422	0.25578	0.28939
Eigenvalues ---	0.29534	0.30646	0.31746	0.32094	0.32652
Eigenvalues ---	0.33797	0.34280	0.34314	0.34344	0.34546
Eigenvalues ---	0.34664	0.34737	0.35038	0.35070	0.35259
Eigenvalues ---	0.35410	0.35583	0.35765	0.35892	0.36422
Eigenvalues ---	0.36624	0.38150	0.39275	0.41976	0.42469
Eigenvalues ---	0.44621	0.45471	0.46227	0.49314	0.55102
Eigenvalues ---	0.58379	0.60603	1.22273		

En-DIIS/RFO-DIIS IScMMF= 0 using points: 17 16 15 14 13
RFO step: Lambda=-1.34759419D-05.
DidBck=F Rises=F RFO-DIIS coefs: 1.97759 -0.74275 -0.48933 0.19460 0.05989
Iteration 1 RMS(Cart)= 0.07375512 RMS(Int)= 0.00180517
Iteration 2 RMS(Cart)= 0.00566882 RMS(Int)= 0.00049291
Iteration 3 RMS(Cart)= 0.00002522 RMS(Int)= 0.00049286
Iteration 4 RMS(Cart)= 0.00000002 RMS(Int)= 0.00049286

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56556	0.00003	-0.00006	-0.00014	-0.00019	2.56537
R2	2.61999	0.00037	0.00004	0.00015	0.00019	2.62018
R3	2.03417	-0.00003	-0.00001	-0.00003	-0.00004	2.03414
R4	2.62604	-0.00020	0.00047	-0.00006	0.00040	2.62644
R5	2.03059	0.00004	0.00001	0.00005	0.00005	2.03064

R6	2.54074	0.00048	-0.00033	0.00038	0.00004	2.54078
R7	2.69817	0.00007	-0.00083	0.00007	-0.00076	2.69741
R8	2.52253	-0.00027	-0.00006	-0.00027	-0.00032	2.52221
R9	2.09554	0.00004	0.00064	-0.00018	0.00046	2.09600
R10	2.78821	-0.00006	0.00014	-0.00024	-0.00011	2.78810
R11	2.89971	0.00026	-0.00101	-0.00003	-0.00104	2.89867
R12	2.06041	0.00000	-0.00009	-0.00001	-0.00010	2.06031
R13	2.05945	0.00004	-0.00002	0.00000	-0.00002	2.05943
R14	2.06824	0.00007	0.00008	0.00008	0.00016	2.06840
R15	2.07659	0.00022	-0.00021	0.00023	0.00003	2.07662
R16	2.75546	-0.00022	0.00087	0.00007	0.00094	2.75641
R17	4.20301	-0.00017	0.00428	0.00499	0.00927	4.21228
R18	2.50639	-0.00004	0.00021	0.00003	0.00024	2.50663
R19	2.05562	0.00011	-0.00005	0.00025	0.00020	2.05583
R20	2.04341	0.00001	-0.00001	0.00002	0.00000	2.04341
R21	2.04709	0.00003	0.00013	0.00007	0.00020	2.04728
R22	1.91374	0.00004	0.00024	0.00008	0.00031	1.91406
R23	1.92513	0.00005	0.00000	-0.00009	-0.00011	1.92501
R24	3.93260	-0.00012	-0.00002	0.00097	0.00097	3.93357
R25	2.77043	0.00008	0.00204	0.00054	0.00122	2.77165
R26	2.72320	0.00011	-0.00206	-0.00112	-0.00269	2.72051
R27	2.05521	0.00002	-0.00002	0.00005	0.00003	2.05525
R28	2.05338	0.00004	0.00045	0.00046	0.00091	2.05429
R29	2.74958	0.00018	0.00114	0.00100	0.00302	2.75261
R30	2.05777	-0.00008	0.00061	0.00004	0.00065	2.05842
R31	2.84067	0.00003	-0.00061	0.00004	-0.00057	2.84010
R32	2.06682	-0.00002	-0.00019	-0.00018	-0.00037	2.06645
R33	2.06762	-0.00003	-0.00016	-0.00007	-0.00022	2.06740
R34	2.06531	0.00002	0.00012	0.00011	0.00023	2.06554
A1	1.87309	0.00008	0.00011	0.00006	0.00017	1.87326
A2	2.27979	-0.00006	-0.00070	-0.00006	-0.00076	2.27902
A3	2.13030	-0.00002	0.00059	0.00002	0.00060	2.13090
A4	1.86309	0.00007	-0.00027	0.00003	-0.00024	1.86285
A5	2.27739	0.00000	0.00132	0.00036	0.00167	2.27906
A6	2.14271	-0.00008	-0.00104	-0.00040	-0.00145	2.14126
A7	1.89892	-0.00015	0.00013	-0.00008	0.00005	1.89896
A8	2.25332	0.00019	-0.00065	-0.00067	-0.00132	2.25200
A9	2.13091	-0.00003	0.00052	0.00077	0.00129	2.13220
A10	1.88898	0.00021	0.00001	0.00002	0.00003	1.88901
A11	2.15663	-0.00139	0.00092	-0.00206	-0.00114	2.15549
A12	2.23683	0.00118	-0.00089	0.00187	0.00098	2.23781
A13	1.90069	-0.00021	0.00001	-0.00001	-0.00001	1.90068
A14	2.20272	0.00028	-0.00147	-0.00052	-0.00202	2.20070
A15	2.17764	-0.00007	0.00197	0.00072	0.00266	2.18029

A16	1.96110	0.00023	0.00075	0.00088	0.00163	1.96273
A17	1.87742	-0.00001	0.00001	0.00054	0.00055	1.87797
A18	1.88198	0.00006	-0.00047	0.00017	-0.00030	1.88168
A19	1.92062	-0.00001	0.00059	-0.00008	0.00052	1.92113
A20	1.92895	-0.00029	-0.00145	-0.00157	-0.00302	1.92594
A21	1.89158	0.00002	0.00058	0.00010	0.00068	1.89226
A22	1.90674	-0.00014	0.00017	0.00007	0.00023	1.90697
A23	1.89647	-0.00020	0.00067	0.00045	0.00112	1.89759
A24	1.88082	0.00035	-0.00146	-0.00039	-0.00185	1.87897
A25	1.87784	0.00002	0.00036	-0.00018	0.00018	1.87802
A26	1.90861	-0.00021	-0.00047	-0.00113	-0.00160	1.90701
A27	1.99225	0.00018	0.00074	0.00117	0.00191	1.99416
A28	2.16189	-0.00013	0.00027	-0.00062	-0.00035	2.16154
A29	1.94660	0.00000	0.00063	0.00034	0.00097	1.94756
A30	2.17470	0.00012	-0.00090	0.00027	-0.00063	2.17407
A31	2.07561	-0.00004	-0.00001	-0.00014	-0.00015	2.07547
A32	2.16226	0.00001	-0.00020	0.00003	-0.00017	2.16209
A33	2.04530	0.00003	0.00020	0.00011	0.00031	2.04562
A34	1.93944	-0.00011	-0.00088	0.00039	-0.00024	1.93920
A35	1.92147	0.00055	-0.00046	-0.00002	-0.00040	1.92107
A36	1.88576	-0.00022	0.00093	0.00036	0.00121	1.88698
A37	2.08889	-0.00008	0.00071	-0.00069	-0.00122	2.08767
A38	2.08222	0.00020	0.00327	0.00257	0.00696	2.08917
A39	1.99889	-0.00010	0.00063	0.00109	0.00148	2.00037
A40	2.00773	0.00016	-0.00022	0.00054	0.00025	2.00798
A41	2.02098	-0.00013	-0.00325	-0.00231	-0.00552	2.01545
A42	2.03276	0.00040	0.00588	0.00461	0.01017	2.04292
A43	2.13119	-0.00004	-0.00126	-0.00051	-0.00162	2.12957
A44	1.97022	0.00029	-0.00108	0.00094	-0.00047	1.96975
A45	2.02666	-0.00003	0.00005	-0.00008	0.00006	2.02672
A46	2.03574	-0.00037	-0.00241	-0.00312	-0.00545	2.03029
A47	2.57438	0.00012	0.01955	0.01633	0.03312	2.60750
A48	2.54771	-0.00002	0.00869	0.00874	0.01278	2.56049
A49	1.93022	0.00001	-0.00039	-0.00082	-0.00121	1.92902
A50	1.91713	-0.00012	-0.00035	-0.00048	-0.00083	1.91630
A51	1.94182	0.00008	-0.00008	0.00101	0.00094	1.94275
A52	1.87889	0.00002	-0.00049	-0.00078	-0.00127	1.87762
A53	1.89534	-0.00001	0.00097	0.00061	0.00158	1.89692
A54	1.89901	0.00003	0.00034	0.00043	0.00077	1.89978
A55	3.35486	0.00064	-0.00172	0.00055	-0.00118	3.35369
A56	2.85610	0.00025	-0.02872	-0.02343	-0.05189	2.80421
A57	2.82274	-0.00022	0.00292	-0.02752	-0.02460	2.79814
A58	3.20123	-0.00008	-0.01689	-0.00817	-0.02510	3.17613
D1	0.00092	0.00009	0.00073	0.00035	0.00108	0.00200

D2	-3.14050	0.00003	-0.00226	-0.00272	-0.00499	3.13770
D3	3.13658	0.00010	0.00146	0.00323	0.00470	3.14128
D4	-0.00484	0.00003	-0.00152	0.00017	-0.00136	-0.00620
D5	-0.00395	-0.00007	-0.00161	0.00211	0.00050	-0.00345
D6	-3.07766	-0.00003	-0.00953	-0.00094	-0.01045	-3.08811
D7	-3.14024	-0.00007	-0.00226	-0.00047	-0.00274	3.14021
D8	0.06924	-0.00003	-0.01018	-0.00352	-0.01369	0.05555
D9	0.00240	-0.00009	0.00038	-0.00267	-0.00229	0.00011
D10	3.13438	0.00001	0.00056	-0.00020	0.00035	3.13473
D11	-3.13935	-0.00003	0.00309	0.00010	0.00319	-3.13617
D12	-0.00737	0.00007	0.00327	0.00257	0.00583	-0.00154
D13	-0.00488	0.00005	-0.00139	0.00401	0.00262	-0.00226
D14	3.09833	0.00013	-0.00013	-0.00057	-0.00069	3.09764
D15	-3.13767	-0.00005	-0.00154	0.00176	0.00021	-3.13746
D16	-0.03447	0.00003	-0.00028	-0.00282	-0.00310	-0.03756
D17	0.12851	-0.00014	0.01728	0.00625	0.02353	0.15204
D18	-3.01539	-0.00012	0.01446	0.00499	0.01945	-2.99593
D19	-3.02382	-0.00002	0.01747	0.00900	0.02647	-2.99735
D20	0.11547	0.00000	0.01465	0.00774	0.02240	0.13787
D21	0.00546	0.00001	0.00185	-0.00379	-0.00194	0.00352
D22	3.08037	-0.00001	0.00946	-0.00085	0.00863	3.08900
D23	-3.09545	0.00000	0.00045	0.00118	0.00164	-3.09382
D24	-0.02054	-0.00002	0.00806	0.00412	0.01220	-0.00834
D25	1.60179	-0.00027	-0.00341	-0.01038	-0.01379	1.58799
D26	-2.56494	-0.00015	-0.00219	-0.00957	-0.01177	-2.57670
D27	-0.52821	-0.00010	-0.00175	-0.00909	-0.01084	-0.53905
D28	-1.46161	-0.00023	-0.01243	-0.01386	-0.02629	-1.48789
D29	0.65486	-0.00010	-0.01121	-0.01305	-0.02426	0.63060
D30	2.69159	-0.00006	-0.01077	-0.01256	-0.02333	2.66825
D31	-1.08645	0.00011	0.01895	0.00800	0.02695	-1.05950
D32	0.95763	-0.00007	0.01985	0.00808	0.02793	0.98556
D33	3.12473	0.00024	0.02026	0.00954	0.02980	-3.12866
D34	3.10519	-0.00002	0.01804	0.00679	0.02483	3.13002
D35	-1.13391	-0.00019	0.01894	0.00687	0.02581	-1.10810
D36	1.03319	0.00011	0.01934	0.00834	0.02768	1.06087
D37	1.01664	0.00014	0.01785	0.00771	0.02556	1.04220
D38	3.06072	-0.00003	0.01875	0.00779	0.02654	3.08726
D39	-1.05537	0.00027	0.01916	0.00926	0.02841	-1.02696
D40	2.77432	0.00003	0.01478	0.01640	0.03112	2.80545
D41	-1.42032	0.00004	0.01508	0.01708	0.03222	-1.38809
D42	0.70351	0.00012	0.01568	0.01718	0.03280	0.73631
D43	2.79206	0.00013	0.01598	0.01786	0.03390	2.82596
D44	-1.40078	0.00013	0.01506	0.01744	0.03245	-1.36833
D45	0.68776	0.00014	0.01537	0.01813	0.03355	0.72131

D46	-3.13389	0.00001	0.00019	0.00019	0.00038	-3.13351
D47	0.01151	-0.00001	0.00088	0.00015	0.00103	0.01254
D48	0.01030	-0.00001	0.00337	0.00161	0.00498	0.01528
D49	-3.12748	-0.00003	0.00407	0.00157	0.00563	-3.12185
D50	1.53111	0.00006	0.08555	0.05089	0.13647	1.66759
D51	-0.58782	-0.00031	0.01414	-0.01158	0.00282	-0.58500
D52	-2.69236	0.00024	0.08436	0.04936	0.13346	-2.55889
D53	1.47189	-0.00014	0.01294	-0.01311	-0.00019	1.47171
D54	-2.70662	0.00007	-0.00421	0.00044	-0.00341	-2.71003
D55	-0.00738	-0.00005	0.00077	0.00217	0.00326	-0.00412
D56	-0.02905	0.00002	-0.00331	-0.00120	-0.00434	-0.03339
D57	2.67019	-0.00011	0.00167	0.00053	0.00232	2.67252
D58	1.66978	-0.00007	-0.06073	-0.05237	-0.11443	1.55535
D59	-0.73557	0.00007	-0.05593	-0.05057	-0.10753	-0.84310
D60	0.80157	-0.00012	0.05923	0.05222	0.11093	0.91249
D61	-1.61578	0.00017	0.06444	0.05626	0.12027	-1.49551
D62	2.54658	0.00001	-0.00154	0.00188	0.00057	2.54715
D63	-1.66516	-0.00004	-0.00260	0.00011	-0.00226	-1.66742
D64	0.43863	-0.00003	-0.00245	0.00098	-0.00124	0.43739
D65	1.35179	0.00005	0.00063	0.00300	0.00340	1.35518
D66	-2.85995	0.00000	-0.00043	0.00124	0.00056	-2.85939
D67	-0.75616	0.00000	-0.00028	0.00211	0.00159	-0.75458
D68	-1.03807	0.00007	0.00543	0.00544	0.01089	-1.02718
D69	1.03338	0.00002	0.00437	0.00367	0.00805	1.04143
D70	3.13717	0.00002	0.00452	0.00455	0.00908	-3.13694

Item	Value	Threshold	Converged?
Maximum Force	0.001389	0.000450	NO
RMS Force	0.000208	0.000300	YES
Maximum Displacement	0.359412	0.001800	NO
RMS Displacement	0.077602	0.001200	NO

Predicted change in Energy=-4.514719D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.818083	2.092464	-0.347672
2	6	0	-3.700513	1.124452	0.008944
3	7	0	-2.966528	-0.043654	0.177739
4	6	0	-1.671652	0.218258	-0.072157
5	7	0	-1.561409	1.508519	-0.395395
6	6	0	-0.290696	2.202658	-0.678711

7	6	0	0.396224	2.710528	0.595295
8	1	0	-2.973597	3.133921	-0.570962
9	1	0	-4.763765	1.168365	0.158166
10	1	0	0.359815	1.499818	-1.199808
11	1	0	-0.507203	3.033784	-1.349552
12	1	0	-0.262687	3.423235	1.101184
13	1	0	0.551332	1.861103	1.274997
14	35	0	0.185929	-2.371177	0.733536
15	1	0	-0.863888	-0.534903	0.030247
16	6	0	-3.419433	-1.342824	0.557903
17	6	0	-4.698578	-1.679043	0.659015
18	1	0	-2.587148	-2.017647	0.746141
19	1	0	-4.952244	-2.685777	0.961344
20	1	0	-5.519020	-1.002556	0.451792
21	7	0	1.623472	3.389922	0.195448
22	1	0	1.954464	4.006240	0.927920
23	1	0	2.354048	2.706881	0.002038
24	6	0	3.808474	-0.103276	-1.243654
25	6	0	3.497281	-0.486550	0.137451
26	8	0	3.296553	0.879995	-0.325146
27	1	0	4.844149	0.048545	-1.538912
28	1	0	3.129508	-0.381330	-2.045798
29	1	0	2.561506	-1.018264	0.305124
30	6	0	4.570733	-0.684496	1.170539
31	1	0	4.215759	-0.373007	2.156821
32	1	0	4.833365	-1.744655	1.233528
33	1	0	5.468943	-0.112166	0.924808

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357537	0.000000			
3	N	2.204788	1.389855	0.000000		
4	C	2.214240	2.223520	1.344525	0.000000	
5	N	1.386542	2.210603	2.170733	1.334695	0.000000
6	C	2.551356	3.641738	3.597152	2.492548	1.475401
7	C	3.406311	4.432008	4.366688	3.306511	2.501723
8	H	1.076418	2.214197	3.264596	3.231866	2.160331
9	H	2.212580	1.074570	2.167817	3.242979	3.267601
10	H	3.343112	4.253028	3.917206	2.653461	2.082849
11	H	2.688869	3.960845	4.225106	3.303766	2.085234
12	H	3.224931	4.277387	4.492530	3.692396	2.755460
13	H	3.746937	4.497080	4.148181	3.074967	2.716283
14	Br	5.487912	5.277204	3.957810	3.287084	4.402240

15	H	3.296173	3.286389	2.164295	1.109153	2.200745
16	C	3.603178	2.543189	1.427407	2.426662	3.534288
17	C	4.332891	3.046032	2.430252	3.646456	4.595015
18	H	4.259433	3.414063	2.088937	2.550884	3.845659
19	H	5.394419	4.122104	3.396751	4.501535	5.561530
20	H	4.184896	2.833239	2.740404	4.070276	4.762973
21	N	4.658946	5.788951	5.732177	4.581366	3.745963
22	H	5.297818	6.413111	6.417209	5.338322	4.511223
23	H	5.220224	6.257942	5.992065	4.733394	4.113979
24	C	7.038133	7.711109	6.922757	5.613161	5.670368
25	C	6.838895	7.376997	6.479090	5.220974	5.463934
26	O	6.233728	7.009302	6.350764	5.018463	4.898956
27	H	8.019131	8.750125	7.997629	6.681006	6.668608
28	H	6.661616	7.289618	6.497676	5.225505	5.319780
29	H	6.248419	6.625091	5.614735	4.426167	4.886081
30	C	8.038101	8.546058	7.629328	6.428580	6.698107
31	H	7.862949	8.338053	7.457244	6.322939	6.590115
32	H	8.704500	9.086168	8.052728	6.919038	7.357286
33	H	8.669164	9.297686	8.468765	7.217425	7.334535

		6	7	8	9	10
6	C	0.000000				
7	C	1.533910	0.000000			
8	H	2.841974	3.590976	0.000000		
9	H	4.666741	5.403224	2.756763	0.000000	
10	H	1.090271	2.165535	3.765285	5.310840	0.000000
11	H	1.089804	2.168664	2.588306	4.885829	1.768388
12	H	2.158383	1.094549	3.198250	5.121857	3.062941
13	H	2.154680	1.098898	4.177649	5.475166	2.508359
14	Br	4.810569	5.087933	6.480002	6.112190	4.330434
15	H	2.885379	3.527036	4.274645	4.257525	2.674056
16	C	4.887602	5.566893	4.638357	2.876298	5.045085
17	C	6.023832	6.725281	5.258615	2.891856	6.256815
18	H	5.011474	5.592754	5.331300	3.903082	4.984363
19	H	6.951015	7.606589	6.334974	3.941450	7.099842
20	H	6.235929	6.985534	4.963431	2.317223	6.599270
21	N	2.416151	1.458627	4.667543	6.762654	2.667595
22	H	3.297713	2.053685	5.224306	7.333530	3.654078
23	H	2.777108	2.045738	5.375360	7.283863	2.622670
24	C	4.737055	4.789852	7.545094	8.778693	3.803299
25	C	4.716644	4.477442	7.448619	8.425204	3.946849
26	O	3.839635	3.551053	6.667487	8.079943	3.126283
27	H	5.634428	5.605804	8.460120	9.820697	4.725509
28	H	4.499302	4.899572	7.195834	8.340429	3.453349
29	H	4.413312	4.321636	6.974635	7.646080	3.667834

30	C	5.948855	5.411435	8.633079	9.570311	5.302981
31	H	5.914594	5.151252	8.451401	9.327503	5.444515
32	H	6.744919	6.320144	9.381116	10.086971	6.038243
33	H	6.411172	5.814522	9.167927	10.340977	5.763305

		11	12	13	14	15
11	H	0.000000				
12	H	2.493504	0.000000			
13	H	3.063321	1.770055	0.000000		
14	Br	5.833806	5.823369	4.282393	0.000000	
15	H	3.842733	4.144297	3.048457	2.229043	0.000000
16	C	5.592331	5.742431	5.152314	3.753264	2.731660
17	C	6.619117	6.775388	6.361888	4.933864	4.050834
18	H	5.851073	5.927256	5.017414	2.795549	2.383413
19	H	7.603421	7.702696	7.145757	5.152833	4.712521
20	H	6.682454	6.902055	6.762202	5.873580	4.697516
21	N	2.655868	2.092621	2.156895	5.962074	4.649570
22	H	3.491755	2.299060	2.586669	6.620948	5.419493
23	H	3.181260	2.927215	2.363377	5.569784	4.567830
24	C	5.336425	5.874428	4.561947	4.709086	4.862108
25	C	5.535325	5.509316	3.934985	3.856448	4.362755
26	O	4.489629	4.601161	3.325548	4.622436	4.408799
27	H	6.130618	6.666215	5.443504	5.719973	5.948476
28	H	5.037205	5.990426	4.764785	4.510969	4.503416
29	H	5.345467	5.323222	3.643104	2.767179	3.470233
30	C	6.779521	6.343518	4.758842	4.718302	5.554976
31	H	6.797591	5.965091	4.381425	4.717834	5.509205
32	H	7.617575	7.259087	5.598126	4.716056	5.947275
33	H	7.126292	6.736599	5.310304	5.748909	6.409656

		16	17	18	19	20
16	C	0.000000				
17	C	1.326454	0.000000			
18	H	1.087896	2.140183	0.000000		
19	H	2.077450	1.081324	2.467061	0.000000	
20	H	2.129627	1.083375	3.116557	1.847732	0.000000
21	N	6.925399	8.116503	6.875637	8.985586	8.388967
22	H	7.591322	8.755440	7.546290	9.617007	9.009312
23	H	7.074050	8.331116	6.876792	9.131425	8.714781
24	C	7.551472	8.858506	6.966210	9.395824	9.522888
25	C	6.982186	8.298565	6.303573	8.769828	9.036524
26	O	7.129178	8.452182	6.645444	9.078130	9.047760
27	H	8.638248	9.943797	8.044550	10.473639	10.604857
28	H	7.112830	8.383257	6.569064	8.925698	9.023354
29	H	5.995070	7.298678	5.263259	7.724485	8.081873
30	C	8.040614	9.336537	7.293330	9.733241	10.120320

31	H	7.860868	9.133158	7.139636	9.530496	9.902999
32	H	8.290151	9.549467	7.441510	9.834528	10.408347
33	H	8.980666	10.290979	8.280301	10.734335	11.034123

		21	22	23	24	25
21	N	0.000000				
22	H	1.012877	0.000000			
23	H	1.018673	1.644767	0.000000		
24	C	4.364365	5.004119	3.400601	0.000000	
25	C	4.305991	4.815630	3.394602	1.466694	0.000000
26	O	3.061038	3.625574	2.081556	1.439632	1.456618
27	H	4.954349	5.486246	3.954982	1.087589	2.215982
28	H	4.638283	5.429042	3.785765	1.087081	2.216507
29	H	4.508219	5.099217	3.743208	2.188800	1.089270
30	C	5.122307	5.376498	4.216696	2.597534	1.502915
31	H	4.972582	5.079513	4.194611	3.435384	2.146382
32	H	6.143688	6.438498	5.242113	3.143399	2.137599
33	H	5.252070	5.414134	4.301291	2.731202	2.155816

		26	27	28	29	30
26	O	0.000000				
27	H	2.135320	0.000000			
28	H	2.139974	1.838946	0.000000		
29	H	2.130944	3.122341	2.501029	0.000000	
30	C	2.511622	2.820148	3.537494	2.212993	0.000000
31	H	2.928330	3.772403	4.340739	2.565481	1.093519
32	H	3.417608	3.301834	3.939005	2.559476	1.094020
33	H	2.695561	2.546785	3.790766	3.107766	1.093035

		31	32	33
31	H	0.000000		
32	H	1.765028	0.000000	
33	H	1.776616	1.778844	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.665840	2.339732	-0.198868
2	6	0	-3.598508	1.367983	-0.029339
3	7	0	-2.922833	0.153986	-0.066348

4	6	0	-1.613009	0.392586	-0.253912
5	7	0	-1.437124	1.712866	-0.339559
6	6	0	-0.130697	2.383365	-0.482702
7	6	0	0.556932	2.621132	0.867674
8	1	0	-2.768721	3.410674	-0.233128
9	1	0	-4.660987	1.436556	0.116050
10	1	0	0.495282	1.753947	-1.115689
11	1	0	-0.296532	3.330582	-0.995492
12	1	0	-0.076714	3.263376	1.487395
13	1	0	0.660436	1.657358	1.385363
14	35	0	0.107535	-2.386980	0.090558
15	1	0	-0.843144	-0.405402	-0.281179
16	6	0	-3.442359	-1.168436	0.070712
17	6	0	-4.737353	-1.454240	0.098721
18	1	0	-2.645840	-1.905981	0.142145
19	1	0	-5.042899	-2.485140	0.213391
20	1	0	-5.521636	-0.712246	0.009013
21	7	0	1.821283	3.300094	0.606870
22	1	0	2.167886	3.758637	1.440851
23	1	0	2.522462	2.627653	0.300495
24	6	0	3.865678	0.017508	-1.416188
25	6	0	3.513017	-0.590682	-0.128971
26	8	0	3.384292	0.844698	-0.340750
27	1	0	4.912276	0.168728	-1.670381
28	1	0	3.188515	-0.079132	-2.261087
29	1	0	2.550695	-1.097310	-0.067542
30	6	0	4.557970	-1.022392	0.861206
31	1	0	4.200835	-0.875151	1.884220
32	1	0	4.769747	-2.088315	0.735352
33	1	0	5.486022	-0.460062	0.729942

Rotational constants (GHZ): 0.4563733 0.2607749 0.1748102

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1297.0556510587 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 4.23D-06 NBF= 482
NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999941 -0.003079 0.001933 0.010273 Ang= -1.25 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3205.64713984 A.U. after 11 cycles
NFock= 11 Conv=0.85D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000469280	0.000067366	0.000319649
2	6	0.000453099	-0.000350305	-0.000023452
3	7	-0.000697852	-0.000191501	0.000438455
4	6	0.001597456	0.001133647	-0.000445495
5	7	-0.000098340	0.000177960	-0.000599376
6	6	-0.000617217	-0.000654561	0.000203371
7	6	0.000988662	0.000492412	-0.000556593
8	1	0.000079455	-0.000000070	0.000027048
9	1	-0.000033581	0.000078876	-0.000070611
10	1	0.000119585	0.000016361	0.000107539
11	1	0.000184273	0.000074893	-0.000123922
12	1	-0.000073649	0.000089649	-0.000109561
13	1	-0.000255352	-0.000172406	0.000232803

14	35	-0.000202014	0.000045458	-0.000139001
15	1	-0.000684443	-0.000418625	0.000372322
16	6	-0.000251330	-0.000688885	-0.000200594
17	6	0.000036834	0.000281059	0.000070649
18	1	0.000209661	0.000057406	-0.000013276
19	1	0.000013390	-0.000018000	0.000000698
20	1	0.000018957	-0.000003848	0.000067177
21	7	-0.000338120	0.000207182	0.000406981
22	1	0.000134326	-0.000213240	0.000083153
23	1	-0.000035433	0.000110557	0.000007171
24	6	0.000087247	-0.000190493	-0.000279090
25	6	-0.000298842	0.000320165	-0.000543133
26	8	-0.000433464	-0.000009801	-0.000003000
27	1	0.000089820	0.000099236	0.000057853
28	1	0.000086531	-0.000123722	0.000102298
29	1	0.000503254	-0.000151820	0.000414974
30	6	0.000000183	0.000011877	0.000210569
31	1	-0.000026249	-0.000052402	-0.000010718
32	1	-0.000049219	-0.000013011	-0.000031787
33	1	-0.000038351	-0.000011415	0.000026897

Cartesian Forces: Max 0.001597456 RMS 0.000345009

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.001337835 RMS 0.000231980
Search for a local minimum.
Step number 18 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 16 17 18
DE= -5.62D-05 DEPred=-4.51D-05 R= 1.24D+00
TightC=F SS= 1.41D+00 RLast= 3.35D-01 DXNew= 1.1563D+00 1.0036D+00
Trust test= 1.24D+00 RLast= 3.35D-01 DXMaxT set to 1.00D+00
ITU= 1 1 1 1 1 1 0 -1 -1 1 1 1 -1 1 0 0 -1 0

Eigenvalues ---	0.00045	0.00267	0.00329	0.00484	0.00694
Eigenvalues ---	0.00724	0.00859	0.01481	0.01541	0.01752
Eigenvalues ---	0.01886	0.02098	0.02126	0.02369	0.02398
Eigenvalues ---	0.02451	0.02502	0.02987	0.03074	0.03105
Eigenvalues ---	0.03221	0.03364	0.03533	0.04000	0.04083

Eigenvalues --- 0.04387 0.04422 0.05084 0.05429 0.05745
Eigenvalues --- 0.05779 0.05953 0.07507 0.07713 0.08632
Eigenvalues --- 0.09542 0.10139 0.12260 0.12359 0.12541
Eigenvalues --- 0.12811 0.13668 0.15360 0.15998 0.16000
Eigenvalues --- 0.16001 0.16003 0.16018 0.16024 0.16060
Eigenvalues --- 0.16208 0.17412 0.18592 0.22084 0.22418
Eigenvalues --- 0.22860 0.23166 0.24258 0.25457 0.28564
Eigenvalues --- 0.29474 0.30287 0.32028 0.32191 0.32722
Eigenvalues --- 0.33751 0.34275 0.34313 0.34341 0.34548
Eigenvalues --- 0.34664 0.34742 0.35059 0.35145 0.35261
Eigenvalues --- 0.35408 0.35579 0.35730 0.35891 0.36420
Eigenvalues --- 0.36621 0.38059 0.39526 0.42137 0.42512
Eigenvalues --- 0.44581 0.45478 0.46213 0.49317 0.54895
Eigenvalues --- 0.58226 0.60615 1.24582
En-DIIS/RFO-DIIS IScMMF= 0 using points: 18 17 16 15 14
RFO step: Lambda=-1.76159987D-05.
DidBck=F Rises=F RFO-DIIS coefs: 0.93843 1.14691 -1.53595 0.02320 0.42740
Iteration 1 RMS(Cart)= 0.03840524 RMS(Int)= 0.00050668
Iteration 2 RMS(Cart)= 0.00150413 RMS(Int)= 0.00016422
Iteration 3 RMS(Cart)= 0.00000141 RMS(Int)= 0.00016422
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00016422

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56537	0.00004	-0.00008	0.00002	-0.00006	2.56532
R2	2.62018	0.00027	0.00053	0.00020	0.00073	2.62092
R3	2.03414	-0.00002	-0.00004	-0.00002	-0.00006	2.03407
R4	2.62644	-0.00028	0.00023	0.00007	0.00029	2.62674
R5	2.03064	0.00003	0.00005	0.00006	0.00011	2.03075
R6	2.54078	0.00051	0.00049	0.00017	0.00066	2.54145
R7	2.69741	0.00031	-0.00056	-0.00005	-0.00062	2.69679
R8	2.52221	-0.00009	-0.00072	-0.00078	-0.00150	2.52071
R9	2.09600	-0.00036	0.00135	-0.00016	0.00119	2.09719
R10	2.78810	-0.00011	-0.00060	-0.00069	-0.00128	2.78682
R11	2.89867	0.00029	-0.00024	-0.00008	-0.00032	2.89835
R12	2.06031	0.00001	-0.00001	-0.00009	-0.00011	2.06021
R13	2.05943	0.00010	0.00016	0.00005	0.00021	2.05964
R14	2.06840	0.00005	0.00021	0.00017	0.00037	2.06877
R15	2.07662	0.00024	0.00051	0.00029	0.00080	2.07742
R16	2.75641	-0.00040	-0.00065	-0.00051	-0.00115	2.75525
R17	4.21228	-0.00018	-0.00658	0.00176	-0.00482	4.20746
R18	2.50663	-0.00012	0.00015	-0.00001	0.00014	2.50678
R19	2.05583	0.00012	-0.00012	0.00012	0.00000	2.05583
R20	2.04341	0.00001	0.00001	0.00002	0.00003	2.04344

R21	2.04728	-0.00003	0.00004	0.00001	0.00005	2.04733
R22	1.91406	-0.00003	0.00020	0.00006	0.00026	1.91432
R23	1.92501	-0.00002	0.00035	0.00009	0.00044	1.92545
R24	3.93357	0.00007	-0.00629	0.00241	-0.00388	3.92969
R25	2.77165	-0.00012	0.00172	-0.00077	0.00146	2.77311
R26	2.72051	0.00029	-0.00039	-0.00022	-0.00083	2.71968
R27	2.05525	0.00008	-0.00002	0.00015	0.00013	2.05537
R28	2.05429	-0.00010	0.00013	0.00021	0.00034	2.05463
R29	2.75261	0.00009	0.00016	0.00126	0.00112	2.75372
R30	2.05842	-0.00029	0.00023	-0.00047	-0.00024	2.05818
R31	2.84010	0.00006	-0.00037	0.00017	-0.00020	2.83989
R32	2.06645	-0.00002	-0.00009	-0.00015	-0.00024	2.06621
R33	2.06740	0.00000	-0.00012	-0.00003	-0.00015	2.06725
R34	2.06554	-0.00004	0.00005	-0.00002	0.00003	2.06557
A1	1.87326	0.00004	-0.00010	-0.00015	-0.00024	1.87302
A2	2.27902	0.00005	-0.00056	0.00011	-0.00045	2.27857
A3	2.13090	-0.00010	0.00066	0.00004	0.00070	2.13160
A4	1.86285	0.00018	0.00015	-0.00004	0.00012	1.86297
A5	2.27906	-0.00018	0.00051	0.00017	0.00068	2.27974
A6	2.14126	0.00001	-0.00067	-0.00014	-0.00081	2.14045
A7	1.89896	-0.00019	-0.00038	-0.00009	-0.00047	1.89850
A8	2.25200	0.00026	0.00026	-0.00017	0.00010	2.25210
A9	2.13220	-0.00007	0.00012	0.00026	0.00039	2.13259
A10	1.88901	0.00017	0.00032	0.00008	0.00042	1.88943
A11	2.15549	-0.00134	-0.00174	-0.00074	-0.00248	2.15301
A12	2.23781	0.00117	0.00159	0.00059	0.00219	2.23999
A13	1.90068	-0.00019	-0.00002	0.00019	0.00017	1.90085
A14	2.20070	0.00031	0.00185	0.00024	0.00207	2.20277
A15	2.18029	-0.00012	-0.00153	-0.00044	-0.00200	2.17830
A16	1.96273	-0.00016	0.00080	-0.00095	-0.00015	1.96258
A17	1.87797	0.00008	-0.00124	-0.00034	-0.00157	1.87639
A18	1.88168	0.00020	0.00147	0.00162	0.00310	1.88478
A19	1.92113	0.00009	-0.00008	0.00002	-0.00005	1.92108
A20	1.92594	-0.00018	-0.00085	-0.00095	-0.00179	1.92415
A21	1.89226	-0.00003	-0.00012	0.00069	0.00057	1.89283
A22	1.90697	-0.00029	-0.00011	0.00018	0.00006	1.90703
A23	1.89759	-0.00024	-0.00050	0.00017	-0.00033	1.89726
A24	1.87897	0.00065	-0.00084	0.00050	-0.00033	1.87865
A25	1.87802	0.00007	-0.00047	-0.00028	-0.00075	1.87727
A26	1.90701	-0.00026	-0.00023	-0.00091	-0.00114	1.90587
A27	1.99416	0.00004	0.00209	0.00035	0.00243	1.99659
A28	2.16154	-0.00016	0.00030	-0.00020	0.00010	2.16164
A29	1.94756	-0.00010	0.00023	0.00012	0.00035	1.94791
A30	2.17407	0.00027	-0.00054	0.00007	-0.00046	2.17360

A31	2.07547	-0.00003	-0.00003	-0.00004	-0.00007	2.07540
A32	2.16209	0.00002	-0.00017	-0.00008	-0.00025	2.16185
A33	2.04562	0.00001	0.00019	0.00013	0.00032	2.04594
A34	1.93920	-0.00007	0.00028	-0.00018	-0.00015	1.93906
A35	1.92107	0.00049	0.00033	-0.00144	-0.00119	1.91988
A36	1.88698	-0.00031	0.00024	-0.00069	-0.00037	1.88661
A37	2.08767	-0.00001	0.00016	-0.00157	-0.00140	2.08627
A38	2.08917	-0.00007	0.00215	0.00137	0.00355	2.09272
A39	2.00037	-0.00025	-0.00104	0.00112	0.00007	2.00044
A40	2.00798	0.00024	0.00067	0.00105	0.00183	2.00981
A41	2.01545	0.00005	-0.00144	-0.00111	-0.00257	2.01288
A42	2.04292	0.00029	0.00409	0.00384	0.00774	2.05066
A43	2.12957	0.00010	-0.00026	0.00029	0.00028	2.12986
A44	1.96975	0.00042	0.00003	0.00184	0.00187	1.97162
A45	2.02672	-0.00019	0.00017	-0.00012	0.00009	2.02681
A46	2.03029	-0.00042	-0.00271	-0.00373	-0.00650	2.02380
A47	2.60750	0.00011	-0.00084	0.01552	0.01611	2.62361
A48	2.56049	0.00002	-0.00372	0.00624	0.00376	2.56425
A49	1.92902	-0.00001	0.00031	-0.00082	-0.00052	1.92850
A50	1.91630	-0.00010	-0.00065	-0.00032	-0.00096	1.91534
A51	1.94275	0.00004	-0.00037	0.00090	0.00053	1.94328
A52	1.87762	0.00002	0.00000	-0.00074	-0.00074	1.87688
A53	1.89692	0.00001	0.00053	0.00060	0.00113	1.89805
A54	1.89978	0.00004	0.00020	0.00035	0.00056	1.90033
A55	3.35369	0.00074	-0.00338	0.00092	-0.00246	3.35123
A56	2.80421	0.00058	-0.00107	-0.01669	-0.01782	2.78639
A57	2.79814	0.00006	0.02714	-0.01651	0.01062	2.80877
A58	3.17613	0.00023	-0.01071	0.00014	-0.01048	3.16565
D1	0.00200	-0.00001	-0.00122	0.00235	0.00112	0.00312
D2	3.13770	0.00002	-0.00040	-0.00093	-0.00134	3.13636
D3	3.14128	0.00004	0.00047	0.00336	0.00381	-3.13809
D4	-0.00620	0.00007	0.00128	0.00008	0.00135	-0.00485
D5	-0.00345	0.00001	-0.00013	-0.00127	-0.00139	-0.00484
D6	-3.08811	0.00012	-0.00482	-0.00110	-0.00596	-3.09406
D7	3.14021	-0.00004	-0.00163	-0.00218	-0.00381	3.13640
D8	0.05555	0.00008	-0.00633	-0.00201	-0.00837	0.04718
D9	0.00011	0.00001	0.00215	-0.00263	-0.00048	-0.00037
D10	3.13473	0.00005	0.00423	-0.00094	0.00330	3.13803
D11	-3.13617	-0.00002	0.00141	0.00032	0.00173	-3.13444
D12	-0.00154	0.00002	0.00350	0.00202	0.00550	0.00396
D13	-0.00226	-0.00001	-0.00225	0.00186	-0.00039	-0.00265
D14	3.09764	0.00010	0.00264	0.00013	0.00278	3.10041
D15	-3.13746	-0.00004	-0.00415	0.00031	-0.00385	-3.14131
D16	-0.03756	0.00006	0.00074	-0.00142	-0.00068	-0.03825

D17	0.15204	-0.00021	-0.00502	0.00259	-0.00242	0.14962
D18	-2.99593	-0.00011	-0.00587	0.00216	-0.00371	-2.99965
D19	-2.99735	-0.00016	-0.00269	0.00449	0.00180	-2.99555
D20	0.13787	-0.00007	-0.00354	0.00405	0.00051	0.13837
D21	0.00352	0.00000	0.00148	-0.00038	0.00110	0.00462
D22	3.08900	-0.00010	0.00632	-0.00052	0.00574	3.09475
D23	-3.09382	-0.00003	-0.00365	0.00150	-0.00213	-3.09594
D24	-0.00834	-0.00013	0.00119	0.00136	0.00252	-0.00582
D25	1.58799	-0.00037	-0.02074	-0.02156	-0.04229	1.54570
D26	-2.57670	-0.00029	-0.02117	-0.02235	-0.04352	-2.62022
D27	-0.53905	-0.00018	-0.02120	-0.02087	-0.04207	-0.58112
D28	-1.48789	-0.00023	-0.02627	-0.02138	-0.04765	-1.53554
D29	0.63060	-0.00016	-0.02670	-0.02217	-0.04888	0.58172
D30	2.66825	-0.00004	-0.02673	-0.02070	-0.04743	2.62083
D31	-1.05950	0.00005	0.00533	-0.00386	0.00148	-1.05803
D32	0.98556	-0.00016	0.00443	-0.00400	0.00043	0.98599
D33	-3.12866	0.00015	0.00615	-0.00316	0.00299	-3.12567
D34	3.13002	-0.00001	0.00642	-0.00282	0.00361	3.13363
D35	-1.10810	-0.00022	0.00552	-0.00296	0.00256	-1.10554
D36	1.06087	0.00008	0.00724	-0.00212	0.00512	1.06599
D37	1.04220	0.00007	0.00716	-0.00309	0.00407	1.04627
D38	3.08726	-0.00014	0.00626	-0.00323	0.00302	3.09028
D39	-1.02696	0.00017	0.00798	-0.00239	0.00558	-1.02138
D40	2.80545	-0.00003	0.01779	0.01948	0.03732	2.84277
D41	-1.38809	-0.00015	0.01848	0.01756	0.03600	-1.35210
D42	0.73631	0.00008	0.01853	0.01949	0.03807	0.77438
D43	2.82596	-0.00004	0.01923	0.01757	0.03674	2.86270
D44	-1.36833	0.00015	0.01790	0.02028	0.03823	-1.33011
D45	0.72131	0.00003	0.01859	0.01836	0.03690	0.75821
D46	-3.13351	0.00005	-0.00067	0.00083	0.00017	-3.13335
D47	0.01254	0.00000	-0.00045	0.00023	-0.00022	0.01232
D48	0.01528	-0.00006	0.00030	0.00133	0.00162	0.01691
D49	-3.12185	-0.00011	0.00052	0.00072	0.00124	-3.12061
D50	1.66759	0.00006	0.01502	0.05675	0.07164	1.73922
D51	-0.58500	-0.00038	0.00801	-0.02762	-0.01974	-0.60474
D52	-2.55889	0.00018	0.01830	0.05119	0.06963	-2.48927
D53	1.47171	-0.00027	0.01129	-0.03317	-0.02175	1.44995
D54	-2.71003	0.00012	-0.00372	0.00268	-0.00110	-2.71113
D55	-0.00412	-0.00008	-0.00153	0.00282	0.00133	-0.00278
D56	-0.03339	0.00009	-0.00200	-0.00079	-0.00278	-0.03617
D57	2.67252	-0.00011	0.00018	-0.00064	-0.00035	2.67217
D58	1.55535	-0.00003	-0.00665	-0.06366	-0.07029	1.48506
D59	-0.84310	-0.00012	-0.00386	-0.06444	-0.06838	-0.91148
D60	0.91249	-0.00018	0.00158	0.06255	0.06393	0.97643

D61	-1.49551	0.00023	0.00577	0.06652	0.07208	-1.42342
D62	2.54715	0.00008	-0.00071	0.00319	0.00246	2.54961
D63	-1.66742	0.00004	-0.00092	0.00157	0.00064	-1.66678
D64	0.43739	0.00005	-0.00134	0.00239	0.00103	0.43843
D65	1.35518	-0.00001	-0.00005	0.00339	0.00340	1.35858
D66	-2.85939	-0.00005	-0.00026	0.00178	0.00157	-2.85781
D67	-0.75458	-0.00005	-0.00068	0.00260	0.00197	-0.75260
D68	-1.02718	0.00005	0.00310	0.00509	0.00816	-1.01902
D69	1.04143	0.00000	0.00289	0.00348	0.00633	1.04777
D70	-3.13694	0.00001	0.00247	0.00430	0.00673	-3.13021

Item	Value	Threshold	Converged?
Maximum Force	0.001338	0.000450	NO
RMS Force	0.000232	0.000300	YES
Maximum Displacement	0.194442	0.001800	NO
RMS Displacement	0.039523	0.001200	NO

Predicted change in Energy=-5.124742D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.790285	2.086787	-0.324904
2	6	0	-3.674534	1.119231	0.028310
3	7	0	-2.943605	-0.052281	0.187785
4	6	0	-1.648545	0.207712	-0.065032
5	7	0	-1.535501	1.498644	-0.381286
6	6	0	-0.263384	2.186083	-0.671031
7	6	0	0.403984	2.740509	0.593720
8	1	0	-2.943365	3.130661	-0.538204
9	1	0	-4.736978	1.165098	0.183027
10	1	0	0.395443	1.465882	-1.156650
11	1	0	-0.469469	2.993461	-1.373586
12	1	0	-0.264650	3.467468	1.065873
13	1	0	0.552040	1.915351	1.304848
14	35	0	0.213781	-2.393423	0.694882
15	1	0	-0.844218	-0.551192	0.028477
16	6	0	-3.399739	-1.352937	0.557643
17	6	0	-4.679768	-1.686029	0.658903
18	1	0	-2.569477	-2.032691	0.736865
19	1	0	-4.935819	-2.694542	0.953248
20	1	0	-5.498404	-1.004933	0.459655
21	7	0	1.632247	3.412510	0.186783

22	1	0	1.969505	4.029105	0.916350
23	1	0	2.358328	2.724369	-0.006693
24	6	0	3.795296	-0.098607	-1.256477
25	6	0	3.450525	-0.487812	0.115787
26	8	0	3.252880	0.878753	-0.349928
27	1	0	4.837819	0.059968	-1.522926
28	1	0	3.142169	-0.378175	-2.079522
29	1	0	2.515087	-1.025023	0.266100
30	6	0	4.497480	-0.680591	1.176519
31	1	0	4.112865	-0.376416	2.153788
32	1	0	4.765836	-1.739033	1.242776
33	1	0	5.397569	-0.100537	0.957116

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357506	0.000000			
3	N	2.204987	1.390010	0.000000		
4	C	2.214052	2.223558	1.344877	0.000000	
5	N	1.386929	2.210698	2.170706	1.333904	0.000000
6	C	2.552429	3.641868	3.596028	2.489951	1.474723
7	C	3.387414	4.425217	4.378448	3.325941	2.500894
8	H	1.076384	2.213911	3.264687	3.231730	2.161061
9	H	2.212943	1.074629	2.167538	3.242921	3.267897
10	H	3.350550	4.253118	3.906605	2.636761	2.081059
11	H	2.703327	3.968689	4.223241	3.295895	2.086998
12	H	3.196775	4.268262	4.509598	3.717542	2.754197
13	H	3.722448	4.486344	4.164005	3.104058	2.715607
14	Br	5.489687	5.282239	3.963228	3.288105	4.400717
15	H	3.297119	3.286488	2.163728	1.109785	2.201728
16	C	3.603058	2.543092	1.427081	2.426939	3.533905
17	C	4.332686	3.045920	2.430093	3.646732	4.594622
18	H	4.259837	3.414353	2.088895	2.551580	3.845737
19	H	5.394266	4.122040	3.396527	4.501794	5.561110
20	H	4.184277	2.832778	2.740156	4.070285	4.762318
21	N	4.645229	5.783266	5.739616	4.593227	3.744358
22	H	5.288564	6.411799	6.428621	5.353171	4.513554
23	H	5.197690	6.242846	5.988163	4.732018	4.099345
24	C	7.000975	7.676729	6.892084	5.581109	5.633345
25	C	6.765389	7.304568	6.409351	5.149463	5.390135
26	O	6.162777	6.941899	6.289069	4.955343	4.828441
27	H	7.983184	8.717140	7.968042	6.649827	6.632673
28	H	6.659485	7.290585	6.502579	5.229950	5.318558
29	H	6.178966	6.554829	5.545239	4.354896	4.816147

30	C	7.938777	8.446275	7.532736	6.332784	6.600961
31	H	7.737232	8.209641	7.332394	6.201469	6.468887
32	H	8.613332	8.993578	7.962011	6.829675	7.268217
33	H	8.571401	9.200738	8.376717	7.126537	7.239901

		6	7	8	9	10
6	C	0.000000				
7	C	1.533741	0.000000			
8	H	2.844674	3.555026	0.000000		
9	H	4.667426	5.392595	2.756930	0.000000	
10	H	1.090214	2.165304	3.781746	5.312904	0.000000
11	H	1.089915	2.167302	2.614736	4.896691	1.768793
12	H	2.158422	1.094747	3.140384	5.107058	3.062952
13	H	2.154601	1.099322	4.134208	5.458486	2.507093
14	Br	4.802632	5.138450	6.481017	6.118421	4.284321
15	H	2.884329	3.565502	4.275932	4.257126	2.647617
16	C	4.885798	5.588015	4.638083	2.875595	5.028712
17	C	6.022161	6.741144	5.258201	2.891134	6.244081
18	H	5.009819	5.625424	5.331585	3.902646	4.961468
19	H	6.949132	7.627748	6.334611	3.940761	7.084007
20	H	6.234298	6.991744	4.962569	2.316318	6.592025
21	N	2.415240	1.458017	4.641257	6.754102	2.669055
22	H	3.301864	2.053151	5.201848	7.329203	3.653096
23	H	2.757620	2.044558	5.343737	7.267096	2.599828
24	C	4.694192	4.794247	7.506906	8.744645	3.743874
25	C	4.643481	4.464515	7.375831	8.352954	3.843117
26	O	3.765146	3.531687	6.595452	8.012731	3.026626
27	H	5.591812	5.596819	8.422925	9.788173	4.673913
28	H	4.489661	4.936605	7.191754	8.341569	3.434639
29	H	4.348484	4.329356	6.907338	7.576013	3.566752
30	C	5.856371	5.366590	8.534172	9.469362	5.184374
31	H	5.804959	5.089679	8.326872	9.196732	5.307758
32	H	6.660498	6.285962	9.290726	9.993023	5.926978
33	H	6.318693	5.756691	9.069057	10.242562	5.651809

		11	12	13	14	15
11	H	0.000000				
12	H	2.493511	0.000000			
13	H	3.062648	1.770074	0.000000		
14	Br	5.810672	5.892077	4.364860	0.000000	
15	H	3.830246	4.190671	3.108455	2.226493	0.000000
16	C	5.586349	5.772641	5.182333	3.762841	2.730110
17	C	6.614776	6.798340	6.384278	4.944545	4.049289
18	H	5.841766	5.972623	5.064929	2.806852	2.381842
19	H	7.597092	7.733232	7.175746	5.164863	4.710664
20	H	6.681176	6.911009	6.771284	5.883221	4.696088

21	N	2.650955	2.091420	2.158333	5.998255	4.676416
22	H	3.502137	2.308515	2.574509	6.661867	5.448347
23	H	3.152340	2.929610	2.374305	5.593128	4.581139
24	C	5.269043	5.881612	4.597295	4.679876	4.835393
25	C	5.450124	5.509032	3.948452	3.800423	4.296098
26	O	4.401789	4.591183	3.332770	4.586380	4.355932
27	H	6.065888	6.659440	5.459547	5.685027	5.921648
28	H	4.991012	6.024027	4.839730	4.509324	4.512746
29	H	5.267291	5.343131	3.684881	2.711528	3.400869
30	C	6.683733	6.316369	4.724603	4.638517	5.465206
31	H	6.692998	5.926352	4.318839	4.625968	5.396310
32	H	7.526637	7.241874	5.578033	4.631373	5.861586
33	H	7.030444	6.693520	5.259645	5.674306	6.326560

		16	17	18	19	20
16	C	0.000000				
17	C	1.326529	0.000000			
18	H	1.087897	2.139995	0.000000		
19	H	2.077486	1.081341	2.466666	0.000000	
20	H	2.129578	1.083400	3.116367	1.847949	0.000000
21	N	6.940310	8.127702	6.899803	9.001280	8.392523
22	H	7.610771	8.771652	7.574955	9.638065	9.017748
23	H	7.078011	8.332433	6.889540	9.137323	8.709386
24	C	7.525484	8.832628	6.944381	9.373054	9.494177
25	C	6.918801	8.236041	6.246024	8.712162	8.970451
26	O	7.075413	8.397783	6.599808	9.028926	8.988252
27	H	8.612923	9.919343	8.022089	10.451927	10.578381
28	H	7.120489	8.390004	6.579693	8.934044	9.027721
29	H	5.931079	7.235825	5.204787	7.666516	8.015853
30	C	7.949914	9.246660	7.208561	9.648471	10.026804
31	H	7.742125	9.014442	7.028842	9.417733	9.779653
32	H	8.203358	9.463781	7.358600	9.752894	10.320213
33	H	8.894982	10.205657	8.200948	10.654003	10.944753

		21	22	23	24	25
21	N	0.000000				
22	H	1.013016	0.000000			
23	H	1.018904	1.644850	0.000000		
24	C	4.369178	5.009261	3.405294	0.000000	
25	C	4.303915	4.820463	3.394997	1.467466	0.000000
26	O	3.055231	3.629770	2.079502	1.439194	1.457208
27	H	4.943515	5.470955	3.942825	1.087656	2.215858
28	H	4.667472	5.456603	3.812716	1.087261	2.219569
29	H	4.525195	5.124909	3.762569	2.194407	1.089144
30	C	5.093389	5.351596	4.191624	2.598315	1.502808
31	H	4.937462	5.053104	4.166646	3.436268	2.145822

32	H	6.121511	6.418523	5.222951	3.143122	2.136750
33	H	5.206972	5.367237	4.259813	2.732632	2.156107

		26	27	28	29	30
26	O	0.000000				
27	H	2.135033	0.000000			
28	H	2.140939	1.837661	0.000000		
29	H	2.132649	3.126164	2.512686	0.000000	
30	C	2.512096	2.819799	3.539792	2.208479	0.000000
31	H	2.929781	3.772826	4.343175	2.556746	1.093392
32	H	3.417389	3.300106	3.940291	2.555304	1.093940
33	H	2.695750	2.547488	3.792768	3.104976	1.093051

		31	32	33
31	H	0.000000		
32	H	1.764381	0.000000	
33	H	1.777244	1.779145	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.632314	2.346468	-0.198280
2	6	0	-3.572737	1.382819	-0.025626
3	7	0	-2.906899	0.163106	-0.058624
4	6	0	-1.595019	0.391061	-0.247568
5	7	0	-1.408677	1.708762	-0.338342
6	6	0	-0.096826	2.364858	-0.491291
7	6	0	0.571061	2.660191	0.857437
8	1	0	-2.726650	3.418152	-0.232889
9	1	0	-4.634460	1.459756	0.121518
10	1	0	0.534155	1.702291	-1.084110
11	1	0	-0.245828	3.289431	-1.048855
12	1	0	-0.069075	3.332221	1.438016
13	1	0	0.661022	1.719836	1.419709
14	35	0	0.113718	-2.398783	0.082010
15	1	0	-0.833166	-0.415460	-0.274518
16	6	0	-3.437444	-1.154512	0.079085
17	6	0	-4.734849	-1.429596	0.106448
18	1	0	-2.647443	-1.899050	0.150368

19	1	0	-5.048912	-2.457866	0.221881
20	1	0	-5.512744	-0.680985	0.015802
21	7	0	1.840838	3.323303	0.585846
22	1	0	2.193805	3.788322	1.413718
23	1	0	2.534369	2.639216	0.287174
24	6	0	3.849986	-0.005902	-1.406499
25	6	0	3.456260	-0.602150	-0.124733
26	8	0	3.339507	0.832205	-0.353756
27	1	0	4.904776	0.138330	-1.629232
28	1	0	3.201060	-0.106218	-2.273084
29	1	0	2.491309	-1.105197	-0.079484
30	6	0	4.468900	-1.028342	0.900620
31	1	0	4.079678	-0.873276	1.910554
32	1	0	4.680727	-2.095787	0.789284
33	1	0	5.402250	-0.469522	0.794140

Rotational constants (GHZ): 0.4530948 0.2649974 0.1762204

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1299.7981977026 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 4.18D-06 NBF= 482

NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999996 0.001707 0.000616 0.001981 Ang= 0.31 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3205.64720242 A.U. after 11 cycles

NFock= 11 Conv=0.41D-08 -V/T= 2.0018

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000387141	0.000047255	0.000309111
2	6	0.000497990	-0.000474199	0.000178936
3	7	-0.000519062	0.000173307	0.000226309
4	6	0.001139582	0.000057058	-0.000264795
5	7	-0.000178636	0.000398874	-0.000629707
6	6	-0.000329145	-0.000222389	0.000315408
7	6	0.000622511	0.000292218	-0.000453113
8	1	0.000120626	-0.000001527	-0.000113644
9	1	-0.000006887	0.000172144	-0.000124903
10	1	0.000199542	0.000055307	0.000157252
11	1	-0.000007865	0.000002135	-0.000173731
12	1	-0.000010607	0.000087999	-0.000074994
13	1	-0.000182792	-0.000150418	0.000130548
14	35	-0.000703425	-0.000240012	-0.000029995
15	1	-0.000594955	-0.000034555	0.000245074
16	6	-0.000265166	-0.000814009	-0.000153713
17	6	0.000106343	0.000282681	0.000126289
18	1	0.000154464	0.000117811	-0.000000994
19	1	-0.000006741	-0.000003804	-0.000039897
20	1	0.000035663	-0.000037273	0.000090182
21	7	0.000022807	0.000158750	0.000314699
22	1	0.000058132	-0.000156678	0.000063584
23	1	-0.000103451	0.000267259	0.000067686
24	6	0.000148369	-0.000673975	-0.000000780
25	6	0.000138631	0.000536914	-0.000413531
26	8	-0.000669789	0.000190784	0.000016614
27	1	0.000130276	0.000148804	0.000109984
28	1	-0.000101051	-0.000123324	0.000381496

29	1	0.000425632	-0.000118673	-0.000344403
30	6	0.000259775	0.000109411	-0.000016446
31	1	-0.000019940	0.000027665	0.000042265
32	1	0.000002030	-0.000049161	-0.000031182
33	1	0.000024278	-0.000026381	0.000090390

Cartesian Forces: Max 0.001139582 RMS 0.000292204

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.003850386 RMS 0.000715627
Search for a local minimum.
Step number 19 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 17 18 19
DE= -6.26D-05 DEPred=-5.12D-05 R= 1.22D+00
TightC=F SS= 1.41D+00 RLast= 2.28D-01 DXNew= 1.6878D+00 6.8444D-01
Trust test= 1.22D+00 RLast= 2.28D-01 DXMaxT set to 1.00D+00
ITU= 1 1 1 1 1 1 1 0 -1 -1 1 1 1 -1 1 0 0 -1 0

Eigenvalues ---	0.00033	0.00256	0.00291	0.00470	0.00689
Eigenvalues ---	0.00724	0.00866	0.01475	0.01581	0.01874
Eigenvalues ---	0.01919	0.02124	0.02198	0.02374	0.02393
Eigenvalues ---	0.02490	0.02887	0.02998	0.03078	0.03107
Eigenvalues ---	0.03232	0.03436	0.03670	0.03979	0.04087
Eigenvalues ---	0.04390	0.04413	0.05101	0.05425	0.05742
Eigenvalues ---	0.05778	0.05960	0.07683	0.08282	0.08612
Eigenvalues ---	0.09506	0.10088	0.12155	0.12392	0.12660
Eigenvalues ---	0.13200	0.13708	0.15773	0.15967	0.15998
Eigenvalues ---	0.16001	0.16002	0.16016	0.16026	0.16086
Eigenvalues ---	0.16203	0.16870	0.17810	0.21461	0.22157
Eigenvalues ---	0.22890	0.23209	0.23878	0.25522	0.27347
Eigenvalues ---	0.29267	0.30239	0.31997	0.32146	0.32702
Eigenvalues ---	0.33665	0.34272	0.34314	0.34342	0.34548
Eigenvalues ---	0.34664	0.34741	0.35062	0.35133	0.35262
Eigenvalues ---	0.35404	0.35574	0.35722	0.35890	0.36418
Eigenvalues ---	0.36619	0.38141	0.39443	0.42053	0.42571
Eigenvalues ---	0.44559	0.45478	0.46171	0.49335	0.54684
Eigenvalues ---	0.57798	0.60615	2.01433		

En-DIIS/RFO-DIIS IScMMF= 0 using points: 19 18 17 16 15
RFO step: Lambda=-6.68441756D-05.

DidBck=F Rises=F RFO-DIIS coefs: 0.94169 1.21365 -2.23981 0.10562 0.97885

Iteration 1 RMS(Cart)= 0.03904241 RMS(Int)= 0.00146790

Iteration 2 RMS(Cart)= 0.00161293 RMS(Int)= 0.00124230

Iteration 3 RMS(Cart)= 0.00000219 RMS(Int)= 0.00124230

Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00124230

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56532	-0.00028	-0.00016	0.00008	-0.00007	2.56524
R2	2.62092	0.00024	0.00087	0.00019	0.00106	2.62197
R3	2.03407	0.00000	-0.00007	-0.00001	-0.00008	2.03400
R4	2.62674	-0.00065	-0.00023	0.00016	-0.00006	2.62668
R5	2.03075	0.00000	0.00013	0.00001	0.00014	2.03089
R6	2.54145	0.00037	0.00145	-0.00020	0.00125	2.54270
R7	2.69679	0.00041	0.00010	-0.00025	-0.00014	2.69665
R8	2.52071	0.00106	-0.00125	-0.00051	-0.00176	2.51895
R9	2.09719	-0.00075	0.00135	-0.00003	0.00132	2.09851
R10	2.78682	0.00062	-0.00116	-0.00091	-0.00207	2.78475
R11	2.89835	0.00048	0.00083	-0.00070	0.00013	2.89848
R12	2.06021	0.00001	0.00005	-0.00030	-0.00025	2.05995
R13	2.05964	0.00011	0.00023	0.00021	0.00045	2.06009
R14	2.06877	0.00003	0.00031	0.00023	0.00054	2.06932
R15	2.07742	0.00017	0.00120	0.00023	0.00143	2.07885
R16	2.75525	0.00032	-0.00177	-0.00042	-0.00219	2.75307
R17	4.20746	-0.00015	-0.01059	0.00190	-0.00868	4.19878
R18	2.50678	-0.00018	-0.00002	0.00003	0.00001	2.50678
R19	2.05583	0.00004	0.00012	0.00006	0.00018	2.05600
R20	2.04344	-0.00001	0.00004	-0.00002	0.00002	2.04346
R21	2.04733	-0.00007	-0.00001	-0.00003	-0.00003	2.04730
R22	1.91432	-0.00003	0.00011	0.00023	0.00034	1.91466
R23	1.92545	0.00011	0.00045	0.00038	0.00092	1.92637
R24	3.92969	0.00011	-0.00881	0.00244	-0.00641	3.92328
R25	2.77311	-0.00111	-0.00152	0.00036	0.00233	2.77543
R26	2.71968	0.00051	0.00150	-0.00051	-0.00028	2.71940
R27	2.05537	0.00012	0.00003	0.00019	0.00022	2.05559
R28	2.05463	-0.00019	0.00013	-0.00028	-0.00015	2.05448
R29	2.75372	0.00026	0.00104	0.00055	-0.00067	2.75306
R30	2.05818	-0.00035	-0.00045	-0.00032	-0.00077	2.05742
R31	2.83989	0.00023	0.00032	-0.00015	0.00016	2.84006
R32	2.06621	0.00005	-0.00008	-0.00014	-0.00022	2.06599
R33	2.06725	0.00005	-0.00005	-0.00003	-0.00007	2.06717
R34	2.06557	-0.00001	0.00003	-0.00009	-0.00006	2.06551
A1	1.87302	0.00045	-0.00018	-0.00037	-0.00056	1.87246
A2	2.27857	-0.00008	-0.00010	0.00019	0.00009	2.27866

A3	2.13160	-0.00037	0.00029	0.00018	0.00047	2.13207
A4	1.86297	0.00013	0.00049	0.00019	0.00070	1.86367
A5	2.27974	-0.00026	-0.00040	-0.00017	-0.00055	2.27919
A6	2.14045	0.00014	-0.00013	-0.00004	-0.00015	2.14029
A7	1.89850	0.00016	-0.00071	-0.00025	-0.00097	1.89753
A8	2.25210	0.00016	0.00044	0.00045	0.00089	2.25298
A9	2.13259	-0.00032	0.00031	-0.00021	0.00009	2.13268
A10	1.88943	-0.00008	0.00044	0.00022	0.00066	1.89009
A11	2.15301	-0.00261	-0.00515	-0.00028	-0.00543	2.14758
A12	2.23999	0.00268	0.00468	0.00011	0.00480	2.24479
A13	1.90085	-0.00066	-0.00003	0.00016	0.00015	1.90100
A14	2.20277	-0.00197	0.00372	0.00013	0.00390	2.20667
A15	2.17830	0.00263	-0.00376	-0.00051	-0.00424	2.17406
A16	1.96258	0.00028	0.00117	-0.00229	-0.00113	1.96144
A17	1.87639	0.00061	-0.00138	-0.00044	-0.00181	1.87458
A18	1.88478	-0.00066	0.00287	0.00214	0.00502	1.88980
A19	1.92108	-0.00009	-0.00086	-0.00118	-0.00204	1.91904
A20	1.92415	-0.00017	-0.00120	0.00079	-0.00041	1.92374
A21	1.89283	0.00004	-0.00062	0.00112	0.00050	1.89333
A22	1.90703	-0.00047	-0.00026	0.00065	0.00039	1.90742
A23	1.89726	-0.00026	-0.00110	-0.00082	-0.00193	1.89533
A24	1.87865	0.00104	0.00044	0.00015	0.00061	1.87926
A25	1.87727	0.00016	-0.00132	-0.00011	-0.00142	1.87586
A26	1.90587	-0.00095	-0.00113	-0.00061	-0.00175	1.90412
A27	1.99659	0.00044	0.00327	0.00075	0.00401	2.00060
A28	2.16164	-0.00010	-0.00047	0.00040	-0.00006	2.16158
A29	1.94791	-0.00014	0.00007	-0.00044	-0.00037	1.94754
A30	2.17360	0.00024	0.00038	0.00006	0.00045	2.17405
A31	2.07540	0.00000	-0.00017	-0.00003	-0.00021	2.07519
A32	2.16185	0.00002	0.00000	-0.00006	-0.00007	2.16178
A33	2.04594	-0.00002	0.00018	0.00010	0.00028	2.04622
A34	1.93906	-0.00135	0.00185	-0.00105	-0.00008	1.93897
A35	1.91988	0.00385	0.00132	-0.00070	0.00031	1.92018
A36	1.88661	-0.00123	-0.00054	0.00047	0.00023	1.88684
A37	2.08627	0.00021	-0.00315	0.00085	0.00038	2.08664
A38	2.09272	-0.00051	0.00285	0.00038	0.00086	2.09358
A39	2.00044	-0.00048	-0.00106	-0.00037	-0.00078	1.99966
A40	2.00981	0.00022	0.00183	-0.00063	0.00134	2.01115
A41	2.01288	0.00025	-0.00031	-0.00052	-0.00091	2.01197
A42	2.05066	-0.00052	0.00260	0.00323	0.00669	2.05735
A43	2.12986	0.00026	0.00085	-0.00008	0.00033	2.13019
A44	1.97162	0.00026	0.00211	0.00140	0.00417	1.97579
A45	2.02681	-0.00052	0.00024	0.00009	0.00021	2.02702
A46	2.02380	0.00019	-0.00387	-0.00285	-0.00696	2.01684

A47	2.62361	-0.00019	-0.01217	0.01344	0.00975	2.63336
A48	2.56425	0.00066	-0.01331	0.00498	0.00266	2.56691
A49	1.92850	-0.00003	-0.00004	-0.00057	-0.00061	1.92789
A50	1.91534	-0.00007	-0.00092	-0.00031	-0.00123	1.91411
A51	1.94328	0.00015	0.00077	-0.00002	0.00075	1.94403
A52	1.87688	0.00003	-0.00023	-0.00026	-0.00049	1.87638
A53	1.89805	-0.00005	0.00011	0.00091	0.00102	1.89907
A54	1.90033	-0.00003	0.00029	0.00026	0.00055	1.90088
A55	3.35123	0.00279	-0.00490	0.00073	-0.00416	3.34707
A56	2.78639	0.00306	0.01046	-0.01086	-0.00144	2.78495
A57	2.80877	-0.00108	0.00275	-0.00224	0.00051	2.80927
A58	3.16565	-0.00040	-0.00506	-0.02410	-0.02905	3.13660
D1	0.00312	-0.00010	-0.00088	0.00277	0.00188	0.00499
D2	3.13636	0.00001	-0.00063	0.00155	0.00095	3.13731
D3	-3.13809	-0.00006	0.00328	0.00074	0.00398	-3.13411
D4	-0.00485	0.00005	0.00353	-0.00047	0.00305	-0.00179
D5	-0.00484	0.00012	0.00345	-0.00668	-0.00322	-0.00807
D6	-3.09406	0.00009	0.00294	-0.00215	0.00071	-3.09336
D7	3.13640	0.00008	-0.00028	-0.00486	-0.00511	3.13129
D8	0.04718	0.00006	-0.00078	-0.00033	-0.00118	0.04600
D9	-0.00037	0.00005	-0.00197	0.00203	0.00008	-0.00029
D10	3.13803	0.00006	0.00386	-0.00186	0.00200	3.14003
D11	-3.13444	-0.00004	-0.00223	0.00312	0.00092	-3.13352
D12	0.00396	-0.00003	0.00360	-0.00076	0.00284	0.00680
D13	-0.00265	0.00002	0.00413	-0.00622	-0.00209	-0.00475
D14	3.10041	0.00010	0.00397	-0.00498	-0.00104	3.09938
D15	-3.14131	0.00001	-0.00120	-0.00266	-0.00386	3.13801
D16	-0.03825	0.00009	-0.00137	-0.00142	-0.00280	-0.04105
D17	0.14962	-0.00021	-0.02242	0.00268	-0.01974	0.12988
D18	-2.99965	-0.00010	-0.02147	0.00589	-0.01558	-3.01522
D19	-2.99555	-0.00019	-0.01591	-0.00166	-0.01759	-3.01313
D20	0.13837	-0.00009	-0.01496	0.00154	-0.01343	0.12495
D21	0.00462	-0.00009	-0.00469	0.00797	0.00328	0.00790
D22	3.09475	-0.00023	-0.00369	0.00354	-0.00026	3.09449
D23	-3.09594	-0.00001	-0.00424	0.00666	0.00245	-3.09350
D24	-0.00582	-0.00015	-0.00325	0.00223	-0.00109	-0.00691
D25	1.54570	-0.00057	-0.03787	-0.02641	-0.06428	1.48142
D26	-2.62022	-0.00010	-0.03913	-0.02960	-0.06873	-2.68895
D27	-0.58112	-0.00008	-0.03910	-0.02740	-0.06650	-0.64762
D28	-1.53554	-0.00048	-0.03874	-0.02121	-0.05994	-1.59548
D29	0.58172	-0.00001	-0.04000	-0.02440	-0.06440	0.51733
D30	2.62083	0.00002	-0.03996	-0.02220	-0.06216	2.55866
D31	-1.05803	0.00080	-0.00568	-0.00018	-0.00586	-1.06389
D32	0.98599	0.00058	-0.00802	-0.00041	-0.00842	0.97756

D33	-3.12567	0.00160	-0.00444	0.00010	-0.00433	-3.13000
D34	3.13363	-0.00009	-0.00413	0.00269	-0.00143	3.13220
D35	-1.10554	-0.00031	-0.00647	0.00246	-0.00400	-1.10954
D36	1.06599	0.00072	-0.00288	0.00297	0.00009	1.06608
D37	1.04627	0.00002	-0.00206	0.00155	-0.00051	1.04576
D38	3.09028	-0.00020	-0.00440	0.00133	-0.00308	3.08721
D39	-1.02138	0.00083	-0.00081	0.00183	0.00102	-1.02036
D40	2.84277	-0.00055	0.02624	0.02797	0.05441	2.89718
D41	-1.35210	-0.00044	0.02762	0.02743	0.05485	-1.29725
D42	0.77438	-0.00006	0.02692	0.02744	0.05456	0.82894
D43	2.86270	0.00005	0.02830	0.02690	0.05500	2.91769
D44	-1.33011	0.00015	0.02725	0.02753	0.05498	-1.27513
D45	0.75821	0.00025	0.02862	0.02698	0.05541	0.81362
D46	-3.13335	0.00002	-0.00090	0.00281	0.00191	-3.13144
D47	0.01232	-0.00001	-0.00165	0.00163	-0.00002	0.01230
D48	0.01691	-0.00009	-0.00198	-0.00081	-0.00279	0.01412
D49	-3.12061	-0.00012	-0.00274	-0.00199	-0.00472	-3.12533
D50	1.73922	-0.00028	-0.02780	0.04838	0.02049	1.75972
D51	-0.60474	-0.00153	-0.01460	-0.04917	-0.06473	-0.66947
D52	-2.48927	0.00093	-0.02330	0.05123	0.02885	-2.46042
D53	1.44995	-0.00031	-0.01010	-0.04633	-0.05637	1.39358
D54	-2.71113	0.00017	0.00181	-0.00080	0.00012	-2.71101
D55	-0.00278	0.00002	0.00004	-0.00068	-0.00135	-0.00414
D56	-0.03617	0.00012	0.00028	0.00076	0.00065	-0.03553
D57	2.67217	-0.00002	-0.00149	0.00089	-0.00082	2.67134
D58	1.48506	0.00002	0.00981	-0.07806	-0.06532	1.41975
D59	-0.91148	-0.00009	0.00937	-0.07603	-0.06449	-0.97597
D60	0.97643	-0.00019	-0.01640	0.07031	0.05520	1.03163
D61	-1.42342	-0.00019	-0.01303	0.07314	0.06120	-1.36223
D62	2.54961	0.00022	0.00359	0.00147	0.00450	2.55412
D63	-1.66678	0.00019	0.00271	0.00061	0.00277	-1.66402
D64	0.43843	0.00020	0.00296	0.00071	0.00312	0.44155
D65	1.35858	-0.00007	0.00234	0.00193	0.00487	1.36345
D66	-2.85781	-0.00010	0.00146	0.00107	0.00313	-2.85468
D67	-0.75260	-0.00009	0.00171	0.00118	0.00349	-0.74912
D68	-1.01902	-0.00009	0.00325	0.00299	0.00618	-1.01284
D69	1.04777	-0.00011	0.00237	0.00213	0.00444	1.05221
D70	-3.13021	-0.00011	0.00262	0.00223	0.00480	-3.12541

Item	Value	Threshold	Converged?
Maximum Force	0.003850	0.000450	NO
RMS Force	0.000716	0.000300	NO
Maximum Displacement	0.148541	0.001800	NO
RMS Displacement	0.038964	0.001200	NO

Predicted change in Energy=-4.380417D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.763080	2.081660	-0.321296
2	6	0	-3.655379	1.118298	0.022877
3	7	0	-2.933803	-0.059215	0.180456
4	6	0	-1.635259	0.193933	-0.064853
5	7	0	-1.512102	1.484066	-0.376620
6	6	0	-0.231806	2.158126	-0.656015
7	6	0	0.390344	2.775096	0.602890
8	1	0	-2.907663	3.128198	-0.527134
9	1	0	-4.718196	1.171176	0.173232
10	1	0	0.443385	1.413624	-1.078046
11	1	0	-0.408025	2.929400	-1.406023
12	1	0	-0.292005	3.527487	1.012046
13	1	0	0.504625	1.985806	1.360609
14	35	0	0.201261	-2.422884	0.693210
15	1	0	-0.839694	-0.574816	0.031480
16	6	0	-3.400343	-1.359102	0.539585
17	6	0	-4.682844	-1.679050	0.651457
18	1	0	-2.575392	-2.048918	0.704918
19	1	0	-4.946725	-2.687768	0.938125
20	1	0	-5.495841	-0.986363	0.469973
21	7	0	1.634197	3.423449	0.209308
22	1	0	1.972707	4.037440	0.940737
23	1	0	2.351090	2.721889	0.027550
24	6	0	3.751211	-0.101385	-1.264677
25	6	0	3.435602	-0.491552	0.115624
26	8	0	3.208573	0.869541	-0.351610
27	1	0	4.786288	0.074313	-1.549269
28	1	0	3.089949	-0.394525	-2.076323
29	1	0	2.514116	-1.044449	0.290316
30	6	0	4.502918	-0.663863	1.159577
31	1	0	4.127639	-0.366645	2.142471
32	1	0	4.790380	-1.717477	1.221873
33	1	0	5.388984	-0.068120	0.925764

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				

2	C	1.357467	0.000000			
3	N	2.205503	1.389978	0.000000		
4	C	2.213878	2.223293	1.345539	0.000000	
5	N	1.387489	2.210660	2.171010	1.332971	0.000000
6	C	2.554454	3.641838	3.594033	2.485399	1.473627
7	C	3.358431	4.410132	4.388818	3.348336	2.499100
8	H	1.076344	2.213886	3.265114	3.231506	2.161808
9	H	2.212695	1.074702	2.167481	3.242867	3.267916
10	H	3.361601	4.254305	3.893389	2.614377	2.078675
11	H	2.727927	3.983359	4.222356	3.284452	2.089892
12	H	3.158232	4.253813	4.531563	3.751883	2.755467
13	H	3.676397	4.455079	4.171051	3.133985	2.708671
14	Br	5.487027	5.278541	3.959606	3.285605	4.398229
15	H	3.298594	3.285542	2.161788	1.110485	2.204013
16	C	3.603618	2.543530	1.427004	2.427505	3.533906
17	C	4.332975	3.045645	2.429990	3.648141	4.595198
18	H	4.260283	3.415085	2.088644	2.550838	3.844774
19	H	5.394616	4.122062	3.396352	4.502884	5.561420
20	H	4.184119	2.831395	2.739975	4.072251	4.763394
21	N	4.627957	5.773048	5.744250	4.603725	3.742154
22	H	5.276882	6.406184	6.436959	5.366673	4.516530
23	H	5.165881	6.216847	5.973944	4.721237	4.076740
24	C	6.934814	7.615970	6.839562	5.526378	5.568193
25	C	6.725770	7.272017	6.384391	5.120166	5.350248
26	O	6.093504	6.878659	6.234939	4.899121	4.760571
27	H	7.907612	8.650046	7.912622	6.591971	6.559896
28	H	6.593145	7.224591	6.441356	5.169128	5.253282
29	H	6.164043	6.543063	5.537380	4.344773	4.800899
30	C	7.907314	8.427692	7.525231	6.317615	6.569168
31	H	7.716629	8.202018	7.335392	6.196574	6.448072
32	H	8.594741	8.989441	7.968525	6.826272	7.247506
33	H	8.522491	9.166421	8.356096	7.098590	7.192390

		6	7	8	9	10
6	C	0.000000				
7	C	1.533808	0.000000			
8	H	2.849186	3.504067	0.000000		
9	H	4.667914	5.371625	2.756534	0.000000	
10	H	1.090080	2.163785	3.804312	5.316615	0.000000
11	H	1.090151	2.167242	2.657096	4.915585	1.769194
12	H	2.158982	1.095034	3.061074	5.083993	3.062303
13	H	2.153787	1.100080	4.063538	5.417689	2.505629
14	Br	4.795165	5.202202	6.478362	6.114631	4.232584
15	H	2.882906	3.614057	4.277950	4.255744	2.613662
16	C	4.882620	5.609359	4.638587	2.876327	5.007892

17	C	6.020394	6.751222	5.258325	2.890283	6.231696
18	H	5.004373	5.663665	5.332062	3.904267	4.927592
19	H	6.946541	7.644578	6.334842	3.940651	7.066799
20	H	6.234239	6.986660	4.962107	2.312522	6.590198
21	N	2.414911	1.456859	4.610641	6.739951	2.667341
22	H	3.307766	2.052200	5.176811	7.319339	3.646741
23	H	2.730648	2.044107	5.303512	7.238836	2.563833
24	C	4.619554	4.801810	7.437391	8.684346	3.643048
25	C	4.589782	4.492440	7.331626	8.321804	3.742714
26	O	3.686369	3.533358	6.522321	7.949849	2.910326
27	H	5.506491	5.590201	8.340735	9.721386	4.569093
28	H	4.423500	4.951015	7.126073	8.275207	3.357121
29	H	4.323438	4.381442	6.890203	7.564988	3.493203
30	C	5.803241	5.389768	8.493611	9.453528	5.079637
31	H	5.762877	5.119396	8.296758	9.191931	5.207188
32	H	6.615823	6.318755	9.262800	9.992847	5.830076
33	H	6.249117	5.759733	9.008979	10.210644	5.538029

		11	12	13	14	15
11	H	0.000000				
12	H	2.493637	0.000000			
13	H	3.062279	1.769998	0.000000		
14	Br	5.781433	5.979288	4.469229	0.000000	
15	H	3.812123	4.253276	3.182855	2.221899	0.000000
16	C	5.579482	5.810657	5.206849	3.758562	2.725839
17	C	6.614009	6.820375	6.390923	4.940599	4.046418
18	H	5.825565	6.033612	5.118148	2.801748	2.374688
19	H	7.592589	7.765390	7.192914	5.160611	4.706832
20	H	6.688680	6.910036	6.755192	5.879661	4.694822
21	N	2.650292	2.089369	2.160612	6.038798	4.705091
22	H	3.521778	2.322511	2.557490	6.703363	5.478070
23	H	3.116233	2.933287	2.393386	5.615475	4.587960
24	C	5.148290	5.890651	4.667849	4.671705	4.793806
25	C	5.365799	5.554395	4.034591	3.811117	4.276935
26	O	4.293552	4.601986	3.389553	4.579917	4.315251
27	H	5.928991	6.653856	5.518499	5.682181	5.879781
28	H	4.871715	6.029744	4.915524	4.486543	4.462896
29	H	5.216125	5.412745	3.790255	2.722445	3.396410
30	C	6.603878	6.370280	4.800782	4.670750	5.461139
31	H	6.635358	5.997948	4.389939	4.663144	5.401298
32	H	7.451357	7.306457	5.665796	4.673017	5.866894
33	H	6.930200	6.723798	5.316452	5.701882	6.312916

		16	17	18	19	20
16	C	0.000000				
17	C	1.326533	0.000000			

18	H	1.087991	2.140330	0.000000		
19	H	2.077374	1.081353	2.466928	0.000000	
20	H	2.129529	1.083382	3.116608	1.848101	0.000000
21	N	6.951868	8.132404	6.921926	9.010365	8.387600
22	H	7.625828	8.778285	7.601616	9.649195	9.013292
23	H	7.070760	8.320682	6.891273	9.129712	8.690294
24	C	7.482108	8.791694	6.906381	9.337870	9.449877
25	C	6.903806	8.222313	6.237364	8.704211	8.952156
26	O	7.031276	8.353198	6.564137	8.990369	8.937908
27	H	8.569651	9.878357	7.986476	10.418626	10.532073
28	H	7.063800	8.337091	6.524447	8.884480	8.974948
29	H	5.928066	7.233904	5.204224	7.667092	8.012183
30	C	7.957970	9.255647	7.226864	9.666488	10.027699
31	H	7.760459	9.031619	7.058840	9.443630	9.787373
32	H	8.226900	9.490459	7.391325	9.789442	10.339547
33	H	8.892021	10.203531	8.209970	10.662531	10.932993

		21	22	23	24	25
21	N	0.000000				
22	H	1.013194	0.000000			
23	H	1.019391	1.645527	0.000000		
24	C	4.367933	5.015656	3.406034	0.000000	
25	C	4.310577	4.830388	3.392658	1.468697	0.000000
26	O	3.052169	3.637734	2.076109	1.439043	1.456855
27	H	4.923920	5.461021	3.927621	1.087771	2.217301
28	H	4.681907	5.476605	3.832001	1.087184	2.221153
29	H	4.554441	5.151871	3.779011	2.199495	1.088737
30	C	5.083177	5.343417	4.168352	2.599702	1.502894
31	H	4.931449	5.048155	4.143436	3.438126	2.145373
32	H	6.116854	6.413844	5.204278	3.142380	2.135907
33	H	5.177141	5.341048	4.221342	2.735221	2.156692

		26	27	28	29	30
26	O	0.000000				
27	H	2.134470	0.000000			
28	H	2.141628	1.837162	0.000000		
29	H	2.134877	3.130251	2.520906	0.000000	
30	C	2.512040	2.821887	3.541196	2.203586	0.000000
31	H	2.931429	3.775871	4.344628	2.548205	1.093276
32	H	3.416230	3.299963	3.939513	2.549929	1.093901
33	H	2.695382	2.551336	3.795342	3.101915	1.093019

		31	32	33
31	H	0.000000		
32	H	1.763936	0.000000	
33	H	1.777774	1.779434	0.000000

Stoichiometry C10H18BrN3O

Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.585783	2.363949	-0.205050
2	6	0	-3.540380	1.414033	-0.034402
3	7	0	-2.892763	0.184492	-0.063721
4	6	0	-1.576555	0.393970	-0.248628
5	7	0	-1.371121	1.707643	-0.342827
6	6	0	-0.047679	2.338269	-0.492458
7	6	0	0.581966	2.702112	0.857998
8	1	0	-2.664172	3.436931	-0.237957
9	1	0	-4.601293	1.506896	0.109908
10	1	0	0.591712	1.632537	-1.022927
11	1	0	-0.161913	3.230947	-1.107687
12	1	0	-0.063825	3.418153	1.376978
13	1	0	0.633158	1.794245	1.477135
14	35	0	0.086242	-2.419347	0.091300
15	1	0	-0.829769	-0.427622	-0.270354
16	6	0	-3.442513	-1.125406	0.071497
17	6	0	-4.743716	-1.379873	0.114011
18	1	0	-2.663272	-1.882341	0.131141
19	1	0	-5.072535	-2.403695	0.227985
20	1	0	-5.510506	-0.618209	0.039050
21	7	0	1.870021	3.328299	0.591082
22	1	0	2.227926	3.792719	1.417388
23	1	0	2.548306	2.623080	0.305155
24	6	0	3.808215	-0.032135	-1.416334
25	6	0	3.440188	-0.622165	-0.122700
26	8	0	3.303681	0.808276	-0.362768
27	1	0	4.857787	0.123687	-1.655848
28	1	0	3.148771	-0.147691	-2.272926
29	1	0	2.484249	-1.138454	-0.052169
30	6	0	4.472501	-1.027797	0.891442
31	1	0	4.093938	-0.872455	1.905252
32	1	0	4.696208	-2.093104	0.783308
33	1	0	5.396894	-0.457493	0.769210

Rotational constants (GHZ): 0.4492969 0.2671271 0.1766495
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 499 symmetry adapted cartesian basis functions of A symmetry.
There are 482 symmetry adapted basis functions of A symmetry.
482 basis functions, 760 primitive gaussians, 499 cartesian basis functions
71 alpha electrons 71 beta electrons
nuclear repulsion energy 1300.4489983210 Hartrees.
NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 482 RedAO= T EigKep= 4.02D-06 NBF= 482
NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999991 0.001860 -0.000303 0.003887 Ang= 0.50 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3205.64731900 A.U. after 11 cycles
NFock= 11 Conv=0.46D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Atomic Forces (Hartrees/Bohr)
Number Number X Y Z

1	6	-0.000149374	-0.000008018	0.000154353
2	6	0.000329153	-0.000448427	0.000330156
3	7	-0.000116020	0.000635556	-0.000025006
4	6	0.000135903	-0.001499546	-0.000179714
5	7	-0.000077827	0.000578872	-0.000203275
6	6	0.000146658	0.000434780	0.000394606
7	6	-0.000084557	-0.000041075	-0.000214890
8	1	0.000098214	-0.000014637	-0.000276790
9	1	0.000023042	0.000216027	-0.000174420
10	1	0.000284715	0.000024297	0.000143742
11	1	-0.000243874	-0.000072212	-0.000152214
12	1	0.000052602	0.000033026	-0.000019572
13	1	-0.000027515	-0.000039809	-0.000018518
14	35	-0.000517156	-0.000322983	-0.000043610
15	1	-0.000322972	0.000516441	0.000047065
16	6	-0.000243826	-0.000632081	0.000058000
17	6	0.000141235	0.000221759	0.000136905
18	1	0.000083125	0.000140513	0.000030823
19	1	-0.000032381	-0.000000779	-0.000106868
20	1	0.000021917	-0.000072649	0.000075310
21	7	0.000610243	0.000017220	0.000104667
22	1	-0.000015930	-0.000078357	-0.000017849
23	1	-0.000242603	0.000601765	0.000163579
24	6	0.000134727	-0.001114611	0.000637075
25	6	0.001014326	0.000632798	-0.000363823
26	8	-0.001215623	0.000159782	0.000058733
27	1	0.000090933	0.000024271	0.000235752
28	1	-0.000261553	-0.000099557	0.000450304
29	1	-0.000263031	0.000017727	-0.001256940
30	6	0.000438363	0.000175078	-0.000232706
31	1	0.000020924	0.000143465	0.000118554
32	1	0.000118903	-0.000074448	-0.000017190
33	1	0.000069259	-0.000054186	0.000163764

Cartesian Forces: Max 0.001499546 RMS 0.000371048

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.002756678 RMS 0.000615051

Search for a local minimum.

Step number 20 out of a maximum of 172

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 18 19 20
DE= -1.17D-04 DEPred=-4.38D-05 R= 2.66D+00
TightC=F SS= 1.41D+00 RLast= 2.64D-01 DXNew= 1.6878D+00 7.9238D-01
Trust test= 2.66D+00 RLast= 2.64D-01 DXMaxT set to 1.00D+00
ITU= 1 1 1 1 1 1 1 1 0 -1 -1 1 1 1 -1 1 0 0 -1 0

Eigenvalues ---	0.00026	0.00183	0.00307	0.00410	0.00688
Eigenvalues ---	0.00726	0.00859	0.01329	0.01506	0.01875
Eigenvalues ---	0.01934	0.02133	0.02238	0.02390	0.02413
Eigenvalues ---	0.02486	0.02856	0.02997	0.03083	0.03103
Eigenvalues ---	0.03241	0.03362	0.03674	0.03991	0.04080
Eigenvalues ---	0.04345	0.04456	0.05121	0.05445	0.05739
Eigenvalues ---	0.05783	0.05977	0.07664	0.08621	0.08917
Eigenvalues ---	0.09479	0.10120	0.12254	0.12353	0.12746
Eigenvalues ---	0.13469	0.13791	0.15221	0.15983	0.15999
Eigenvalues ---	0.16001	0.16002	0.16015	0.16024	0.16080
Eigenvalues ---	0.16257	0.17453	0.18085	0.22091	0.22646
Eigenvalues ---	0.22879	0.22964	0.24228	0.25545	0.26981
Eigenvalues ---	0.29201	0.31112	0.31810	0.32164	0.33639
Eigenvalues ---	0.34179	0.34278	0.34324	0.34518	0.34588
Eigenvalues ---	0.34697	0.34863	0.35066	0.35224	0.35387
Eigenvalues ---	0.35522	0.35573	0.35890	0.35900	0.36425
Eigenvalues ---	0.36628	0.38819	0.39377	0.41964	0.42582
Eigenvalues ---	0.44805	0.45476	0.46487	0.49358	0.54841
Eigenvalues ---	0.58416	0.60621	1.93582		

En-DIIS/RFO-DIIS IScMMF= 0 using points: 20 19 18 17 16
RFO step: Lambda=-5.57957979D-05.
DidBck=F Rises=F RFO-DIIS coefs: 1.48588 0.35108 0.45018 -3.22229 1.93516
Iteration 1 RMS(Cart)= 0.10456664 RMS(Int)= 0.00786247
Iteration 2 RMS(Cart)= 0.02322052 RMS(Int)= 0.00170190
Iteration 3 RMS(Cart)= 0.00020480 RMS(Int)= 0.00169991
Iteration 4 RMS(Cart)= 0.00000299 RMS(Int)= 0.00169991
Iteration 5 RMS(Cart)= 0.00000004 RMS(Int)= 0.00169991

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56524	-0.00031	-0.00021	-0.00023	-0.00045	2.56479
R2	2.62197	-0.00002	0.00145	0.00054	0.00197	2.62395
R3	2.03400	0.00003	-0.00012	-0.00002	-0.00014	2.03385
R4	2.62668	-0.00053	-0.00001	-0.00035	-0.00035	2.62633
R5	2.03089	-0.00004	0.00022	0.00002	0.00023	2.03112
R6	2.54270	0.00008	0.00185	0.00068	0.00254	2.54524
R7	2.69665	0.00037	-0.00023	0.00021	-0.00002	2.69663

R8	2.51895	0.00152	-0.00276	0.00031	-0.00246	2.51649
R9	2.09851	-0.00074	0.00164	-0.00018	0.00146	2.09997
R10	2.78475	0.00079	-0.00283	-0.00097	-0.00380	2.78096
R11	2.89848	0.00019	0.00016	-0.00094	-0.00077	2.89771
R12	2.05995	0.00010	-0.00027	-0.00006	-0.00033	2.05963
R13	2.06009	0.00009	0.00045	0.00055	0.00100	2.06109
R14	2.06932	-0.00002	0.00072	0.00039	0.00111	2.07042
R15	2.07885	0.00001	0.00188	0.00099	0.00287	2.08172
R16	2.75307	0.00057	-0.00285	-0.00058	-0.00344	2.74963
R17	4.19878	0.00001	-0.00766	0.00516	-0.00250	4.19628
R18	2.50678	-0.00015	0.00009	-0.00001	0.00007	2.50686
R19	2.05600	-0.00002	0.00033	0.00051	0.00083	2.05684
R20	2.04346	-0.00002	0.00007	-0.00004	0.00003	2.04349
R21	2.04730	-0.00008	0.00002	-0.00002	0.00000	2.04729
R22	1.91466	-0.00007	0.00042	0.00038	0.00080	1.91546
R23	1.92637	-0.00026	0.00092	-0.00007	0.00119	1.92756
R24	3.92328	0.00023	-0.00723	0.00425	-0.00315	3.92013
R25	2.77543	-0.00195	-0.00045	-0.00124	-0.00630	2.76913
R26	2.71940	0.00061	-0.00002	0.00035	0.00181	2.72120
R27	2.05559	0.00003	0.00024	0.00017	0.00041	2.05600
R28	2.05448	-0.00015	0.00048	-0.00043	0.00005	2.05453
R29	2.75306	0.00024	0.00269	0.00045	0.00631	2.75937
R30	2.05742	0.00001	-0.00095	0.00037	-0.00058	2.05684
R31	2.84006	0.00046	0.00031	0.00062	0.00092	2.84098
R32	2.06599	0.00014	-0.00042	0.00003	-0.00040	2.06560
R33	2.06717	0.00010	-0.00018	0.00008	-0.00010	2.06707
R34	2.06551	-0.00001	0.00006	-0.00013	-0.00007	2.06543
A1	1.87246	0.00044	-0.00060	-0.00029	-0.00090	1.87155
A2	2.27866	-0.00008	-0.00017	0.00038	0.00022	2.27888
A3	2.13207	-0.00036	0.00075	-0.00009	0.00067	2.13273
A4	1.86367	0.00010	0.00068	0.00082	0.00150	1.86517
A5	2.27919	-0.00030	0.00009	-0.00123	-0.00116	2.27803
A6	2.14029	0.00020	-0.00080	0.00048	-0.00033	2.13996
A7	1.89753	0.00029	-0.00115	-0.00057	-0.00172	1.89580
A8	2.25298	0.00004	0.00032	0.00045	0.00074	2.25373
A9	2.13268	-0.00033	0.00089	0.00011	0.00097	2.13365
A10	1.89009	-0.00027	0.00079	0.00021	0.00099	1.89108
A11	2.14758	-0.00155	-0.00799	-0.00401	-0.01200	2.13559
A12	2.24479	0.00182	0.00710	0.00398	0.01109	2.25588
A13	1.90100	-0.00056	0.00027	-0.00018	0.00011	1.90110
A14	2.20667	-0.00218	0.00445	-0.00018	0.00434	2.21101
A15	2.17406	0.00274	-0.00490	0.00041	-0.00441	2.16965
A16	1.96144	0.00021	-0.00029	-0.00211	-0.00235	1.95910
A17	1.87458	0.00060	-0.00220	0.00124	-0.00099	1.87359

A18	1.88980	-0.00074	0.00647	0.00173	0.00818	1.89797
A19	1.91904	-0.00018	-0.00167	-0.00309	-0.00479	1.91425
A20	1.92374	0.00004	-0.00267	0.00093	-0.00176	1.92198
A21	1.89333	0.00006	0.00054	0.00148	0.00201	1.89534
A22	1.90742	-0.00028	0.00047	0.00128	0.00176	1.90918
A23	1.89533	-0.00019	-0.00139	-0.00261	-0.00399	1.89134
A24	1.87926	0.00076	0.00004	0.00102	0.00098	1.88024
A25	1.87586	0.00013	-0.00179	-0.00116	-0.00295	1.87291
A26	1.90412	-0.00072	-0.00268	-0.00204	-0.00469	1.89943
A27	2.00060	0.00027	0.00525	0.00348	0.00876	2.00936
A28	2.16158	0.00000	-0.00058	-0.00010	-0.00068	2.16090
A29	1.94754	-0.00015	0.00021	-0.00123	-0.00101	1.94653
A30	2.17405	0.00016	0.00035	0.00134	0.00170	2.17575
A31	2.07519	0.00001	-0.00032	-0.00036	-0.00067	2.07452
A32	2.16178	0.00005	-0.00015	0.00041	0.00025	2.16203
A33	2.04622	-0.00006	0.00047	-0.00005	0.00042	2.04664
A34	1.93897	-0.00102	0.00075	-0.00041	0.00074	1.93971
A35	1.92018	0.00276	-0.00040	-0.00010	-0.00035	1.91983
A36	1.88684	-0.00082	-0.00010	0.00212	0.00187	1.88872
A37	2.08664	0.00006	-0.00433	0.00023	-0.00636	2.08028
A38	2.09358	-0.00054	0.00612	0.00202	0.00998	2.10356
A39	1.99966	-0.00032	0.00020	-0.00086	-0.00298	1.99668
A40	2.01115	-0.00006	0.00348	-0.00219	0.00248	2.01363
A41	2.01197	0.00039	-0.00346	-0.00037	-0.00368	2.00829
A42	2.05735	-0.00104	0.01135	0.00309	0.00969	2.06704
A43	2.13019	-0.00003	0.00060	-0.00163	0.00338	2.13357
A44	1.97579	-0.00035	0.00568	0.00038	0.00566	1.98146
A45	2.02702	-0.00054	0.00034	0.00050	0.00016	2.02719
A46	2.01684	0.00099	-0.01138	-0.00156	-0.01250	2.00434
A47	2.63336	0.00011	0.02059	0.01984	0.02813	2.66149
A48	2.56691	0.00082	0.00108	0.00543	-0.00517	2.56174
A49	1.92789	0.00000	-0.00151	-0.00028	-0.00179	1.92610
A50	1.91411	0.00003	-0.00185	-0.00080	-0.00266	1.91146
A51	1.94403	0.00023	0.00211	0.00044	0.00256	1.94659
A52	1.87638	0.00002	-0.00144	-0.00001	-0.00147	1.87491
A53	1.89907	-0.00015	0.00159	0.00082	0.00240	1.90147
A54	1.90088	-0.00014	0.00104	-0.00017	0.00087	1.90175
A55	3.34707	0.00242	0.00045	0.01640	0.01686	3.36392
A56	2.78495	0.00222	-0.02234	-0.03846	-0.06272	2.72224
A57	2.80927	-0.00071	-0.01683	0.03077	0.01394	2.82322
A58	3.13660	-0.00027	-0.03192	-0.05122	-0.08391	3.05269
D1	0.00499	-0.00015	0.00826	-0.00789	0.00036	0.00535
D2	3.13731	-0.00001	-0.00034	0.00132	0.00098	3.13829
D3	-3.13411	-0.00013	0.01125	-0.00661	0.00463	-3.12949

D4	-0.00179	0.00001	0.00265	0.00260	0.00525	0.00345
D5	-0.00807	0.00025	-0.00493	0.00269	-0.00223	-0.01030
D6	-3.09336	0.00010	-0.00439	0.00169	-0.00276	-3.09612
D7	3.13129	0.00023	-0.00762	0.00154	-0.00606	3.12523
D8	0.04600	0.00008	-0.00709	0.00054	-0.00659	0.03941
D9	-0.00029	0.00001	-0.00882	0.01042	0.00160	0.00131
D10	3.14003	0.00003	0.00023	0.00689	0.00712	-3.13604
D11	-3.13352	-0.00011	-0.00108	0.00212	0.00105	-3.13247
D12	0.00680	-0.00009	0.00798	-0.00140	0.00656	0.01336
D13	-0.00475	0.00014	0.00582	-0.00883	-0.00302	-0.00777
D14	3.09938	0.00013	0.00341	-0.00398	-0.00060	3.09878
D15	3.13801	0.00013	-0.00248	-0.00560	-0.00808	3.12993
D16	-0.04105	0.00011	-0.00489	-0.00075	-0.00565	-0.04670
D17	0.12988	-0.00011	-0.01731	-0.00689	-0.02421	0.10568
D18	-3.01522	-0.00006	-0.01571	-0.00373	-0.01944	-3.03466
D19	-3.01313	-0.00009	-0.00719	-0.01084	-0.01803	-3.03116
D20	0.12495	-0.00004	-0.00559	-0.00767	-0.01326	0.11168
D21	0.00790	-0.00024	-0.00060	0.00385	0.00325	0.01115
D22	3.09449	-0.00030	-0.00065	0.00481	0.00411	3.09860
D23	-3.09350	-0.00012	0.00240	-0.00112	0.00128	-3.09221
D24	-0.00691	-0.00018	0.00235	-0.00017	0.00214	-0.00477
D25	1.48142	-0.00034	-0.08386	-0.06252	-0.14639	1.33503
D26	-2.68895	-0.00003	-0.08760	-0.06683	-0.15443	-2.84338
D27	-0.64762	-0.00002	-0.08477	-0.06353	-0.14831	-0.79593
D28	-1.59548	-0.00037	-0.08354	-0.06365	-0.14720	-1.74268
D29	0.51733	-0.00006	-0.08728	-0.06796	-0.15523	0.36209
D30	2.55866	-0.00005	-0.08445	-0.06466	-0.14912	2.40954
D31	-1.06389	0.00071	-0.00231	0.00919	0.00688	-1.05700
D32	0.97756	0.00060	-0.00497	0.00704	0.00209	0.97965
D33	-3.13000	0.00129	0.00061	0.01033	0.01096	-3.11905
D34	3.13220	-0.00007	0.00180	0.01109	0.01288	-3.13811
D35	-1.10954	-0.00018	-0.00086	0.00895	0.00809	-1.10145
D36	1.06608	0.00051	0.00472	0.01224	0.01695	1.08303
D37	1.04576	-0.00006	0.00388	0.01062	0.01449	1.06025
D38	3.08721	-0.00017	0.00122	0.00848	0.00970	3.09690
D39	-1.02036	0.00052	0.00679	0.01176	0.01856	-1.00180
D40	2.89718	-0.00039	0.07530	0.06399	0.13918	3.03636
D41	-1.29725	-0.00028	0.07539	0.06631	0.14176	-1.15549
D42	0.82894	-0.00009	0.07618	0.06300	0.13910	0.96804
D43	2.91769	0.00002	0.07627	0.06532	0.14168	3.05938
D44	-1.27513	0.00009	0.07692	0.06366	0.14049	-1.13463
D45	0.81362	0.00021	0.07701	0.06598	0.14308	0.95670
D46	-3.13144	-0.00006	0.00149	-0.00016	0.00133	-3.13011
D47	0.01230	-0.00002	-0.00056	0.00078	0.00022	0.01251

D48	0.01412	-0.00012	-0.00032	-0.00374	-0.00406	0.01006
D49	-3.12533	-0.00008	-0.00238	-0.00279	-0.00517	-3.13050
D50	1.75972	-0.00022	0.08637	0.07489	0.16243	1.92215
D51	-0.66947	-0.00103	-0.06342	-0.07826	-0.14252	-0.81199
D52	-2.46042	0.00067	0.09015	0.08146	0.17240	-2.28801
D53	1.39358	-0.00015	-0.05964	-0.07170	-0.13255	1.26103
D54	-2.71101	0.00011	0.00376	-0.00197	0.00332	-2.70769
D55	-0.00414	0.00013	0.00285	-0.00255	0.00184	-0.00229
D56	-0.03553	0.00001	-0.00111	0.00248	0.00216	-0.03336
D57	2.67134	0.00002	-0.00203	0.00190	0.00069	2.67203
D58	1.41975	0.00008	-0.11714	-0.13714	-0.25748	1.16227
D59	-0.97597	-0.00010	-0.11593	-0.13294	-0.25092	-1.22689
D60	1.03163	0.00036	0.10577	0.12336	0.22366	1.25529
D61	-1.36223	-0.00019	0.11686	0.12484	0.23685	-1.12537
D62	2.55412	0.00027	0.00835	0.00294	0.01234	2.56646
D63	-1.66402	0.00032	0.00451	0.00226	0.00783	-1.65618
D64	0.44155	0.00031	0.00595	0.00179	0.00880	0.45035
D65	1.36345	-0.00020	0.00857	0.00278	0.01039	1.37384
D66	-2.85468	-0.00015	0.00473	0.00210	0.00588	-2.84880
D67	-0.74912	-0.00016	0.00617	0.00163	0.00685	-0.74227
D68	-1.01284	-0.00018	0.01256	0.00344	0.01590	-0.99694
D69	1.05221	-0.00013	0.00872	0.00276	0.01139	1.06360
D70	-3.12541	-0.00014	0.01016	0.00230	0.01236	-3.11305

Item	Value	Threshold	Converged?
Maximum Force	0.002757	0.000450	NO
RMS Force	0.000615	0.000300	NO
Maximum Displacement	0.443798	0.001800	NO
RMS Displacement	0.118806	0.001200	NO

Predicted change in Energy=-9.167136D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.654017	2.048069	-0.317037
2	6	0	-3.566964	1.098534	0.010049
3	7	0	-2.867182	-0.088676	0.189958
4	6	0	-1.558439	0.146840	-0.024080
5	7	0	-1.409956	1.431806	-0.340548
6	6	0	-0.112976	2.079020	-0.594745
7	6	0	0.390695	2.867047	0.620429
8	1	0	-2.778807	3.096258	-0.526995

9	1	0	-4.632343	1.167497	0.134375
10	1	0	0.599534	1.292573	-0.843198
11	1	0	-0.214362	2.741101	-1.455534
12	1	0	-0.330510	3.653736	0.868155
13	1	0	0.438312	2.182783	1.482423
14	35	0	0.187023	-2.528642	0.749959
15	1	0	-0.784461	-0.641059	0.098644
16	6	0	-3.361531	-1.381834	0.535894
17	6	0	-4.651057	-1.676832	0.635358
18	1	0	-2.550226	-2.086961	0.706962
19	1	0	-4.936600	-2.681975	0.913762
20	1	0	-5.448767	-0.966950	0.452493
21	7	0	1.654676	3.487361	0.253406
22	1	0	1.986551	4.102710	0.987315
23	1	0	2.362192	2.769979	0.094589
24	6	0	3.640353	-0.068073	-1.315259
25	6	0	3.312976	-0.485401	0.050738
26	8	0	3.052565	0.878008	-0.402551
27	1	0	4.676813	0.139949	-1.572548
28	1	0	3.009251	-0.364494	-2.149446
29	1	0	2.409034	-1.069994	0.211427
30	6	0	4.362968	-0.640457	1.115461
31	1	0	3.952963	-0.379904	2.094645
32	1	0	4.684449	-1.684944	1.162352
33	1	0	5.232957	-0.009707	0.915761

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357231	0.000000			
3	N	2.206391	1.389794	0.000000		
4	C	2.213772	2.222849	1.346882	0.000000	
5	N	1.388532	2.210582	2.171822	1.331667	0.000000
6	C	2.556359	3.641039	3.591701	2.479585	1.471618
7	C	3.289352	4.377587	4.419883	3.407937	2.495142
8	H	1.076269	2.213710	3.265828	3.231298	2.163081
9	H	2.212003	1.074824	2.167222	3.242798	3.267903
10	H	3.381303	4.257392	3.872129	2.576917	2.076076
11	H	2.779998	4.010724	4.213400	3.253582	2.094491
12	H	3.062929	4.211893	4.571685	3.821284	2.750116
13	H	3.580322	4.402921	4.213820	3.225155	2.702459
14	Br	5.491473	5.272218	3.949077	3.286940	4.407346
15	H	3.301430	3.282736	2.156663	1.111255	2.209277
16	C	3.604484	2.543804	1.426994	2.429312	3.534595

17	C	4.332449	3.044491	2.429574	3.650333	4.595733
18	H	4.261199	3.415672	2.088276	2.551065	3.844374
19	H	5.394291	4.121268	3.395819	4.504855	5.561808
20	H	4.182481	2.828986	2.739502	4.074593	4.763921
21	N	4.578406	5.747281	5.765350	4.643294	3.737653
22	H	5.240015	6.389183	6.462369	5.407289	4.520311
23	H	5.084579	6.160825	5.960483	4.718716	4.026059
24	C	6.715177	7.420433	6.679380	5.361041	5.357734
25	C	6.492976	7.060034	6.194444	4.912841	5.112228
26	O	5.825928	6.636041	6.027350	4.683930	4.497180
27	H	7.678431	8.448867	7.750520	6.424652	6.343144
28	H	6.422677	7.074635	6.330983	5.063835	5.101783
29	H	5.969596	6.360472	5.366740	4.156559	4.598734
30	C	7.649726	8.193281	7.310000	6.081238	6.304037
31	H	7.440662	7.942331	7.087103	5.928069	6.162252
32	H	8.365230	8.784154	7.779509	6.613373	7.008182
33	H	8.243701	8.915555	8.132975	6.857905	6.912638

		6	7	8	9	10
6	C	0.000000				
7	C	1.533401	0.000000			
8	H	2.854124	3.378589	0.000000		
9	H	4.667674	5.325001	2.755563	0.000000	
10	H	1.089907	2.159811	3.842714	5.323893	0.000000
11	H	1.090682	2.166005	2.750401	4.952030	1.770767
12	H	2.160354	1.095621	2.872522	5.022508	3.060850
13	H	2.151584	1.101597	3.901545	5.344117	2.495391
14	Br	4.809239	5.401085	6.485851	6.104644	4.160529
15	H	2.886263	3.736316	4.282100	4.251865	2.557624
16	C	4.879443	5.669156	4.639247	2.876677	4.974373
17	C	6.017787	6.787217	5.257259	2.888173	6.210652
18	H	4.999003	5.761830	5.332978	3.905709	4.872908
19	H	6.943344	7.697906	6.334022	3.939347	7.037949
20	H	6.232601	6.987636	4.959611	2.307295	6.585302
21	N	2.413996	1.455041	4.518602	6.702429	2.670759
22	H	3.317567	2.051396	5.100463	7.290593	3.629251
23	H	2.660651	2.042727	5.188709	7.175867	2.483774
24	C	4.383677	4.787703	7.199998	8.489145	3.364637
25	C	4.327823	4.483658	7.090267	8.115859	3.364979
26	O	3.391168	3.476826	6.240275	7.709080	2.526539
27	H	5.259104	5.533265	8.088215	9.519970	4.299384
28	H	4.258657	4.997190	6.936193	8.121379	3.202951
29	H	4.114211	4.443114	6.694521	7.388727	3.157253
30	C	5.509486	5.322274	8.225914	9.227506	4.662230
31	H	5.459944	5.040412	8.017071	8.941174	4.761679

32	H	6.345873	6.280974	9.022970	9.797743	5.438233
33	H	5.934932	5.640075	8.713033	9.965969	5.124303

		11	12	13	14	15
11	H	0.000000				
12	H	2.499185	0.000000			
13	H	3.060930	1.769779	0.000000		
14	Br	5.726736	6.205128	4.774639	0.000000	
15	H	3.765567	4.386740	3.374034	2.220577	0.000000
16	C	5.555993	5.886803	5.295396	3.735402	2.716841
17	C	6.601078	6.865587	6.443277	4.913831	4.038744
18	H	5.782978	6.157006	5.269099	2.772988	2.361908
19	H	7.571186	7.833223	7.271790	5.128533	4.697873
20	H	6.692475	6.907972	6.755685	5.855724	4.689048
21	N	2.640205	2.084841	2.166090	6.212315	4.797623
22	H	3.558863	2.363165	2.515610	6.875280	5.565213
23	H	3.007049	2.937700	2.443808	5.765089	4.640757
24	C	4.771788	5.864036	4.811074	4.716462	4.680428
25	C	5.012114	5.574551	4.175239	3.799385	4.100673
26	O	3.905471	4.556815	3.477051	4.598355	4.157106
27	H	5.541054	6.586123	5.609893	5.716085	5.764405
28	H	4.529671	6.033746	5.127262	4.588578	4.418443
29	H	4.917866	5.500002	4.009954	2.712011	3.224145
30	C	6.244750	6.366317	4.848533	4.597538	5.246899
31	H	6.301669	6.010214	4.392602	4.539555	5.147369
32	H	7.102222	7.330612	5.752516	4.594424	5.668346
33	H	6.547005	6.661475	5.302522	5.642160	6.105375

		16	17	18	19	20
16	C	0.000000				
17	C	1.326573	0.000000			
18	H	1.088432	2.141687	0.000000		
19	H	2.077016	1.081368	2.468115	0.000000	
20	H	2.129704	1.083381	3.117807	1.848349	0.000000
21	N	6.996512	8.159476	6.997140	9.052165	8.386860
22	H	7.673720	8.808225	7.679386	9.693678	9.015068
23	H	7.084723	8.321792	6.935179	9.146978	8.666246
24	C	7.360646	8.668361	6.818251	9.239326	9.302958
25	C	6.751890	8.073854	6.113326	8.580516	8.784159
26	O	6.864997	8.182314	6.435318	8.844937	8.741145
27	H	8.448451	9.756264	7.898441	10.322921	10.385249
28	H	6.988053	8.255766	6.483343	8.825559	8.869673
29	H	5.788086	7.098792	5.086652	7.553151	7.862173
30	C	7.781608	9.086101	7.074708	9.523153	9.839526
31	H	7.545554	8.822738	6.865214	9.258420	9.562103
32	H	8.076021	9.350372	7.260132	9.675766	10.183393

33	H	8.711616	10.027545	8.058319	10.514795	10.734532
		21	22	23	24	25
21	N	0.000000				
22	H	1.013617	0.000000			
23	H	1.020019	1.647495	0.000000		
24	C	4.364027	5.043049	3.417002	0.000000	
25	C	4.309741	4.866965	3.391668	1.465362	0.000000
26	O	3.032012	3.669717	2.074444	1.440000	1.460195
27	H	4.865448	5.430827	3.879932	1.087989	2.210468
28	H	4.737653	5.553477	3.908874	1.087209	2.224337
29	H	4.619556	5.247605	3.842035	2.202444	1.088431
30	C	5.011673	5.306733	4.083669	2.599653	1.503383
31	H	4.860866	5.018643	4.056172	3.438372	2.144357
32	H	6.062874	6.387976	5.136081	3.137350	2.134368
33	H	5.047009	5.239871	4.079494	2.741759	2.158906
		26	27	28	29	30
26	O	0.000000				
27	H	2.133496	0.000000			
28	H	2.144138	1.835221	0.000000		
29	H	2.141450	3.128793	2.536081	0.000000	
30	C	2.515403	2.816545	3.545183	2.195368	0.000000
31	H	2.937523	3.773925	4.347773	2.531097	1.093066
32	H	3.417702	3.287852	3.939274	2.541641	1.093847
33	H	2.698165	2.554090	3.803451	3.097554	1.092980
		31	32	33		
31	H	0.000000				
32	H	1.762774	0.000000			
33	H	1.779100	1.779912	0.000000		

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.370662	2.457880	-0.232873
2	6	0	-3.385331	1.569833	-0.078299
3	7	0	-2.815539	0.302213	-0.080089
4	6	0	-1.483272	0.429747	-0.231380
5	7	0	-1.195173	1.725793	-0.334343

6	6	0	0.168352	2.265117	-0.459192
7	6	0	0.708178	2.793407	0.875281
8	1	0	-2.381777	3.533327	-0.273440
9	1	0	-4.441842	1.729850	0.037566
10	1	0	0.805630	1.457447	-0.818973
11	1	0	0.163245	3.062093	-1.203766
12	1	0	0.062303	3.602345	1.234238
13	1	0	0.657541	1.980114	1.616569
14	35	0	-0.044036	-2.503023	0.131158
15	1	0	-0.797433	-0.444587	-0.224078
16	6	0	-3.449351	-0.970183	0.044816
17	6	0	-4.764691	-1.139993	0.073792
18	1	0	-2.719647	-1.774833	0.113777
19	1	0	-5.159515	-2.140881	0.181929
20	1	0	-5.480002	-0.330236	-0.005816
21	7	0	2.039946	3.327656	0.634208
22	1	0	2.407592	3.780685	1.463075
23	1	0	2.676243	2.574122	0.373913
24	6	0	3.707425	-0.123310	-1.452674
25	6	0	3.294052	-0.714921	-0.177368
26	8	0	3.188084	0.722788	-0.409600
27	1	0	4.767623	0.012704	-1.655651
28	1	0	3.077841	-0.215890	-2.334194
29	1	0	2.330786	-1.219276	-0.128104
30	6	0	4.286804	-1.146130	0.866023
31	1	0	3.872723	-1.002279	1.867340
32	1	0	4.499318	-2.212798	0.749578
33	1	0	5.222278	-0.586713	0.785120

Rotational constants (GHZ): 0.4329555 0.2796700 0.1796875

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1305.7725679068 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 3.73D-06 NBF= 482

NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999753 0.002593 0.000810 0.022040 Ang= 2.54 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3205.64737507 A.U. after 12 cycles
NFock= 12 Conv=0.74D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000381371	-0.000159279	0.000023171
2	6	-0.000152333	-0.000534481	0.000265923
3	7	0.000557897	0.001564957	-0.000473950
4	6	-0.001721722	-0.003817419	0.000421110
5	7	-0.000147435	0.000866826	0.000508800
6	6	0.000628629	0.001416052	0.000415006
7	6	-0.001637904	-0.000547489	-0.000030737
8	1	0.000101417	-0.000058379	-0.000452824
9	1	0.000090399	0.000220588	-0.000206511
10	1	0.000472310	0.000232173	-0.000180429
11	1	-0.000650926	-0.000138610	-0.000194204
12	1	0.000014349	-0.000050600	0.000276990
13	1	0.000526959	0.000144933	-0.000277299
14	35	-0.000304758	-0.000525295	0.000018963
15	1	0.000151294	0.001531397	-0.000577244

16	6	-0.000123398	-0.000315927	0.000505724
17	6	0.000257743	0.000086412	0.000119523
18	1	-0.000160223	0.000132465	-0.000055140
19	1	-0.000081782	0.000008923	-0.000147392
20	1	-0.000034125	-0.000126535	0.000055236
21	7	0.001984634	-0.000410938	-0.000109832
22	1	-0.000217426	0.000061207	-0.000247036
23	1	-0.000453756	0.001460156	0.000485199
24	6	0.002030468	-0.000301965	-0.000694028
25	6	0.001118920	0.000347626	0.001991053
26	8	-0.001739100	-0.001517313	0.000158671
27	1	-0.000066473	0.000151715	-0.000057178
28	1	-0.000667222	-0.000294225	0.000823305
29	1	-0.000945781	0.000256714	-0.001887361
30	6	0.000450267	0.000183276	-0.000707964
31	1	0.000062651	0.000247190	0.000122502
32	1	0.000200262	-0.000067948	0.000026958
33	1	0.000074792	-0.000046206	0.000080993

Cartesian Forces: Max 0.003817419 RMS 0.000790449

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.003821949 RMS 0.000791099
Search for a local minimum.
Step number 21 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 20 21
DE= -5.61D-05 DEPred=-9.17D-05 R= 6.12D-01
TightC=F SS= 1.41D+00 RLast= 7.76D-01 DXNew= 1.6878D+00 2.3267D+00
Trust test= 6.12D-01 RLast= 7.76D-01 DXMaxT set to 1.69D+00
ITU= 1 1 1 1 1 1 1 1 1 0 -1 -1 1 1 1 -1 1 0 0 -1
ITU= 0

Eigenvalues ---	0.00079	0.00198	0.00333	0.00409	0.00724
Eigenvalues ---	0.00733	0.00862	0.01307	0.01528	0.01874
Eigenvalues ---	0.01937	0.02151	0.02282	0.02390	0.02404
Eigenvalues ---	0.02496	0.02938	0.02991	0.03083	0.03097
Eigenvalues ---	0.03273	0.03325	0.03666	0.03984	0.04150
Eigenvalues ---	0.04343	0.04452	0.05118	0.05468	0.05727
Eigenvalues ---	0.05781	0.06002	0.07631	0.08643	0.09440

Eigenvalues --- 0.09756 0.10051 0.12222 0.12510 0.12736
Eigenvalues --- 0.13428 0.13859 0.15172 0.15956 0.15998
Eigenvalues --- 0.16000 0.16002 0.16012 0.16016 0.16028
Eigenvalues --- 0.16103 0.17231 0.18576 0.22091 0.22840
Eigenvalues --- 0.22949 0.22962 0.24221 0.25529 0.27209
Eigenvalues --- 0.29188 0.31061 0.31796 0.32087 0.33639
Eigenvalues --- 0.33974 0.34278 0.34322 0.34476 0.34555
Eigenvalues --- 0.34693 0.34764 0.35063 0.35222 0.35389
Eigenvalues --- 0.35440 0.35577 0.35843 0.35890 0.36423
Eigenvalues --- 0.36629 0.38810 0.39456 0.41915 0.42545
Eigenvalues --- 0.44706 0.45477 0.46440 0.49360 0.54856
Eigenvalues --- 0.58463 0.60617 1.77402
En-DIIS/RFO-DIIS IScMMF= 0 using points: 21 20 19 18 17
RFO step: Lambda=-1.18324848D-04.
DidBck=T Rises=F RFO-DIIS coefs: 0.53121 0.01185 -0.32815 -0.49055 1.27565
Iteration 1 RMS(Cart)= 0.16388587 RMS(Int)= 0.02117994
Iteration 2 RMS(Cart)= 0.04010223 RMS(Int)= 0.00370975
Iteration 3 RMS(Cart)= 0.00147545 RMS(Int)= 0.00359846
Iteration 4 RMS(Cart)= 0.00003662 RMS(Int)= 0.00359846
Iteration 5 RMS(Cart)= 0.00000051 RMS(Int)= 0.00359846

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56479	-0.00031	0.00053	-0.00005	0.00049	2.56528
R2	2.62395	-0.00043	-0.00223	0.00032	-0.00191	2.62204
R3	2.03385	0.00002	0.00020	-0.00009	0.00011	2.03397
R4	2.62633	-0.00054	-0.00055	-0.00025	-0.00080	2.62553
R5	2.03112	-0.00010	-0.00033	-0.00003	-0.00036	2.03077
R6	2.54524	-0.00039	-0.00234	0.00053	-0.00181	2.54342
R7	2.69663	0.00036	0.00153	0.00007	0.00160	2.69823
R8	2.51649	0.00223	0.00354	-0.00030	0.00324	2.51973
R9	2.09997	-0.00088	-0.00281	0.00028	-0.00253	2.09744
R10	2.78096	0.00152	0.00387	0.00017	0.00404	2.78500
R11	2.89771	0.00006	0.00188	-0.00010	0.00175	2.89946
R12	2.05963	0.00018	0.00048	0.00016	0.00064	2.06027
R13	2.06109	0.00013	-0.00081	0.00021	-0.00060	2.06049
R14	2.07042	0.00002	-0.00126	0.00039	-0.00088	2.06954
R15	2.08172	-0.00028	-0.00266	0.00026	-0.00240	2.07931
R16	2.74963	0.00163	0.00232	0.00045	0.00277	2.75240
R17	4.19628	0.00032	-0.00290	0.00473	0.00182	4.19810
R18	2.50686	-0.00013	-0.00046	0.00008	-0.00038	2.50648
R19	2.05684	-0.00021	-0.00073	0.00002	-0.00071	2.05612
R20	2.04349	-0.00002	-0.00005	0.00002	-0.00003	2.04346
R21	2.04729	-0.00007	-0.00027	0.00007	-0.00020	2.04709

R22	1.91546	-0.00021	-0.00114	-0.00001	-0.00115	1.91431
R23	1.92756	-0.00007	-0.00118	0.00003	-0.00153	1.92603
R24	3.92013	0.00103	0.00622	0.00796	0.01437	3.93450
R25	2.76913	-0.00065	-0.00081	-0.00031	0.00956	2.77869
R26	2.72120	0.00083	0.00336	0.00064	0.00019	2.72139
R27	2.05600	-0.00002	-0.00043	-0.00011	-0.00054	2.05546
R28	2.05453	-0.00016	-0.00138	0.00032	-0.00107	2.05346
R29	2.75937	-0.00021	-0.00739	0.00156	-0.01285	2.74652
R30	2.05684	0.00037	-0.00002	0.00102	0.00101	2.05784
R31	2.84098	0.00018	0.00038	0.00008	0.00046	2.84144
R32	2.06560	0.00015	0.00095	0.00000	0.00095	2.06654
R33	2.06707	0.00012	0.00049	0.00000	0.00049	2.06756
R34	2.06543	0.00002	-0.00025	0.00017	-0.00008	2.06535
A1	1.87155	0.00059	0.00065	0.00028	0.00092	1.87248
A2	2.27888	-0.00013	0.00118	-0.00038	0.00081	2.27970
A3	2.13273	-0.00046	-0.00184	0.00011	-0.00173	2.13100
A4	1.86517	-0.00006	-0.00081	-0.00013	-0.00095	1.86422
A5	2.27803	-0.00024	-0.00187	0.00030	-0.00155	2.27648
A6	2.13996	0.00030	0.00271	-0.00020	0.00253	2.14249
A7	1.89580	0.00059	0.00156	0.00003	0.00158	1.89738
A8	2.25373	-0.00024	0.00085	-0.00015	0.00074	2.25446
A9	2.13365	-0.00035	-0.00244	0.00009	-0.00231	2.13134
A10	1.89108	-0.00051	-0.00113	0.00014	-0.00102	1.89006
A11	2.13559	-0.00005	0.01151	-0.00109	0.01042	2.14601
A12	2.25588	0.00055	-0.01036	0.00076	-0.00959	2.24629
A13	1.90110	-0.00061	-0.00024	-0.00025	-0.00049	1.90061
A14	2.21101	-0.00293	-0.00286	0.00081	-0.00201	2.20899
A15	2.16965	0.00356	0.00218	-0.00015	0.00205	2.17170
A16	1.95910	-0.00025	-0.00034	0.00015	-0.00034	1.95876
A17	1.87359	0.00100	0.00183	0.00152	0.00339	1.87698
A18	1.89797	-0.00097	-0.00817	0.00025	-0.00788	1.89010
A19	1.91425	-0.00009	0.00256	-0.00127	0.00133	1.91558
A20	1.92198	0.00038	0.00627	-0.00012	0.00620	1.92818
A21	1.89534	-0.00007	-0.00249	-0.00051	-0.00299	1.89235
A22	1.90918	-0.00082	-0.00134	-0.00001	-0.00139	1.90780
A23	1.89134	0.00020	0.00158	0.00013	0.00165	1.89300
A24	1.88024	0.00146	0.00188	0.00088	0.00294	1.88318
A25	1.87291	0.00023	0.00238	-0.00077	0.00163	1.87454
A26	1.89943	-0.00066	0.00594	0.00091	0.00679	1.90622
A27	2.00936	-0.00047	-0.01028	-0.00112	-0.01146	1.99790
A28	2.16090	0.00017	0.00071	0.00012	0.00083	2.16173
A29	1.94653	-0.00008	-0.00087	0.00020	-0.00068	1.94586
A30	2.17575	-0.00009	0.00017	-0.00031	-0.00015	2.17560
A31	2.07452	0.00004	0.00065	-0.00025	0.00040	2.07492

A32	2.16203	0.00011	0.00032	0.00038	0.00070	2.16273
A33	2.04664	-0.00015	-0.00098	-0.00013	-0.00111	2.04553
A34	1.93971	-0.00138	0.00012	0.00108	-0.00020	1.93951
A35	1.91983	0.00382	0.00147	0.00090	0.00193	1.92176
A36	1.88872	-0.00144	-0.00225	-0.00101	-0.00279	1.88592
A37	2.08028	0.00089	0.00547	-0.00018	0.01180	2.09208
A38	2.10356	-0.00137	-0.01673	0.00164	-0.02063	2.08292
A39	1.99668	0.00010	-0.00019	-0.00012	0.00289	1.99957
A40	2.01363	-0.00030	-0.00353	-0.00040	-0.00467	2.00896
A41	2.00829	0.00048	0.01121	-0.00103	0.00987	2.01816
A42	2.06704	-0.00159	-0.02664	0.00027	-0.02086	2.04619
A43	2.13357	-0.00017	0.00011	-0.00149	-0.00585	2.12772
A44	1.98146	-0.00077	-0.00543	-0.00205	-0.00593	1.97552
A45	2.02719	-0.00055	-0.00032	0.00064	0.00082	2.02801
A46	2.00434	0.00173	0.02109	0.00151	0.02176	2.02610
A47	2.66149	-0.00037	-0.07254	0.00186	-0.04970	2.61179
A48	2.56174	0.00081	-0.01804	-0.00294	0.01216	2.57390
A49	1.92610	0.00004	0.00307	0.00008	0.00316	1.92925
A50	1.91146	0.00019	0.00362	-0.00026	0.00337	1.91482
A51	1.94659	0.00008	-0.00315	0.00050	-0.00265	1.94393
A52	1.87491	0.00000	0.00312	-0.00001	0.00313	1.87804
A53	1.90147	-0.00015	-0.00450	-0.00009	-0.00459	1.89689
A54	1.90175	-0.00017	-0.00208	-0.00024	-0.00232	1.89943
A55	3.36392	0.00208	-0.00257	-0.00503	-0.00759	3.35633
A56	2.72224	0.00315	0.11024	-0.00975	0.10340	2.82564
A57	2.82322	-0.00049	0.01627	-0.01851	-0.00224	2.82097
A58	3.05269	0.00075	0.09285	0.00679	0.10073	3.15342
D1	0.00535	-0.00014	-0.00328	0.00438	0.00111	0.00646
D2	3.13829	-0.00003	0.00652	0.00001	0.00653	-3.13837
D3	-3.12949	-0.00020	-0.01297	0.00294	-0.01000	-3.13949
D4	0.00345	-0.00008	-0.00318	-0.00143	-0.00459	-0.00114
D5	-0.01030	0.00034	0.00297	0.00167	0.00463	-0.00566
D6	-3.09612	0.00000	0.01898	-0.00624	0.01282	-3.08330
D7	3.12523	0.00039	0.01166	0.00296	0.01461	3.13984
D8	0.03941	0.00005	0.02766	-0.00495	0.02279	0.06220
D9	0.00131	-0.00009	0.00250	-0.00889	-0.00641	-0.00510
D10	-3.13604	-0.00006	-0.00729	-0.00221	-0.00950	3.13764
D11	-3.13247	-0.00019	-0.00633	-0.00495	-0.01129	3.13942
D12	0.01336	-0.00017	-0.01613	0.00173	-0.01438	-0.00102
D13	-0.00777	0.00031	-0.00066	0.01002	0.00938	0.00161
D14	3.09878	0.00023	-0.00055	0.00481	0.00425	3.10303
D15	3.12993	0.00028	0.00830	0.00389	0.01221	-3.14104
D16	-0.04670	0.00021	0.00842	-0.00132	0.00708	-0.03962
D17	0.10568	-0.00002	-0.00775	-0.00058	-0.00832	0.09735

D18	-3.03466	-0.00008	-0.00567	-0.00289	-0.00856	-3.04322
D19	-3.03116	0.00001	-0.01869	0.00691	-0.01179	-3.04295
D20	0.11168	-0.00005	-0.01661	0.00459	-0.01202	0.09966
D21	0.01115	-0.00041	-0.00141	-0.00726	-0.00868	0.00247
D22	3.09860	-0.00033	-0.01732	0.00045	-0.01681	3.08179
D23	-3.09221	-0.00030	-0.00214	-0.00153	-0.00371	-3.09593
D24	-0.00477	-0.00022	-0.01805	0.00619	-0.01184	-0.01661
D25	1.33503	-0.00019	0.14880	-0.01236	0.13645	1.47148
D26	-2.84338	0.00020	0.15298	-0.01283	0.14014	-2.70324
D27	-0.79593	0.00016	0.14677	-0.01248	0.13430	-0.66163
D28	-1.74268	-0.00042	0.16734	-0.02142	0.14594	-1.59674
D29	0.36209	-0.00002	0.17152	-0.02189	0.14963	0.51172
D30	2.40954	-0.00006	0.16531	-0.02154	0.14379	2.55334
D31	-1.05700	0.00093	-0.03609	-0.00156	-0.03765	-1.09465
D32	0.97965	0.00086	-0.03310	-0.00241	-0.03554	0.94412
D33	-3.11905	0.00133	-0.04352	-0.00314	-0.04669	3.11745
D34	-3.13811	-0.00011	-0.03989	-0.00273	-0.04259	3.10249
D35	-1.10145	-0.00017	-0.03690	-0.00358	-0.04048	-1.14193
D36	1.08303	0.00029	-0.04732	-0.00431	-0.05163	1.03140
D37	1.06025	-0.00021	-0.04237	-0.00123	-0.04358	1.01667
D38	3.09690	-0.00027	-0.03937	-0.00208	-0.04147	3.05543
D39	-1.00180	0.00020	-0.04979	-0.00281	-0.05262	-1.05442
D40	3.03636	-0.00098	-0.15911	0.01361	-0.14517	2.89119
D41	-1.15549	-0.00116	-0.16088	0.01363	-0.14752	-1.30301
D42	0.96804	-0.00047	-0.16187	0.01263	-0.14894	0.81910
D43	3.05938	-0.00064	-0.16364	0.01265	-0.15130	2.90808
D44	-1.13463	0.00005	-0.16239	0.01370	-0.14837	-1.28300
D45	0.95670	-0.00013	-0.16416	0.01372	-0.15072	0.80598
D46	-3.13011	-0.00016	-0.00211	-0.00256	-0.00467	-3.13478
D47	0.01251	-0.00005	-0.00123	-0.00106	-0.00229	0.01022
D48	0.01006	-0.00009	-0.00445	0.00005	-0.00440	0.00566
D49	-3.13050	0.00002	-0.00358	0.00156	-0.00202	-3.13252
D50	1.92215	-0.00012	-0.31584	0.03277	-0.28553	1.63661
D51	-0.81199	-0.00171	0.10829	-0.04142	0.06800	-0.74399
D52	-2.28801	0.00106	-0.31892	0.02880	-0.29113	-2.57914
D53	1.26103	-0.00052	0.10521	-0.04539	0.06241	1.32344
D54	-2.70769	-0.00027	0.00360	-0.00249	-0.00178	-2.70947
D55	-0.00229	0.00003	-0.00545	-0.00133	-0.00936	-0.01165
D56	-0.03336	-0.00012	0.00641	-0.00173	0.00332	-0.03005
D57	2.67203	0.00018	-0.00264	-0.00057	-0.00426	2.66777
D58	1.16227	0.00027	0.35171	-0.05414	0.30539	1.46766
D59	-1.22689	-0.00027	0.33795	-0.05186	0.29150	-0.93539
D60	1.25529	0.00041	-0.32177	0.04402	-0.27076	0.98453
D61	-1.12537	-0.00081	-0.34901	0.04327	-0.29977	-1.42514

D62	2.56646	0.00014	-0.01050	-0.00014	-0.01260	2.55386
D63	-1.65618	0.00029	-0.00255	-0.00026	-0.00478	-1.66097
D64	0.45035	0.00025	-0.00478	-0.00041	-0.00716	0.44319
D65	1.37384	-0.00017	-0.01410	-0.00005	-0.01220	1.36163
D66	-2.84880	-0.00003	-0.00614	-0.00018	-0.00438	-2.85319
D67	-0.74227	-0.00007	-0.00838	-0.00033	-0.00676	-0.74903
D68	-0.99694	-0.00031	-0.03057	0.00074	-0.02980	-1.02675
D69	1.06360	-0.00017	-0.02262	0.00061	-0.02198	1.04162
D70	-3.11305	-0.00021	-0.02485	0.00046	-0.02436	-3.13741

Item	Value	Threshold	Converged?
Maximum Force	0.003822	0.000450	NO
RMS Force	0.000791	0.000300	NO
Maximum Displacement	0.785971	0.001800	NO
RMS Displacement	0.181234	0.001200	NO

Predicted change in Energy=-5.541715D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.798105	2.104984	-0.313433
2	6	0	-3.684414	1.134043	0.024962
3	7	0	-2.960616	-0.045456	0.148456
4	6	0	-1.666572	0.212199	-0.117191
5	7	0	-1.547916	1.509556	-0.401264
6	6	0	-0.269145	2.188981	-0.675287
7	6	0	0.358905	2.778119	0.594610
8	1	0	-2.946163	3.154493	-0.500763
9	1	0	-4.745565	1.184719	0.186923
10	1	0	0.406269	1.453849	-1.113508
11	1	0	-0.449076	2.973318	-1.411039
12	1	0	-0.307166	3.543741	1.006361
13	1	0	0.443833	1.977756	1.344891
14	35	0	0.169744	-2.437704	0.516684
15	1	0	-0.871533	-0.559547	-0.052094
16	6	0	-3.419332	-1.353396	0.491385
17	6	0	-4.697225	-1.669259	0.654129
18	1	0	-2.590930	-2.050140	0.601660
19	1	0	-4.954330	-2.685298	0.920375
20	1	0	-5.513459	-0.967357	0.533388
21	7	0	1.625529	3.393932	0.223330
22	1	0	1.969519	3.995451	0.962268

23	1	0	2.326789	2.675183	0.048912
24	6	0	3.700349	-0.174226	-1.207117
25	6	0	3.504004	-0.508819	0.211203
26	8	0	3.225182	0.827393	-0.287955
27	1	0	4.703801	0.001451	-1.588324
28	1	0	2.971520	-0.510792	-1.939462
29	1	0	2.605085	-1.065300	0.472192
30	6	0	4.659113	-0.633195	1.165741
31	1	0	4.368881	-0.297125	2.165095
32	1	0	4.961789	-1.681673	1.244143
33	1	0	5.516352	-0.042515	0.832943

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357490	0.000000			
3	N	2.205480	1.389371	0.000000		
4	C	2.213936	2.222991	1.345922	0.000000	
5	N	1.387524	2.210725	2.171630	1.333384	0.000000
6	C	2.556098	3.642431	3.593783	2.484339	1.473757
7	C	3.353262	4.401808	4.380736	3.345618	2.497395
8	H	1.076328	2.214411	3.265174	3.231342	2.161206
9	H	2.211299	1.074636	2.168145	3.243221	3.267483
10	H	3.366320	4.258178	3.895688	2.613621	2.080681
11	H	2.734352	3.989040	4.225264	3.283309	2.090381
12	H	3.164910	4.263284	4.545232	3.769552	2.767449
13	H	3.643678	4.415483	4.137042	3.115876	2.689857
14	Br	5.489375	5.277661	3.956969	3.285703	4.401574
15	H	3.298439	3.284278	2.160736	1.109917	2.204677
16	C	3.604725	2.544636	1.427840	2.427678	3.534900
17	C	4.334483	3.046332	2.430689	3.649613	4.597485
18	H	4.259738	3.415744	2.088257	2.547423	3.842548
19	H	5.396145	4.123326	3.396987	4.503486	5.563020
20	H	4.186829	2.831923	2.741365	4.075923	4.768041
21	N	4.638754	5.774248	5.733038	4.591002	3.743225
22	H	5.285028	6.405713	6.426309	5.357180	4.517880
23	H	5.169232	6.205662	5.947137	4.694764	4.071201
24	C	6.944305	7.600283	6.798721	5.490091	5.570350
25	C	6.842791	7.376112	6.481509	5.230924	5.474563
26	O	6.157343	6.923472	6.262301	4.933242	4.822929
27	H	7.894858	8.616705	7.858874	6.541429	6.539683
28	H	6.540246	7.132033	6.306043	5.035403	5.183932
29	H	6.313665	6.677943	5.667620	4.497380	4.963892
30	C	8.080575	8.604589	7.709772	6.509601	6.750859

31	H	7.954805	8.454820	7.606031	6.472630	6.697670
32	H	8.773869	9.174502	8.163470	7.026746	7.434216
33	H	8.663494	9.310812	8.504559	7.249968	7.337307

		6	7	8	9	10
6	C	0.000000				
7	C	1.534330	0.000000			
8	H	2.851157	3.502138	0.000000		
9	H	4.668007	5.362905	2.755135	0.000000	
10	H	1.090248	2.161851	3.808733	5.320240	0.000000
11	H	1.090363	2.171075	2.663995	4.920609	1.768877
12	H	2.159805	1.095155	3.063860	5.092725	3.061124
13	H	2.152689	1.100325	4.035247	5.375839	2.513884
14	Br	4.797878	5.219834	6.482032	6.114815	4.225832
15	H	2.881952	3.615552	4.277789	4.255316	2.610200
16	C	4.881930	5.599567	4.639968	2.879865	5.009145
17	C	6.021732	6.734030	5.260092	2.892371	6.238910
18	H	4.999142	5.658061	5.331953	3.908807	4.919649
19	H	6.946632	7.627943	6.336838	3.944435	7.071438
20	H	6.239087	6.965415	4.964889	2.311089	6.604369
21	N	2.418513	1.456507	4.634868	6.743351	2.652856
22	H	3.310066	2.052108	5.197268	7.320774	3.634877
23	H	2.738563	2.044737	5.323148	7.229019	2.555635
24	C	4.650211	4.809138	7.466955	8.667384	3.675643
25	C	4.722355	4.565371	7.451939	8.421642	3.899088
26	O	3.770181	3.577680	6.598952	7.992872	3.003373
27	H	5.509002	5.599393	8.345442	9.687216	4.561106
28	H	4.403273	4.905529	7.107962	8.182278	3.335045
29	H	4.490907	4.453334	7.040571	7.692595	3.700723
30	C	5.970074	5.518609	8.658177	9.628649	5.257129
31	H	5.979948	5.291829	8.516474	9.443631	5.432995
32	H	6.784456	6.441909	9.432333	10.176770	6.011887
33	H	6.381716	5.883200	9.144057	10.355211	5.669279

		11	12	13	14	15
11	H	0.000000				
12	H	2.487839	0.000000			
13	H	3.063263	1.769438	0.000000		
14	Br	5.777388	6.020374	4.500815	0.000000	
15	H	3.808718	4.275021	3.181142	2.221541	0.000000
16	C	5.582302	5.825180	5.171952	3.749378	2.723389
17	C	6.623082	6.824372	6.341005	4.929177	4.045507
18	H	5.820105	6.055647	5.097659	2.789041	2.367612
19	H	7.599522	7.772030	7.145939	5.145911	4.704651
20	H	6.705050	6.905013	6.694890	5.870349	4.696443
21	N	2.674334	2.090667	2.158671	6.017752	4.684140

22	H	3.539342	2.321482	2.558361	6.695014	5.463379
23	H	3.150519	2.934079	2.389872	5.568955	4.550049
24	C	5.212134	5.897706	4.663547	4.534313	4.731242
25	C	5.512149	5.619656	4.102798	3.864092	4.383745
26	O	4.400737	4.640181	3.424241	4.543567	4.331548
27	H	5.951097	6.662581	5.536864	5.562213	5.810256
28	H	4.911082	5.988897	4.834154	4.194710	4.281774
29	H	5.402305	5.478120	3.833119	2.795775	3.552117
30	C	6.763160	6.491234	4.961628	4.881799	5.663621
31	H	6.833538	6.161195	4.610187	4.993204	5.696204
32	H	7.615537	7.424512	5.814938	4.905556	6.080054
33	H	7.051031	6.841393	5.483980	5.867126	6.469598

		16	17	18	19	20
16	C	0.000000				
17	C	1.326373	0.000000			
18	H	1.088054	2.141098	0.000000		
19	H	2.077068	1.081353	2.467927	0.000000	
20	H	2.129826	1.083274	3.117411	1.847621	0.000000
21	N	6.932503	8.111640	6.896345	8.985402	8.371507
22	H	7.607339	8.753820	7.581352	9.621530	8.989347
23	H	7.031581	8.281137	6.842380	9.083440	8.658655
24	C	7.413852	8.730326	6.809619	9.259328	9.410243
25	C	6.980286	8.294755	6.298917	8.762614	9.034860
26	O	7.036531	8.359744	6.549715	8.983511	8.958771
27	H	8.493885	9.808117	7.887849	10.334006	10.480108
28	H	6.889266	8.177922	6.306167	8.702082	8.849763
29	H	6.031332	7.329502	5.290108	7.744031	8.119365
30	C	8.138472	9.427420	7.408715	9.833088	10.197685
31	H	8.035750	9.293011	7.345500	9.704378	10.038542
32	H	8.421259	9.677026	7.588948	9.972036	10.523605
33	H	9.037783	10.343859	8.355362	10.799404	11.072570

		21	22	23	24	25
21	N	0.000000				
22	H	1.013008	0.000000			
23	H	1.019209	1.644679	0.000000		
24	C	4.368387	5.008813	3.403440	0.000000	
25	C	4.331314	4.817384	3.398535	1.470420	0.000000
26	O	3.067152	3.629923	2.082046	1.440098	1.453397
27	H	4.926131	5.471184	3.934408	1.087703	2.222203
28	H	4.662212	5.452547	3.810478	1.086645	2.215604
29	H	4.572331	5.123994	3.774629	2.194014	1.088964
30	C	5.129183	5.357208	4.199096	2.600065	1.503626
31	H	4.992027	5.062602	4.181266	3.440037	2.147213
32	H	6.159096	6.423618	5.230105	3.142023	2.137216

33	H	5.226787	5.376050	4.263085	2.734422	2.157208
		26	27	28	29	30
26	O	0.000000				
27	H	2.135288	0.000000			
28	H	2.140691	1.840242	0.000000		
29	H	2.131814	3.128625	2.501566	0.000000	
30	C	2.510519	2.826596	3.536275	2.210601	0.000000
31	H	2.930878	3.780142	4.341159	2.562614	1.093566
32	H	3.414461	3.304896	3.932872	2.555363	1.094105
33	H	2.694924	2.554351	3.792320	3.106720	1.092939
		31	32	33		
31	H	0.000000				
32	H	1.765408	0.000000			
33	H	1.776554	1.778613	0.000000		

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.653571	2.331141	-0.206883
2	6	0	-3.583574	1.363454	-0.003275
3	7	0	-2.911638	0.147733	-0.032891
4	6	0	-1.605215	0.381781	-0.256460
5	7	0	-1.428873	1.698847	-0.366706
6	6	0	-0.119772	2.352372	-0.543114
7	6	0	0.519703	2.741858	0.796117
8	1	0	-2.755164	3.401580	-0.255064
9	1	0	-4.643222	1.438310	0.159160
10	1	0	0.528344	1.652624	-1.071260
11	1	0	-0.258856	3.233603	-1.169995
12	1	0	-0.117519	3.474876	1.302080
13	1	0	0.563048	1.846960	1.434862
14	35	0	0.110763	-2.405417	0.031274
15	1	0	-0.844254	-0.425519	-0.289957
16	6	0	-3.428763	-1.172823	0.132769
17	6	0	-4.720468	-1.451702	0.246741
18	1	0	-2.631756	-1.913220	0.154083
19	1	0	-5.023039	-2.481818	0.375730

20	1	0	-5.504994	-0.705349	0.215786
21	7	0	1.814966	3.345684	0.514868
22	1	0	2.176574	3.829471	1.328117
23	1	0	2.486915	2.626392	0.250500
24	6	0	3.751347	-0.090122	-1.363553
25	6	0	3.526606	-0.599295	-0.002536
26	8	0	3.309676	0.801712	-0.322668
27	1	0	4.765160	0.090496	-1.713780
28	1	0	3.016411	-0.295707	-2.137117
29	1	0	2.602332	-1.145792	0.178855
30	6	0	4.665650	-0.897862	0.932518
31	1	0	4.379755	-0.683722	1.966101
32	1	0	4.922867	-1.959667	0.873554
33	1	0	5.550460	-0.306259	0.684260

Rotational constants (GHZ): 0.4521714 0.2627628 0.1747797

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1297.3845601449 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 3.91D-06 NBF= 482

NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999558 0.001452 -0.003614 -0.029486 Ang= 3.41 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0

NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3205.64731882 A.U. after 12 cycles

NFock= 12 Conv=0.98D-08 -V/T= 2.0018

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000189659	0.000110115	-0.000106102
2	6	0.000121073	0.000055658	0.000370816
3	7	0.000147437	0.000087962	-0.000614161
4	6	-0.000433553	-0.000914056	0.000748613
5	7	0.000191792	-0.000186828	-0.000490765
6	6	0.000440876	0.000797454	0.000317737
7	6	-0.000077587	-0.000296889	0.000372950
8	1	-0.000025023	0.000025950	-0.000094375
9	1	-0.000004294	0.000055141	0.000012650
10	1	-0.000275631	-0.000301869	0.000074047
11	1	-0.000095141	-0.000057441	0.000010918
12	1	0.000224497	0.000062560	-0.000091294
13	1	-0.000096873	-0.000064684	-0.000107541
14	35	-0.000075643	-0.000041099	-0.000081776
15	1	0.000126552	0.000278118	-0.000000318
16	6	-0.000052269	-0.000055712	-0.000035849
17	6	0.000061699	0.000033295	-0.000033081
18	1	0.000011978	-0.000009913	0.000028994
19	1	-0.000006077	0.000016730	0.000030606
20	1	0.000009921	0.000002936	0.000014846
21	7	0.000081455	0.000174346	-0.000361953
22	1	-0.000041317	0.000058485	0.000016750
23	1	-0.000039870	0.000290082	0.000184225
24	6	-0.000855390	-0.001357038	0.001825423
25	6	0.001766425	0.000108173	-0.001534428
26	8	-0.001209400	0.000934880	0.000051596
27	1	0.000107942	-0.000200948	0.000470279
28	1	-0.000086287	0.000024163	0.000041730
29	1	-0.000306687	0.000128945	-0.001208893

30	6	0.000023036	0.000149960	0.000006406
31	1	0.000098723	0.000111818	0.000126847
32	1	0.000086754	-0.000003571	-0.000015139
33	1	-0.000008777	-0.000016727	0.000070247

Cartesian Forces: Max 0.001825423 RMS 0.000449978

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.002585937 RMS 0.000315013
Search for a local minimum.
Step number 22 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 18 19 20 21 22
DE= 5.62D-05 DEPred=-5.54D-05 R=-1.01D+00
Trust test=-1.01D+00 RLast= 9.05D-01 DXMaxT set to 8.44D-01
ITU= -1 1 1 1 1 1 1 1 1 1 0 -1 -1 1 1 1 -1 1 0 0
ITU= -1 0

Eigenvalues ---	0.00063	0.00158	0.00307	0.00411	0.00717
Eigenvalues ---	0.00728	0.00890	0.01269	0.01522	0.01881
Eigenvalues ---	0.02009	0.02165	0.02313	0.02390	0.02406
Eigenvalues ---	0.02476	0.02956	0.03003	0.03090	0.03115
Eigenvalues ---	0.03267	0.03398	0.03796	0.03961	0.04118
Eigenvalues ---	0.04324	0.04472	0.05114	0.05450	0.05741
Eigenvalues ---	0.05803	0.05964	0.07566	0.08011	0.08667
Eigenvalues ---	0.09580	0.10241	0.12288	0.12508	0.12846
Eigenvalues ---	0.13386	0.13772	0.15062	0.15985	0.15998
Eigenvalues ---	0.16001	0.16001	0.16017	0.16043	0.16140
Eigenvalues ---	0.16272	0.17438	0.18032	0.22096	0.22818
Eigenvalues ---	0.22933	0.23109	0.25294	0.25525	0.27188
Eigenvalues ---	0.29199	0.30953	0.31758	0.32143	0.33640
Eigenvalues ---	0.34230	0.34310	0.34320	0.34539	0.34664
Eigenvalues ---	0.34733	0.34987	0.35083	0.35285	0.35395
Eigenvalues ---	0.35570	0.35704	0.35890	0.36348	0.36505
Eigenvalues ---	0.36636	0.39037	0.41881	0.41915	0.42968
Eigenvalues ---	0.45247	0.45478	0.46922	0.49397	0.55321
Eigenvalues ---	0.59065	0.60632	1.46132		

En-DIIS/RFO-DIIS IScMMF= 0 using points: 22 21 20 19 18
RFO step: Lambda=-3.22172409D-05.

DidBck=F Rises=F RFO-DIIS coefs: 1.08977 0.42790 -1.16727 0.67347 -0.02387

Iteration 1 RMS(Cart)= 0.03479537 RMS(Int)= 0.00085433

Iteration 2 RMS(Cart)= 0.00168791 RMS(Int)= 0.00075778

Iteration 3 RMS(Cart)= 0.00000098 RMS(Int)= 0.00075778

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56528	-0.00009	-0.00014	0.00002	-0.00012	2.56517
R2	2.62204	-0.00020	0.00018	-0.00004	0.00014	2.62218
R3	2.03397	0.00005	-0.00002	0.00001	-0.00001	2.03396
R4	2.62553	0.00005	-0.00021	-0.00040	-0.00061	2.62493
R5	2.03077	0.00001	0.00000	0.00004	0.00004	2.03081
R6	2.54342	-0.00024	0.00035	0.00026	0.00061	2.54404
R7	2.69823	0.00000	0.00021	0.00073	0.00094	2.69917
R8	2.51973	0.00059	0.00012	0.00007	0.00019	2.51992
R9	2.09744	-0.00013	-0.00030	-0.00122	-0.00152	2.09592
R10	2.78500	-0.00005	-0.00029	-0.00086	-0.00114	2.78385
R11	2.89946	-0.00020	-0.00033	0.00014	-0.00019	2.89927
R12	2.06027	0.00000	0.00005	-0.00013	-0.00008	2.06019
R13	2.06049	-0.00003	0.00018	0.00012	0.00030	2.06079
R14	2.06954	-0.00013	0.00015	-0.00003	0.00012	2.06967
R15	2.07931	-0.00003	0.00036	0.00026	0.00062	2.07993
R16	2.75240	-0.00009	-0.00014	-0.00073	-0.00087	2.75153
R17	4.19810	-0.00002	0.00439	0.00800	0.01240	4.21050
R18	2.50648	-0.00007	0.00000	-0.00016	-0.00015	2.50633
R19	2.05612	0.00002	0.00025	0.00044	0.00069	2.05682
R20	2.04346	-0.00001	0.00000	0.00006	0.00005	2.04352
R21	2.04709	-0.00001	0.00000	0.00003	0.00003	2.04712
R22	1.91431	0.00003	0.00010	-0.00002	0.00008	1.91439
R23	1.92603	-0.00044	-0.00011	-0.00023	-0.00039	1.92563
R24	3.93450	-0.00001	0.00373	0.01037	0.01413	3.94863
R25	2.77869	-0.00259	-0.00388	-0.00357	-0.00564	2.77305
R26	2.72139	0.00041	0.00112	0.00156	0.00212	2.72351
R27	2.05546	-0.00010	0.00003	-0.00003	-0.00001	2.05545
R28	2.05346	0.00002	0.00003	-0.00008	-0.00005	2.05342
R29	2.74652	0.00053	0.00257	0.00122	0.00251	2.74903
R30	2.05784	-0.00010	0.00028	-0.00060	-0.00032	2.05752
R31	2.84144	0.00025	0.00041	-0.00008	0.00032	2.84176
R32	2.06654	0.00012	0.00002	0.00010	0.00011	2.06665
R33	2.06756	0.00003	0.00004	-0.00003	0.00000	2.06756
R34	2.06535	-0.00004	0.00000	-0.00010	-0.00011	2.06525
A1	1.87248	-0.00002	-0.00002	-0.00029	-0.00031	1.87216
A2	2.27970	0.00000	0.00012	0.00035	0.00047	2.28016
A3	2.13100	0.00001	-0.00010	-0.00006	-0.00015	2.13085

A4	1.86422	0.00008	0.00024	0.00052	0.00075	1.86497
A5	2.27648	-0.00009	-0.00036	-0.00051	-0.00087	2.27560
A6	2.14249	0.00001	0.00013	-0.00001	0.00013	2.14261
A7	1.89738	0.00009	-0.00013	-0.00036	-0.00050	1.89688
A8	2.25446	-0.00009	-0.00012	-0.00014	-0.00026	2.25420
A9	2.13134	-0.00001	0.00025	0.00051	0.00077	2.13210
A10	1.89006	-0.00018	0.00000	0.00013	0.00012	1.89018
A11	2.14601	0.00016	-0.00181	-0.00221	-0.00402	2.14199
A12	2.24629	0.00003	0.00181	0.00232	0.00413	2.25043
A13	1.90061	0.00003	-0.00008	0.00000	-0.00008	1.90053
A14	2.20899	-0.00074	-0.00042	-0.00027	-0.00067	2.20832
A15	2.17170	0.00072	0.00061	-0.00011	0.00050	2.17220
A16	1.95876	0.00041	-0.00051	0.00052	-0.00002	1.95874
A17	1.87698	-0.00037	0.00093	-0.00210	-0.00115	1.87583
A18	1.89010	-0.00018	0.00034	0.00077	0.00112	1.89121
A19	1.91558	0.00012	-0.00104	0.00065	-0.00037	1.91521
A20	1.92818	-0.00010	-0.00013	0.00028	0.00015	1.92834
A21	1.89235	0.00011	0.00046	-0.00020	0.00026	1.89261
A22	1.90780	0.00031	0.00053	-0.00010	0.00043	1.90822
A23	1.89300	-0.00003	-0.00067	0.00006	-0.00062	1.89238
A24	1.88318	-0.00052	0.00037	-0.00067	-0.00027	1.88291
A25	1.87454	-0.00002	-0.00048	0.00041	-0.00007	1.87447
A26	1.90622	-0.00009	-0.00071	-0.00114	-0.00186	1.90436
A27	1.99790	0.00036	0.00096	0.00141	0.00236	2.00026
A28	2.16173	-0.00009	-0.00024	-0.00108	-0.00132	2.16041
A29	1.94586	0.00005	-0.00034	-0.00009	-0.00042	1.94543
A30	2.17560	0.00004	0.00056	0.00117	0.00173	2.17734
A31	2.07492	0.00002	-0.00018	-0.00021	-0.00039	2.07452
A32	2.16273	-0.00002	0.00023	0.00028	0.00051	2.16324
A33	2.04553	0.00000	-0.00005	-0.00006	-0.00011	2.04541
A34	1.93951	0.00011	0.00041	0.00049	0.00062	1.94013
A35	1.92176	-0.00066	-0.00024	-0.00214	-0.00247	1.91929
A36	1.88592	0.00030	0.00056	-0.00078	-0.00013	1.88580
A37	2.09208	-0.00058	-0.00251	-0.00186	-0.00239	2.08968
A38	2.08292	0.00011	0.00284	0.00024	0.00128	2.08421
A39	1.99957	-0.00030	-0.00078	-0.00044	-0.00033	1.99924
A40	2.00896	-0.00013	0.00004	0.00029	-0.00008	2.00887
A41	2.01816	0.00031	-0.00049	0.00093	0.00038	2.01854
A42	2.04619	-0.00077	-0.00102	-0.00331	-0.00240	2.04379
A43	2.12772	-0.00013	0.00102	0.00133	0.00058	2.12830
A44	1.97552	-0.00051	-0.00027	0.00011	0.00028	1.97580
A45	2.02801	-0.00034	0.00002	-0.00091	-0.00091	2.02710
A46	2.02610	0.00085	-0.00015	0.00144	0.00112	2.02721
A47	2.61179	0.00064	0.00415	0.00687	0.01473	2.62652

A48	2.57390	0.00075	-0.00323	0.00628	0.00912	2.58301
A49	1.92925	0.00015	-0.00026	0.00095	0.00069	1.92995
A50	1.91482	0.00005	-0.00030	-0.00022	-0.00052	1.91431
A51	1.94393	0.00002	0.00061	-0.00065	-0.00004	1.94390
A52	1.87804	-0.00003	-0.00018	0.00008	-0.00009	1.87795
A53	1.89689	-0.00012	0.00020	-0.00011	0.00008	1.89697
A54	1.89943	-0.00006	-0.00010	-0.00005	-0.00015	1.89928
A55	3.35633	0.00047	0.01069	0.00846	0.01915	3.37548
A56	2.82564	-0.00022	-0.02268	-0.01460	-0.03696	2.78868
A57	2.82097	0.00013	0.00694	-0.00037	0.00657	2.82755
A58	3.15342	-0.00003	-0.01577	0.00882	-0.00678	3.14664
D1	0.00646	-0.00014	-0.00091	-0.00133	-0.00224	0.00423
D2	-3.13837	0.00000	0.00045	0.00105	0.00149	-3.13688
D3	-3.13949	-0.00012	-0.00100	-0.00184	-0.00284	3.14086
D4	-0.00114	0.00001	0.00035	0.00054	0.00089	-0.00025
D5	-0.00566	0.00004	0.00132	-0.00475	-0.00344	-0.00910
D6	-3.08330	0.00001	-0.00088	0.00154	0.00065	-3.08265
D7	3.13984	0.00003	0.00140	-0.00430	-0.00290	3.13694
D8	0.06220	0.00000	-0.00080	0.00200	0.00119	0.06338
D9	-0.00510	0.00019	0.00019	0.00692	0.00711	0.00200
D10	3.13764	0.00010	0.00161	0.00260	0.00421	-3.14133
D11	3.13942	0.00007	-0.00102	0.00476	0.00373	-3.14003
D12	-0.00102	-0.00003	0.00039	0.00045	0.00084	-0.00018
D13	0.00161	-0.00017	0.00063	-0.00995	-0.00932	-0.00771
D14	3.10303	0.00000	0.00081	-0.00381	-0.00301	3.10002
D15	-3.14104	-0.00008	-0.00067	-0.00600	-0.00667	3.13548
D16	-0.03962	0.00009	-0.00049	0.00014	-0.00035	-0.03997
D17	0.09735	0.00003	-0.00052	-0.00125	-0.00177	0.09558
D18	-3.04322	0.00007	-0.00080	0.00141	0.00061	-3.04262
D19	-3.04295	-0.00008	0.00108	-0.00608	-0.00501	-3.04796
D20	0.09966	-0.00004	0.00079	-0.00342	-0.00263	0.09703
D21	0.00247	0.00008	-0.00120	0.00911	0.00791	0.01038
D22	3.08179	0.00004	0.00093	0.00297	0.00388	3.08567
D23	-3.09593	-0.00011	-0.00131	0.00265	0.00134	-3.09459
D24	-0.01661	-0.00015	0.00081	-0.00349	-0.00270	-0.01930
D25	1.47148	-0.00009	-0.02279	-0.01092	-0.03370	1.43777
D26	-2.70324	0.00005	-0.02375	-0.01118	-0.03494	-2.73818
D27	-0.66163	-0.00011	-0.02253	-0.01213	-0.03466	-0.69629
D28	-1.59674	-0.00009	-0.02530	-0.00369	-0.02899	-1.62573
D29	0.51172	0.00006	-0.02626	-0.00396	-0.03022	0.48150
D30	2.55334	-0.00010	-0.02504	-0.00491	-0.02994	2.52339
D31	-1.09465	-0.00011	0.00403	-0.00643	-0.00241	-1.09706
D32	0.94412	0.00003	0.00338	-0.00597	-0.00260	0.94152
D33	3.11745	0.00012	0.00437	-0.00462	-0.00026	3.11719

D34	3.10249	0.00001	0.00386	-0.00457	-0.00070	3.10179
D35	-1.14193	0.00015	0.00321	-0.00411	-0.00089	-1.14282
D36	1.03140	0.00024	0.00420	-0.00276	0.00144	1.03285
D37	1.01667	-0.00014	0.00402	-0.00490	-0.00088	1.01579
D38	3.05543	0.00000	0.00337	-0.00444	-0.00108	3.05436
D39	-1.05442	0.00009	0.00436	-0.00310	0.00126	-1.05316
D40	2.89119	0.00012	0.02456	-0.00067	0.02396	2.91515
D41	-1.30301	0.00013	0.02537	-0.00274	0.02258	-1.28043
D42	0.81910	0.00009	0.02410	0.00047	0.02464	0.84374
D43	2.90808	0.00010	0.02491	-0.00159	0.02326	2.93134
D44	-1.28300	-0.00007	0.02461	-0.00017	0.02451	-1.25849
D45	0.80598	-0.00005	0.02542	-0.00223	0.02313	0.82911
D46	-3.13478	0.00005	-0.00097	0.00343	0.00246	-3.13232
D47	0.01022	0.00001	-0.00008	0.00080	0.00071	0.01094
D48	0.00566	0.00001	-0.00065	0.00042	-0.00023	0.00543
D49	-3.13252	-0.00003	0.00024	-0.00222	-0.00198	-3.13450
D50	1.63661	-0.00003	0.04685	0.00173	0.04822	1.68484
D51	-0.74399	0.00033	-0.02610	-0.05360	-0.07963	-0.82362
D52	-2.57914	-0.00019	0.04603	-0.00543	0.04055	-2.53858
D53	1.32344	0.00018	-0.02691	-0.06075	-0.08730	1.23614
D54	-2.70947	0.00022	0.00145	0.00303	0.00371	-2.70576
D55	-0.01165	0.00029	0.00102	0.00196	0.00220	-0.00946
D56	-0.03005	-0.00009	0.00093	0.00160	0.00205	-0.02800
D57	2.66777	-0.00003	0.00050	0.00053	0.00054	2.66831
D58	1.46766	0.00007	-0.06512	-0.04505	-0.10786	1.35979
D59	-0.93539	0.00008	-0.06347	-0.04638	-0.10799	-1.04339
D60	0.98453	0.00077	0.05714	0.04801	0.10748	1.09201
D61	-1.42514	0.00041	0.05767	0.04660	0.10640	-1.31874
D62	2.55386	0.00024	0.00239	0.00086	0.00278	2.55664
D63	-1.66097	0.00032	0.00184	0.00141	0.00278	-1.65819
D64	0.44319	0.00028	0.00191	0.00079	0.00223	0.44541
D65	1.36163	-0.00029	0.00120	-0.00047	0.00117	1.36281
D66	-2.85319	-0.00021	0.00065	0.00008	0.00117	-2.85202
D67	-0.74903	-0.00025	0.00072	-0.00055	0.00062	-0.74842
D68	-1.02675	-0.00008	0.00174	-0.00132	0.00044	-1.02630
D69	1.04162	0.00000	0.00119	-0.00078	0.00044	1.04206
D70	-3.13741	-0.00003	0.00126	-0.00140	-0.00011	-3.13752

Item	Value	Threshold	Converged?
Maximum Force	0.002586	0.000450	NO
RMS Force	0.000315	0.000300	NO
Maximum Displacement	0.128520	0.001800	NO
RMS Displacement	0.035888	0.001200	NO

Predicted change in Energy=-7.283716D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.771046	2.103415	-0.294214
2	6	0	-3.657133	1.131027	0.040338
3	7	0	-2.936263	-0.051570	0.146502
4	6	0	-1.641688	0.207370	-0.116950
5	7	0	-1.522524	1.506245	-0.394271
6	6	0	-0.244763	2.186204	-0.668424
7	6	0	0.367342	2.803131	0.595926
8	1	0	-2.917879	3.154782	-0.471820
9	1	0	-4.717480	1.182756	0.207301
10	1	0	0.438082	1.444845	-1.083941
11	1	0	-0.419489	2.954856	-1.422005
12	1	0	-0.305141	3.575201	0.984747
13	1	0	0.445609	2.017974	1.363284
14	35	0	0.159995	-2.483876	0.463142
15	1	0	-0.851287	-0.568598	-0.059791
16	6	0	-3.397833	-1.362817	0.474732
17	6	0	-4.676326	-1.674878	0.639420
18	1	0	-2.570502	-2.063053	0.574000
19	1	0	-4.936336	-2.692705	0.895950
20	1	0	-5.490263	-0.968261	0.531165
21	7	0	1.634503	3.417192	0.225384
22	1	0	1.979928	4.017600	0.964617
23	1	0	2.333171	2.695952	0.052067
24	6	0	3.641123	-0.202158	-1.202904
25	6	0	3.464627	-0.518013	0.219225
26	8	0	3.157172	0.807458	-0.295388
27	1	0	4.638827	-0.016962	-1.594538
28	1	0	2.911947	-0.561575	-1.923923
29	1	0	2.578439	-1.087522	0.494557
30	6	0	4.630379	-0.607669	1.164946
31	1	0	4.343110	-0.264481	2.162802
32	1	0	4.953659	-1.649155	1.253653
33	1	0	5.473155	-0.005346	0.816626

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357429	0.000000			

3	N	2.205785	1.389051	0.000000		
4	C	2.214015	2.222589	1.346247	0.000000	
5	N	1.387599	2.210482	2.172069	1.333486	0.000000
6	C	2.555189	3.641429	3.593871	2.484212	1.473152
7	C	3.336380	4.393291	4.389204	3.358924	2.496798
8	H	1.076325	2.214584	3.265479	3.231383	2.161181
9	H	2.210822	1.074657	2.167947	3.242994	3.267152
10	H	3.369849	4.258318	3.890945	2.606120	2.079276
11	H	2.743481	3.993387	4.222910	3.278052	2.090789
12	H	3.143657	4.254614	4.558391	3.787134	2.768446
13	H	3.619595	4.401062	4.147364	3.134675	2.687827
14	Br	5.496165	5.274159	3.950086	3.290193	4.414418
15	H	3.298497	3.282000	2.158008	1.109111	2.206221
16	C	3.605399	2.544640	1.428338	2.428912	3.536024
17	C	4.333273	3.044791	2.430208	3.650202	4.597230
18	H	4.260689	3.415803	2.088684	2.548514	3.843917
19	H	5.395159	4.121816	3.396698	4.504565	5.563270
20	H	4.184565	2.829892	2.740657	4.075989	4.766819
21	N	4.626539	5.767339	5.738505	4.599302	3.741993
22	H	5.274516	6.400238	6.434003	5.366912	4.518921
23	H	5.150150	6.191354	5.943461	4.692666	4.059680
24	C	6.874394	7.522471	6.716069	5.408799	5.498707
25	C	6.783740	7.312373	6.418274	5.168524	5.417164
26	O	6.068218	6.830238	6.169533	4.839525	4.732613
27	H	7.816205	8.533091	7.772670	6.455886	6.459338
28	H	6.484947	7.062297	6.224815	4.959034	5.126426
29	H	6.278633	6.634051	5.621946	4.456474	4.933106
30	C	8.016247	8.542287	7.655099	6.453400	6.690142
31	H	7.890188	8.393818	7.556458	6.421660	6.639258
32	H	8.726324	9.129473	8.125818	6.987405	7.390070
33	H	8.581824	9.233425	8.436203	7.178984	7.258836

		6	7	8	9	10
6	C	0.000000				
7	C	1.534227	0.000000			
8	H	2.849972	3.472236	0.000000		
9	H	4.666797	5.350894	2.754752	0.000000	
10	H	1.090204	2.161457	3.815894	5.321260	0.000000
11	H	1.090523	2.171214	2.680443	4.926226	1.769138
12	H	2.160077	1.095221	3.020718	5.079070	3.061089
13	H	2.152383	1.100652	3.996622	5.356433	2.513452
14	Br	4.822232	5.292737	6.491681	6.107324	4.231506
15	H	2.885696	3.644664	4.278332	4.252767	2.601021
16	C	4.883052	5.616614	4.640583	2.879744	5.002666
17	C	6.021391	6.744853	5.258574	2.890413	6.233763

18	H	5.000886	5.684290	5.332937	3.908869	4.909755
19	H	6.947077	7.643509	6.335461	3.942250	7.065668
20	H	6.237381	6.967003	4.962118	2.308452	6.601282
21	N	2.417823	1.456046	4.612932	6.733552	2.652528
22	H	3.312112	2.052146	5.176516	7.311986	3.632209
23	H	2.724829	2.042487	5.297028	7.212873	2.539123
24	C	4.592391	4.794287	7.404325	8.589116	3.603643
25	C	4.675499	4.556871	7.396171	8.357011	3.835496
26	O	3.689615	3.544051	6.515159	7.899600	2.901987
27	H	5.437011	5.567462	8.271896	9.603459	4.477036
28	H	4.369369	4.913847	7.064473	8.111286	3.294132
29	H	4.476637	4.476204	7.010031	7.646379	3.672284
30	C	5.910498	5.489155	8.591347	9.565834	5.181280
31	H	5.922016	5.260425	8.447162	9.381512	5.358393
32	H	6.740026	6.425710	9.381693	10.131411	5.952110
33	H	6.301020	5.831430	9.058474	10.277739	5.573793

		11	12	13	14	15
11	H	0.000000				
12	H	2.488043	0.000000			
13	H	3.063328	1.769709	0.000000		
14	Br	5.785273	6.099249	4.599835	0.000000	
15	H	3.802211	4.308179	3.224505	2.228102	0.000000
16	C	5.577674	5.848835	5.195316	3.730287	2.720550
17	C	6.618502	6.840309	6.355733	4.906684	4.042731
18	H	5.812943	6.090196	5.135628	2.764958	2.364485
19	H	7.594062	7.793748	7.167582	5.118937	4.702436
20	H	6.702124	6.908999	6.696611	5.850396	4.693512
21	N	2.673300	2.088976	2.160115	6.087142	4.706060
22	H	3.547195	2.327588	2.551779	6.769994	5.486201
23	H	3.133219	2.933200	2.396212	5.632255	4.561860
24	C	5.148137	5.884493	4.661075	4.483325	4.650025
25	C	5.462675	5.617079	4.105432	3.852882	4.325219
26	O	4.321237	4.613758	3.401340	4.515674	4.244617
27	H	5.869245	6.633187	5.520213	5.511773	5.727224
28	H	4.869875	5.993574	4.852074	4.119048	4.199639
29	H	5.385314	5.504208	3.866232	2.792788	3.512777
30	C	6.699632	6.472112	4.944253	4.898675	5.616953
31	H	6.774756	6.143062	4.586866	5.031204	5.658106
32	H	7.564839	7.417626	5.812260	4.929593	6.048978
33	H	6.964016	6.799801	5.446915	5.873478	6.409675

		16	17	18	19	20
16	C	0.000000				
17	C	1.326291	0.000000			
18	H	1.088421	2.142301	0.000000		

19	H	2.076782	1.081382	2.469268	0.000000	
20	H	2.130053	1.083292	3.118559	1.847597	0.000000
21	N	6.945146	8.119554	6.916407	8.997579	8.371857
22	H	7.622938	8.764460	7.604823	9.636785	8.991687
23	H	7.035386	8.281435	6.853215	9.088207	8.652289
24	C	7.328607	8.645404	6.723437	9.175011	9.326099
25	C	6.918983	8.233468	6.239855	8.704218	8.971626
26	O	6.947752	8.270401	6.465440	8.898050	8.866481
27	H	8.407205	9.721693	7.801504	10.249189	10.393365
28	H	6.797709	8.086535	6.208969	8.607493	8.762989
29	H	5.982642	7.279944	5.241142	7.694776	8.069667
30	C	8.093134	9.382423	7.370213	9.794987	10.146876
31	H	7.998632	9.255275	7.318277	9.675190	9.992635
32	H	8.392623	9.649587	7.566124	9.951329	10.491001
33	H	8.980760	10.287405	8.306230	10.751080	11.009325

		21	22	23	24	25
21	N	0.000000				
22	H	1.013051	0.000000			
23	H	1.019001	1.644470	0.000000		
24	C	4.377924	5.026338	3.418294	0.000000	
25	C	4.339957	4.830292	3.411408	1.467436	0.000000
26	O	3.066013	3.643971	2.089524	1.441221	1.454726
27	H	4.912381	5.467788	3.922660	1.087698	2.218003
28	H	4.699146	5.493739	3.853699	1.086621	2.213693
29	H	4.610413	5.161534	3.817149	2.189644	1.088795
30	C	5.104660	5.334616	4.174874	2.598034	1.503797
31	H	4.964358	5.035523	4.154421	3.438699	2.147906
32	H	6.143451	6.406147	5.214472	3.138666	2.136993
33	H	5.176734	5.329974	4.212014	2.733785	2.157291

		26	27	28	29	30
26	O	0.000000				
27	H	2.136062	0.000000			
28	H	2.141614	1.840438	0.000000		
29	H	2.133047	3.123398	2.497377	0.000000	
30	C	2.511075	2.822013	3.535003	2.211365	0.000000
31	H	2.932269	3.777078	4.340255	2.564078	1.093626
32	H	3.414943	3.297782	3.930446	2.556037	1.094107
33	H	2.694625	2.551460	3.792069	3.107123	1.092883

		31	32	33
31	H	0.000000		
32	H	1.765401	0.000000	
33	H	1.776611	1.778476	0.000000

Stoichiometry C10H18BrN3O

Framework group C1[X(C10H18BrN3O)]

Deg. of freedom 93

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.606387	2.353267	-0.206364
2	6	0	-3.543409	1.394755	0.007776
3	7	0	-2.883694	0.172736	-0.022323
4	6	0	-1.575117	0.394535	-0.247736
5	7	0	-1.388296	1.709180	-0.370183
6	6	0	-0.075356	2.350667	-0.556894
7	6	0	0.553592	2.783534	0.773859
8	1	0	-2.698627	3.424289	-0.260028
9	1	0	-4.601530	1.480460	0.174879
10	1	0	0.573880	1.629237	-1.053456
11	1	0	-0.203574	3.210073	-1.215848
12	1	0	-0.083483	3.538020	1.247562
13	1	0	0.584507	1.911052	1.444124
14	35	0	0.083654	-2.434214	0.020645
15	1	0	-0.825126	-0.421979	-0.278471
16	6	0	-3.413623	-1.142719	0.147686
17	6	0	-4.707764	-1.406471	0.268858
18	1	0	-2.623405	-1.890925	0.167822
19	1	0	-5.020983	-2.432768	0.403002
20	1	0	-5.484193	-0.651567	0.240606
21	7	0	1.853658	3.371475	0.483646
22	1	0	2.220927	3.862944	1.289775
23	1	0	2.517175	2.640865	0.230039
24	6	0	3.691667	-0.153303	-1.350444
25	6	0	3.484775	-0.623947	0.023986
26	8	0	3.249339	0.766529	-0.332911
27	1	0	4.701413	0.025447	-1.713143
28	1	0	2.953002	-0.388362	-2.111934
29	1	0	2.568407	-1.175938	0.226592
30	6	0	4.634658	-0.882779	0.957892
31	1	0	4.354504	-0.644502	1.987822
32	1	0	4.904536	-1.942576	0.925226
33	1	0	5.510074	-0.287496	0.686458

Rotational constants (GHZ): 0.4456761 0.2674696 0.1758086

Standard basis: 6-311++G(d,p) (5D, 7F)
There are 499 symmetry adapted cartesian basis functions of A symmetry.
There are 482 symmetry adapted basis functions of A symmetry.
482 basis functions, 760 primitive gaussians, 499 cartesian basis functions
71 alpha electrons 71 beta electrons
nuclear repulsion energy 1299.2684158959 Hartrees.
NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 482 RedAO= T EigKep= 3.88D-06 NBF= 482
NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999986 0.002869 -0.000533 0.004309 Ang= 0.60 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
EnCoef did 1 forward-backward iterations
SCF Done: E(RB3LYP) = -3205.64746097 A.U. after 11 cycles
NFock= 11 Conv=0.38D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Atomic Forces (Hartrees/Bohr)
Number Number X Y Z

1	6	0.000279738	-0.000016035	-0.000233778
2	6	-0.000248231	0.000084571	-0.000170078
3	7	0.000503051	0.000355059	0.000100167
4	6	-0.001159097	-0.001263146	0.000061478
5	7	0.000205600	-0.000239603	0.000333687
6	6	0.000657528	0.000808079	0.000217785
7	6	-0.000518677	-0.000207964	0.000381353
8	1	-0.000057197	0.000014749	-0.000082197
9	1	-0.000010487	0.000016790	-0.000027225
10	1	-0.000072263	-0.000263546	0.000174237
11	1	-0.000141950	-0.000060095	0.000078725
12	1	0.000137838	-0.000023867	-0.000006058
13	1	0.000048875	0.000048380	-0.000185928
14	35	-0.000082843	0.000001547	-0.000064037
15	1	0.000500086	0.000270437	-0.000309805
16	6	0.000126151	0.000305668	0.000279743
17	6	0.000014421	-0.000097322	0.000060724
18	1	-0.000119097	-0.000018720	-0.000089021
19	1	-0.000025478	0.000002100	-0.000058296
20	1	0.000030097	-0.000001493	-0.000018841
21	7	0.000397606	-0.000027286	-0.000408650
22	1	-0.000120594	0.000127592	0.000039442
23	1	0.000141009	0.000314050	0.000159531
24	6	-0.000299125	-0.000738454	0.000510699
25	6	0.001456456	0.000094078	-0.000129686
26	8	-0.001297271	0.000188435	-0.000105702
27	1	0.000069505	-0.000029482	0.000291624
28	1	-0.000103927	-0.000019120	0.000166295
29	1	-0.000468188	0.000212308	-0.001054880
30	6	-0.000081636	0.000051985	-0.000035960
31	1	0.000086320	0.000128660	0.000066912
32	1	0.000127300	-0.000017145	0.000002799
33	1	0.000024480	-0.000001209	0.000054939

Cartesian Forces: Max 0.001456456 RMS 0.000363328

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.001131095 RMS 0.000246808

Search for a local minimum.

Step number 23 out of a maximum of 172

All quantities printed in internal units (Hartrees-Bohrs-Radians)

```
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swapping is turned off.
 Update second derivatives using D2CorX and points     19     20     22     23
 DE= -1.42D-04 DEPred=-7.28D-05 R= 1.95D+00
 TightC=F SS=    1.41D+00    RLast= 2.77D-01 DXNew= 1.4193D+00 8.3106D-01
 Trust test= 1.95D+00 RLast= 2.77D-01 DXMaxT set to 8.44D-01
 ITU=    1 -1    1    1    1    1    1    1    1    1    1    0 -1 -1    1    1    1 -1    1    0
 ITU=    0 -1    0
      Eigenvalues ---      0.00002     0.00149     0.00277     0.00426     0.00701
      Eigenvalues ---      0.00727     0.00817     0.01295     0.01601     0.01882
      Eigenvalues ---      0.02072     0.02157     0.02295     0.02389     0.02440
      Eigenvalues ---      0.02772     0.02881     0.03073     0.03098     0.03214
      Eigenvalues ---      0.03321     0.03586     0.03890     0.04023     0.04206
      Eigenvalues ---      0.04375     0.04780     0.05441     0.05701     0.05753
      Eigenvalues ---      0.05934     0.06160     0.07550     0.08667     0.08779
      Eigenvalues ---      0.09656     0.10166     0.12225     0.12342     0.12637
      Eigenvalues ---      0.13549     0.13773     0.15332     0.15984     0.16000
      Eigenvalues ---      0.16000     0.16003     0.16024     0.16046     0.16074
      Eigenvalues ---      0.16139     0.17342     0.18775     0.22125     0.22579
      Eigenvalues ---      0.22883     0.23418     0.24818     0.26200     0.28099
      Eigenvalues ---      0.29530     0.30470     0.31782     0.32412     0.33621
      Eigenvalues ---      0.34273     0.34312     0.34359     0.34537     0.34668
      Eigenvalues ---      0.34728     0.35020     0.35078     0.35269     0.35329
      Eigenvalues ---      0.35561     0.35726     0.35890     0.36420     0.36622
      Eigenvalues ---      0.37598     0.38822     0.41814     0.42417     0.44653
      Eigenvalues ---      0.45466     0.46218     0.49343     0.54686     0.57952
      Eigenvalues ---      0.60218     0.62137     1.34174
 Eigenvalue     1 is      2.07D-05 Eigenvector:
                              D58         D59         D60         D61         D53
   1                      -0.38498    -0.38422     0.37778     0.37557    -0.31151
                              D51         D50         D52         D26         D27
   1                      -0.28929     0.16964     0.14742    -0.13675    -0.13456
 En-DIIS/RFO-DIIS IScMMF=          0 using points:     23     22     21     20     19
 RFO step:    Lambda=-4.58228039D-05.
 DidBck=T  Rises=F      En-DIIS  coefs:          0.54140          0.00000          0.45860          0.00000
0.00000
 Iteration    1 RMS(Cart)=    0.19505645 RMS(Int)=    0.18158199
 Iteration    2 RMS(Cart)=    0.15220175 RMS(Int)=    0.13265683
 Iteration    3 RMS(Cart)=    0.08708963 RMS(Int)=    0.09345085
 Iteration    4 RMS(Cart)=    0.06538485 RMS(Int)=    0.05981154
 Iteration    5 RMS(Cart)=    0.07065393 RMS(Int)=    0.03678227
 Iteration    6 RMS(Cart)=    0.03218262 RMS(Int)=    0.03264382
 Iteration    7 RMS(Cart)=    0.00491446 RMS(Int)=    0.03266040
 Iteration    8 RMS(Cart)=    0.00143511 RMS(Int)=    0.03268196
```

Iteration 9 RMS(Cart)= 0.00040040 RMS(Int)= 0.03268958
Iteration 10 RMS(Cart)= 0.00013006 RMS(Int)= 0.03269210
Iteration 11 RMS(Cart)= 0.00004082 RMS(Int)= 0.03269291
Iteration 12 RMS(Cart)= 0.00001295 RMS(Int)= 0.03269316
Iteration 13 RMS(Cart)= 0.00000410 RMS(Int)= 0.03269325
Iteration 14 RMS(Cart)= 0.00000130 RMS(Int)= 0.03269327
Iteration 15 RMS(Cart)= 0.00000041 RMS(Int)= 0.03269328

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56517	-0.00013	-0.00017	-0.00110	-0.00130	2.56387
R2	2.62218	-0.00017	0.00081	0.00115	0.00200	2.62419
R3	2.03396	0.00004	-0.00005	-0.00006	-0.00010	2.03386
R4	2.62493	0.00011	0.00064	-0.00627	-0.00568	2.61925
R5	2.03081	0.00001	0.00014	0.00032	0.00047	2.03128
R6	2.54404	-0.00033	0.00055	0.00547	0.00596	2.54999
R7	2.69917	-0.00014	-0.00116	0.00927	0.00810	2.70727
R8	2.51992	0.00048	-0.00158	0.00268	0.00106	2.52099
R9	2.09592	0.00009	0.00186	-0.01435	-0.01249	2.08342
R10	2.78385	0.00025	-0.00133	-0.00929	-0.01067	2.77318
R11	2.89927	-0.00030	-0.00072	-0.00307	-0.00357	2.89570
R12	2.06019	0.00007	-0.00026	-0.00038	-0.00063	2.05955
R13	2.06079	-0.00007	0.00014	0.00309	0.00323	2.06402
R14	2.06967	-0.00010	0.00035	0.00138	0.00173	2.07139
R15	2.07993	-0.00016	0.00082	0.00577	0.00659	2.08652
R16	2.75153	0.00017	-0.00087	-0.00711	-0.00805	2.74348
R17	4.21050	-0.00005	-0.00652	0.11620	0.10968	4.32018
R18	2.50633	0.00000	0.00024	-0.00158	-0.00134	2.50499
R19	2.05682	-0.00009	0.00001	0.00626	0.00627	2.06309
R20	2.04352	-0.00001	-0.00001	0.00047	0.00046	2.04398
R21	2.04712	-0.00002	0.00008	0.00017	0.00024	2.04737
R22	1.91439	0.00006	0.00049	0.00087	0.00136	1.91575
R23	1.92563	-0.00039	0.00088	-0.00397	0.00859	1.93422
R24	3.94863	-0.00002	-0.01307	0.15390	0.13532	4.08395
R25	2.77305	-0.00113	-0.00180	-0.05603	-0.14091	2.63214
R26	2.72351	0.00029	-0.00106	0.02502	0.05428	2.77780
R27	2.05545	-0.00005	0.00025	-0.00015	0.00010	2.05555
R28	2.05342	-0.00003	0.00051	-0.00146	-0.00095	2.05246
R29	2.74903	0.00012	0.00474	0.02395	0.07629	2.82532
R30	2.05752	0.00000	-0.00032	-0.00255	-0.00287	2.05466
R31	2.84176	0.00017	-0.00036	0.00345	0.00310	2.84486
R32	2.06665	0.00008	-0.00049	0.00139	0.00090	2.06756
R33	2.06756	0.00006	-0.00023	0.00042	0.00019	2.06775
R34	2.06525	0.00000	0.00008	-0.00101	-0.00093	2.06432
A1	1.87216	0.00007	-0.00028	-0.00262	-0.00306	1.86910

A2	2.28016	-0.00007	-0.00059	0.00444	0.00393	2.28410
A3	2.13085	0.00001	0.00086	-0.00187	-0.00092	2.12993
A4	1.86497	-0.00009	0.00009	0.00659	0.00631	1.87128
A5	2.27560	0.00002	0.00111	-0.00952	-0.00839	2.26722
A6	2.14261	0.00007	-0.00122	0.00292	0.00171	2.14432
A7	1.89688	0.00022	-0.00049	-0.00399	-0.00480	1.89208
A8	2.25420	-0.00018	-0.00022	-0.00208	-0.00217	2.25203
A9	2.13210	-0.00004	0.00071	0.00605	0.00690	2.13900
A10	1.89018	-0.00022	0.00041	0.00046	0.00010	1.89028
A11	2.14199	0.00056	-0.00294	-0.03346	-0.03663	2.10536
A12	2.25043	-0.00034	0.00250	0.03478	0.03699	2.28741
A13	1.90053	0.00002	0.00026	-0.00094	-0.00090	1.89963
A14	2.20832	-0.00085	0.00123	-0.00758	-0.00641	2.20191
A15	2.17220	0.00084	-0.00117	0.00686	0.00584	2.17804
A16	1.95874	0.00058	0.00016	-0.00012	0.00118	1.95992
A17	1.87583	-0.00022	-0.00103	-0.00864	-0.00988	1.86595
A18	1.89121	-0.00032	0.00310	0.00894	0.01148	1.90270
A19	1.91521	-0.00011	-0.00044	-0.00730	-0.00799	1.90722
A20	1.92834	-0.00012	-0.00292	0.00318	-0.00018	1.92816
A21	1.89261	0.00018	0.00125	0.00396	0.00540	1.89801
A22	1.90822	0.00039	0.00044	0.00645	0.00695	1.91518
A23	1.89238	0.00007	-0.00048	-0.00690	-0.00672	1.88566
A24	1.88291	-0.00074	-0.00122	-0.00305	-0.00574	1.87717
A25	1.87447	-0.00007	-0.00072	-0.00105	-0.00188	1.87259
A26	1.90436	0.00006	-0.00226	-0.01593	-0.01794	1.88642
A27	2.00026	0.00031	0.00417	0.02044	0.02526	2.02552
A28	2.16041	0.00004	0.00023	-0.01165	-0.01146	2.14895
A29	1.94543	0.00005	0.00050	-0.00453	-0.00407	1.94136
A30	2.17734	-0.00009	-0.00073	0.01612	0.01535	2.19269
A31	2.07452	0.00005	0.00000	-0.00359	-0.00361	2.07091
A32	2.16324	-0.00005	-0.00056	0.00520	0.00462	2.16786
A33	2.04541	0.00000	0.00056	-0.00159	-0.00105	2.04436
A34	1.94013	0.00000	-0.00019	0.00734	0.03386	1.97399
A35	1.91929	-0.00052	0.00025	-0.02224	-0.00839	1.91090
A36	1.88580	0.00038	0.00134	-0.00014	-0.01195	1.87384
A37	2.08968	-0.00033	-0.00431	-0.02123	0.05555	2.14523
A38	2.08421	0.00002	0.00887	0.00658	-0.07233	2.01188
A39	1.99924	-0.00007	-0.00118	-0.00595	-0.04876	1.95048
A40	2.00887	-0.00015	0.00218	-0.00350	0.02580	2.03468
A41	2.01854	0.00025	-0.00470	0.00933	0.00742	2.02596
A42	2.04379	-0.00066	0.01067	-0.03494	-0.11070	1.93309
A43	2.12830	-0.00011	0.00242	0.00541	0.09379	2.22209
A44	1.97580	-0.00054	0.00259	-0.00327	0.02567	2.00147
A45	2.02710	-0.00014	0.00004	-0.00816	-0.04981	1.97729

A46	2.02721	0.00076	-0.01049	0.02120	0.01475	2.04196
A47	2.62652	0.00038	0.01604	0.11531	-0.12266	2.50386
A48	2.58301	0.00023	-0.00976	0.07008	-0.13365	2.44936
A49	1.92995	0.00009	-0.00177	0.00802	0.00625	1.93620
A50	1.91431	0.00012	-0.00131	-0.00330	-0.00461	1.90970
A51	1.94390	0.00001	0.00123	-0.00158	-0.00036	1.94353
A52	1.87795	-0.00003	-0.00139	0.00078	-0.00060	1.87736
A53	1.89697	-0.00011	0.00207	-0.00111	0.00095	1.89792
A54	1.89928	-0.00009	0.00113	-0.00286	-0.00173	1.89755
A55	3.37548	0.00037	-0.00530	0.19140	0.18610	3.56158
A56	2.78868	-0.00040	-0.03047	-0.36730	-0.41675	2.37193
A57	2.82755	0.00007	-0.00199	0.07444	0.07245	2.90000
A58	3.14664	-0.00032	-0.04309	-0.08281	-0.13348	3.01316
D1	0.00423	-0.00003	0.00052	-0.01500	-0.01435	-0.01012
D2	-3.13688	-0.00005	-0.00368	0.01782	0.01406	-3.12282
D3	3.14086	0.00000	0.00589	-0.02656	-0.02078	3.12008
D4	-0.00025	-0.00002	0.00170	0.00626	0.00763	0.00738
D5	-0.00910	0.00017	-0.00055	-0.02094	-0.02174	-0.03084
D6	-3.08265	0.00000	-0.00618	0.00501	-0.00180	-3.08446
D7	3.13694	0.00014	-0.00537	-0.01061	-0.01602	3.12091
D8	0.06338	-0.00002	-0.01100	0.01534	0.00391	0.06730
D9	0.00200	-0.00012	-0.00032	0.04557	0.04510	0.04711
D10	-3.14133	-0.00004	0.00243	0.03201	0.03415	-3.10718
D11	-3.14003	-0.00010	0.00347	0.01584	0.01915	-3.12088
D12	-0.00018	-0.00003	0.00621	0.00228	0.00820	0.00802
D13	-0.00771	0.00022	-0.00003	-0.05908	-0.05902	-0.06673
D14	3.10002	0.00018	-0.00057	-0.00710	-0.00903	3.09099
D15	3.13548	0.00016	-0.00254	-0.04665	-0.04892	3.08656
D16	-0.03997	0.00011	-0.00309	0.00533	0.00107	-0.03890
D17	0.09558	-0.00002	0.00463	-0.05082	-0.04601	0.04957
D18	-3.04262	-0.00010	0.00365	-0.03329	-0.02958	-3.07220
D19	-3.04796	0.00006	0.00770	-0.06600	-0.05835	-3.10631
D20	0.09703	-0.00002	0.00672	-0.04847	-0.04192	0.05510
D21	0.01038	-0.00024	0.00035	0.04963	0.05013	0.06051
D22	3.08567	-0.00016	0.00593	0.02365	0.02995	3.11561
D23	-3.09459	-0.00021	0.00109	-0.00477	-0.00490	-3.09949
D24	-0.01930	-0.00013	0.00667	-0.03075	-0.02508	-0.04439
D25	1.43777	0.00001	-0.04712	-0.35400	-0.40117	1.03661
D26	-2.73818	0.00008	-0.04824	-0.36885	-0.41679	3.12821
D27	-0.69629	0.00001	-0.04569	-0.36412	-0.40977	-1.10606
D28	-1.62573	-0.00013	-0.05363	-0.32380	-0.37783	-2.00355
D29	0.48150	-0.00006	-0.05476	-0.33865	-0.39345	0.08805
D30	2.52339	-0.00014	-0.05221	-0.33392	-0.38643	2.13696
D31	-1.09706	0.00001	0.01837	-0.02667	-0.00821	-1.10527

D32	0.94152	0.00019	0.01749	-0.02825	-0.01043	0.93108
D33	3.11719	0.00015	0.02153	-0.00944	0.01268	3.12987
D34	3.10179	-0.00001	0.01985	-0.01084	0.00871	3.11050
D35	-1.14282	0.00017	0.01897	-0.01242	0.00648	-1.13634
D36	1.03285	0.00013	0.02301	0.00640	0.02960	1.06245
D37	1.01579	-0.00009	0.02039	-0.01310	0.00719	1.02298
D38	3.05436	0.00009	0.01951	-0.01468	0.00497	3.05933
D39	-1.05316	0.00004	0.02355	0.00413	0.02808	-1.02508
D40	2.91515	0.00013	0.05559	0.24360	0.29406	-3.07397
D41	-1.28043	0.00028	0.05730	0.23362	0.29521	-0.98523
D42	0.84374	0.00005	0.05701	0.24651	0.29880	1.14254
D43	2.93134	0.00019	0.05872	0.23652	0.29995	-3.05190
D44	-1.25849	-0.00012	0.05680	0.24585	0.29774	-0.96075
D45	0.82911	0.00003	0.05851	0.23587	0.29889	1.12799
D46	-3.13232	-0.00010	0.00101	0.01348	0.01454	-3.11777
D47	0.01094	-0.00003	0.00072	0.00160	0.00237	0.01331
D48	0.00543	-0.00001	0.00212	-0.00642	-0.00435	0.00108
D49	-3.13450	0.00006	0.00184	-0.01830	-0.01652	3.13216
D50	1.68484	-0.00003	0.10883	0.40972	0.55022	2.23505
D51	-0.82362	0.00025	0.00533	-0.88515	-0.88383	-1.70745
D52	-2.53858	-0.00013	0.11491	0.33749	0.45747	-2.08112
D53	1.23614	0.00015	0.01141	-0.95738	-0.97658	0.25957
D54	-2.70576	-0.00004	-0.00089	0.03048	0.03499	-2.67077
D55	-0.00946	0.00013	0.00328	0.01443	0.02762	0.01817
D56	-0.02800	-0.00012	-0.00246	0.02017	0.01374	-0.01425
D57	2.66831	0.00005	0.00171	0.00411	0.00638	2.67468
D58	1.35979	0.00003	-0.09058	-1.09577	-1.12244	0.23736
D59	-1.04339	-0.00011	-0.08416	-1.09964	-1.10674	-2.15013
D60	1.09201	0.00074	0.07488	1.08308	1.07391	2.16591
D61	-1.31874	0.00032	0.08868	1.06220	1.07836	-0.24038
D62	2.55664	0.00010	0.00450	0.02422	0.03994	2.59657
D63	-1.65819	0.00019	0.00092	0.02803	0.04014	-1.61805
D64	0.44541	0.00017	0.00226	0.02123	0.03469	0.48011
D65	1.36281	-0.00020	0.00506	0.00571	0.00357	1.36638
D66	-2.85202	-0.00011	0.00148	0.00952	0.00378	-2.84824
D67	-0.74842	-0.00014	0.00282	0.00272	-0.00167	-0.75009
D68	-1.02630	-0.00007	0.01346	-0.00503	0.00444	-1.02186
D69	1.04206	0.00002	0.00988	-0.00123	0.00465	1.04670
D70	-3.13752	-0.00001	0.01122	-0.00803	-0.00080	-3.13833

Item	Value	Threshold	Converged?
Maximum Force	0.001131	0.000450	NO
RMS Force	0.000247	0.000300	YES
Maximum Displacement	1.663191	0.001800	NO
RMS Displacement	0.425641	0.001200	NO

Predicted change in Energy=-3.894017D-03
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.384655	2.023759	-0.165888
2	6	0	-3.299726	1.061256	0.111565
3	7	0	-2.625589	-0.149442	0.141061
4	6	0	-1.312208	0.089226	-0.056282
5	7	0	-1.153867	1.392929	-0.290744
6	6	0	0.136987	2.051282	-0.522776
7	6	0	0.489479	3.047176	0.587182
8	1	0	-2.497054	3.086499	-0.293593
9	1	0	-4.360836	1.141816	0.263139
10	1	0	0.892122	1.266068	-0.554755
11	1	0	0.111256	2.553278	-1.492469
12	1	0	-0.248242	3.857704	0.605122
13	1	0	0.420787	2.519415	1.554585
14	35	0	0.038674	-2.928813	0.147801
15	1	0	-0.580486	-0.734805	-0.023711
16	6	0	-3.146284	-1.467063	0.353593
17	6	0	-4.438307	-1.718902	0.509878
18	1	0	-2.345222	-2.208039	0.387434
19	1	0	-4.749986	-2.739139	0.688449
20	1	0	-5.214137	-0.963254	0.480136
21	7	0	1.783007	3.622196	0.264961
22	1	0	2.128143	4.251330	0.981065
23	1	0	2.472513	2.873320	0.158143
24	6	0	2.906050	-0.286746	-1.169250
25	6	0	2.970345	-0.537110	0.199424
26	8	0	2.389449	0.757161	-0.272520
27	1	0	3.758704	0.063572	-1.746712
28	1	0	2.167982	-0.869188	-1.713003
29	1	0	2.236458	-1.285175	0.489224
30	6	0	4.160258	-0.360595	1.104566
31	1	0	3.844785	-0.091463	2.117042
32	1	0	4.710660	-1.304029	1.170006
33	1	0	4.834054	0.413145	0.729538

Distance matrix (angstroms):

	1	2	3	4	5

1	C	0.000000				
2	C	1.356741	0.000000			
3	N	2.207956	1.386045	0.000000		
4	C	2.214628	2.218838	1.349398	0.000000	
5	N	1.388659	2.208296	2.175162	1.334049	0.000000
6	C	2.546921	3.632291	3.593841	2.483435	1.467506
7	C	3.142474	4.304436	4.485648	3.522725	2.491560
8	H	1.076270	2.215862	3.267531	3.231690	2.161559
9	H	2.206169	1.074905	2.166410	3.241005	3.264123
10	H	3.385644	4.249414	3.855142	2.548039	2.066850
11	H	2.875723	4.053869	4.178928	3.187544	2.095493
12	H	2.919258	4.168366	4.682344	3.971260	2.774499
13	H	3.328094	4.248618	4.289668	3.391753	2.674648
14	Br	5.522580	5.202584	3.850097	3.312867	4.504656
15	H	3.299230	3.261657	2.133600	1.102500	2.219758
16	C	3.610510	2.544507	1.432627	2.440055	3.544637
17	C	4.322229	3.030561	2.425939	3.655456	4.594784
18	H	4.268001	3.416939	2.092159	2.557621	3.853080
19	H	5.386083	4.108413	3.393999	4.513601	5.564610
20	H	4.164801	2.810598	2.734565	4.076826	4.757274
21	N	4.484422	5.693516	5.803130	4.708018	3.728762
22	H	5.161678	6.355656	6.532255	5.498656	4.534263
23	H	4.941542	6.050165	5.926890	4.703326	3.942549
24	C	5.859755	6.478368	5.686369	4.378784	4.480626
25	C	5.947060	6.471188	5.609649	4.335659	4.579786
26	O	4.940416	5.710228	5.113080	3.767647	3.599948
27	H	6.639443	7.366818	6.660950	5.345312	5.293429
28	H	5.611525	6.078773	5.189788	3.971775	4.263176
29	H	5.721268	6.024757	5.005058	3.844423	4.390319
30	C	7.080614	7.658921	6.857160	5.612290	5.767293
31	H	6.963609	7.509643	6.765618	5.599157	5.743463
32	H	7.949987	8.419095	7.497489	6.302371	6.618161
33	H	7.450210	8.182928	7.503937	6.204754	6.152735

		6	7	8	9	10
6	C	0.000000				
7	C	1.532338	0.000000			
8	H	2.839432	3.113951	0.000000		
9	H	4.655664	5.221203	2.750532	0.000000	
10	H	1.089868	2.153714	3.855994	5.317703	0.000000
11	H	1.092230	2.170699	2.919745	5.007394	1.773688
12	H	2.164190	1.096135	2.541574	4.940286	3.059791
13	H	2.148283	1.104137	3.500163	5.140966	2.498469
14	Br	5.026000	6.009053	6.542837	5.994916	4.338085
15	H	2.919951	3.977612	4.283507	4.230253	2.540487

16	C	4.891487	5.801008	4.644919	2.879161	4.960225
17	C	6.017806	6.855987	5.244608	2.872384	6.201369
18	H	5.013148	5.974337	5.340316	3.911480	4.841233
19	H	6.949656	7.806644	6.322829	3.923537	7.029981
20	H	6.223166	6.973253	4.937783	2.281782	6.582346
21	N	2.407838	1.451788	4.349469	6.625640	2.648953
22	H	3.326627	2.071316	4.937006	7.231276	3.577468
23	H	2.567894	2.036351	4.994608	7.050092	2.364131
24	C	3.681305	4.476594	6.429548	7.543220	2.616245
25	C	3.905030	4.376317	6.577694	7.521241	2.852936
26	O	2.609782	3.097279	5.413333	6.782422	1.606434
27	H	4.308810	5.003677	7.098180	8.433804	3.329272
28	H	3.751096	4.842119	6.278912	7.111592	2.743843
29	H	4.069873	4.672343	6.490799	7.033185	3.066916
30	C	4.965088	5.035395	7.626081	8.693348	4.009999
31	H	5.030682	4.842479	7.491964	8.502361	4.207090
32	H	5.919637	6.090241	8.565629	9.439100	4.915428
33	H	5.129738	5.082687	7.870118	9.235502	4.232695

		11	12	13	14	15
11	H	0.000000				
12	H	2.496128	0.000000			
13	H	3.062922	1.772032	0.000000		
14	Br	5.722681	6.807956	5.639879	0.000000	
15	H	3.667049	4.647253	3.752801	2.286141	0.000000
16	C	5.493875	6.067541	5.482553	3.510417	2.694788
17	C	6.554346	6.975977	6.531887	4.651704	4.016958
18	H	5.677892	6.421678	5.600167	2.501979	2.335327
19	H	7.509844	7.986926	7.425596	4.822815	4.680733
20	H	6.679595	6.922238	6.710872	5.618354	4.666560
21	N	2.650641	2.072957	2.175983	6.780276	4.965168
22	H	3.615188	2.437926	2.498703	7.524271	5.762620
23	H	2.898704	2.927681	2.506966	6.291933	4.729952
24	C	3.997634	5.502220	4.633611	4.115456	3.697154
25	C	4.537333	5.462443	4.204646	3.783860	3.563323
26	O	3.147138	4.164257	3.212395	4.391949	3.332924
27	H	4.423477	5.998515	5.298247	5.136357	4.736529
28	H	3.999003	5.792698	5.021200	3.498370	3.228906
29	H	4.814282	5.712825	4.348167	2.765568	2.915679
30	C	5.624026	6.121958	4.741373	4.949605	4.887504
31	H	5.827732	5.885125	4.342442	5.139546	4.957795
32	H	6.566743	7.180063	5.759309	5.050968	5.453916
33	H	5.641126	6.140863	4.959234	5.873905	5.585912

		16	17	18	19	20
16	C	0.000000				

17	C	1.325584	0.000000			
18	H	1.091738	2.152964	0.000000		
19	H	2.074166	1.081626	2.481042	0.000000	
20	H	2.132101	1.083421	3.128699	1.847322	0.000000
21	N	7.085642	8.203175	7.144852	9.128304	8.368554
22	H	7.804698	8.887292	7.879520	9.811266	9.019529
23	H	7.102676	8.304918	7.005951	9.162173	8.596952
24	C	6.351610	7.668776	5.804350	8.251071	8.313578
25	C	6.188839	7.508738	5.575177	8.043108	8.200375
26	O	5.998628	7.304882	5.625394	8.007441	7.832040
27	H	7.377872	8.686795	6.853664	9.283480	9.301888
28	H	5.733210	7.021842	5.154936	7.557908	7.701584
29	H	5.387522	6.688874	4.674808	7.138915	7.457553
30	C	7.427907	8.725479	6.800632	9.231635	9.414479
31	H	7.340100	8.593087	6.766655	9.106105	9.246813
32	H	7.900929	9.182129	7.156474	9.580985	9.954580
33	H	8.207455	9.516856	7.650466	10.089222	10.145089

		21	22	23	24	25
21	N	0.000000				
22	H	1.013772	0.000000			
23	H	1.023545	1.641555	0.000000		
24	C	4.312542	5.081646	3.454843	0.000000	
25	C	4.325956	4.924370	3.446820	1.392869	0.000000
26	O	2.977429	3.721420	2.161133	1.469947	1.495095
27	H	4.540266	5.257073	3.630075	1.087752	2.183981
28	H	4.922710	5.786129	4.195270	1.086117	2.100342
29	H	4.933376	5.559364	4.178327	2.048353	1.087279
30	C	4.713691	5.041289	3.768607	2.597833	1.505435
31	H	4.633832	4.805950	3.809245	3.423314	2.154184
32	H	5.801548	6.129201	4.845968	3.124677	2.135157
33	H	4.452272	4.702859	3.457719	2.795075	2.158105

		26	27	28	29	30
26	O	0.000000				
27	H	2.128185	0.000000			
28	H	2.183816	1.844336	0.000000		
29	H	2.185131	3.022543	2.242217	0.000000	
30	C	2.506294	2.910490	3.488055	2.221373	0.000000
31	H	2.923726	3.867822	4.252737	2.580979	1.094104
32	H	3.423070	3.359137	3.868597	2.566222	1.094209
33	H	2.664312	2.722204	3.836447	3.112803	1.092392

		31	32	33
31	H	0.000000		
32	H	1.765484	0.000000	
33	H	1.777203	1.777055	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.346487	2.913409	-0.215712
2	6	0	-2.553313	2.345759	0.033472
3	7	0	-2.367878	0.972177	0.036180
4	6	0	-1.055435	0.719005	-0.148952
5	7	0	-0.429174	1.879583	-0.350303
6	6	0	1.015900	2.025986	-0.559827
7	6	0	1.692496	2.800530	0.576113
8	1	0	-1.061633	3.946286	-0.317594
9	1	0	-3.513806	2.804916	0.181952
10	1	0	1.432819	1.020151	-0.607653
11	1	0	1.188168	2.523275	-1.516904
12	1	0	1.301213	3.823868	0.610614
13	1	0	1.422953	2.313785	1.529813
14	35	0	-0.901794	-2.587514	-0.013252
15	1	0	-0.675345	-0.315786	-0.133321
16	6	0	-3.336259	-0.068591	0.213544
17	6	0	-4.633072	0.165399	0.357406
18	1	0	-2.861328	-1.051424	0.232830
19	1	0	-5.297901	-0.674175	0.509175
20	1	0	-5.079214	1.152588	0.342700
21	7	0	3.110866	2.870321	0.274378
22	1	0	3.652091	3.314596	1.007473
23	1	0	3.480954	1.923863	0.152325
24	6	0	2.749378	-1.147272	-1.250840
25	6	0	2.699456	-1.432946	0.111505
26	8	0	2.637276	-0.006190	-0.330998
27	1	0	3.678761	-1.120214	-1.815393
28	1	0	1.857067	-1.408305	-1.812348
29	1	0	1.739383	-1.867426	0.379204
30	6	0	3.859436	-1.722392	1.026383
31	1	0	3.650315	-1.378312	2.043703
32	1	0	4.026714	-2.802816	1.071054
33	1	0	4.774082	-1.240259	0.673835

```
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.4054808           0.3259130           0.1896908
 Standard basis: 6-311++G(d,p) (5D, 7F)
 There are     499 symmetry adapted cartesian basis functions of A      symmetry.
 There are     482 symmetry adapted basis functions of A      symmetry.
    482 basis functions,      760 primitive gaussians,      499 cartesian basis functions
     71 alpha electrons             71 beta electrons
          nuclear repulsion energy           1334.1921026612 Hartrees.
 NAtoms=       33 NActive=       33 NUniq=       33 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      482 RedAO= T EigKep=    3.32D-06    NBF=      482
 NBsUse=      482 1.00D-06 EigRej= -1.00D+00 NBFU=      482
 Initial                guess                from                the                checkpoint                file:
"/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"
 B after Tr=          0.000000        0.000000        0.000000
             Rot=        0.986109        0.018100      -0.006976        0.164962 Ang=    19.12 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn=                5 AccDes=
0.00D+00
 Harris functional with IExCor=    402 and IRadAn=             5 diagonalized for initial guess.
 HarFok:    IExCor=    402 AccDes= 0.00D+00 IRadAn=                5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=    3500011 ScaDFX=    1.000000    1.000000    1.000000    1.000000
 FoFCou: FMM=F IPFlag=                  0 FMFlag=           100000 FMFlg1=                  0
             NFxFlg=                  0 DoJE=T BraDBF=F KetDBF=T FulRan=T
             wScrn=      0.000000  ICntrl=             500  IOpCl=      0  I1Cent=        200000004  NGrid=
0
             NMat0=         1 NMatS0=            1 NMatT0=         0 NMatD0=         1 NMtDS0=         0
NMtDT0=         0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                       energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3205.62489385          A.U. after      13 cycles
                  NFock= 13    Conv=0.51D-08         -V/T= 2.0017
 Calling FoFJK, ICntrl=              2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 ---------------------------------------------------------------------
 Center          Atomic                             Forces (Hartrees/Bohr)
 Number          Number                       X                      Y                      Z
```

1	6	0.000856756	-0.002829628	-0.001556658
2	6	-0.004132245	0.001042822	-0.003749954
3	7	0.001814558	0.000838382	0.004395249
4	6	-0.006312206	-0.002680190	-0.004568418
5	7	-0.002453818	0.003122856	0.007312550
6	6	-0.011315715	0.006599315	-0.004518103
7	6	-0.006064659	-0.000462434	-0.000573295
8	1	-0.000186169	-0.000430147	0.000087689
9	1	-0.000001990	-0.000573739	-0.000059898
10	1	-0.009656143	0.005327820	-0.000775690
11	1	-0.002185704	0.001494440	0.000134521
12	1	-0.000422789	-0.000028133	0.001802899
13	1	0.002262166	0.000976663	-0.000397554
14	35	0.004034558	-0.001060930	-0.000430426
15	1	0.001975828	0.002702517	-0.002288539
16	6	0.000911041	0.004191220	0.002806663
17	6	-0.000789131	-0.001408293	0.000642222
18	1	-0.002050383	-0.000022463	-0.000857343
19	1	-0.000231390	-0.000048752	-0.000647345
20	1	0.000117057	0.000011649	-0.000253630
21	7	0.010730670	-0.004608910	-0.001669950
22	1	-0.003236019	0.000686856	0.000586891
23	1	-0.003148349	0.004641199	0.000832671
24	6	0.010438021	0.018195304	-0.047904332
25	6	0.006415211	-0.000621459	0.050015149
26	8	0.018645710	-0.036636120	0.000642998
27	1	0.000737096	-0.002751922	0.000314884
28	1	-0.003104218	0.004774582	-0.003836722
29	1	-0.004984386	0.004249379	0.010086815
30	6	0.001441926	-0.004286126	-0.004281761
31	1	-0.000974116	-0.000270988	-0.001470874
32	1	0.000733094	-0.000023522	0.000733917
33	1	0.000135739	-0.000111248	-0.000554625

Cartesian Forces: Max 0.050015149 RMS 0.009009349

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.090024104 RMS 0.014898505

Search for a local minimum.

Step number 24 out of a maximum of 172

All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 19 20 22 24 23
DE= 2.26D-02 DEPred=-3.89D-03 R=-5.80D+00
Trust test=-5.80D+00 RLast= 2.99D+00 DXMaxT set to 4.22D-01
ITU= -1 1 -1 1 1 1 1 1 1 1 1 1 0 -1 -1 1 1 1 -1 1
ITU= 0 0 -1 0
Use linear search instead of GDIIS.
Energy rises -- skip Quadratic/GDIIS search.
Quartic linear search produced a step of -0.55511.
Iteration 1 RMS(Cart)= 0.20278358 RMS(Int)= 0.07150473
Iteration 2 RMS(Cart)= 0.05470826 RMS(Int)= 0.03149642
Iteration 3 RMS(Cart)= 0.05231080 RMS(Int)= 0.00798626
Iteration 4 RMS(Cart)= 0.00365118 RMS(Int)= 0.00781480
Iteration 5 RMS(Cart)= 0.00020840 RMS(Int)= 0.00781477
Iteration 6 RMS(Cart)= 0.00000586 RMS(Int)= 0.00781477
Iteration 7 RMS(Cart)= 0.00000021 RMS(Int)= 0.00781477

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56387	0.00075	0.00072	0.00000	0.00074	2.56461
R2	2.62419	-0.00068	-0.00111	0.00000	-0.00113	2.62306
R3	2.03386	-0.00042	0.00006	0.00000	0.00006	2.03391
R4	2.61925	0.00141	0.00315	0.00000	0.00318	2.62242
R5	2.03128	-0.00005	-0.00026	0.00000	-0.00026	2.03102
R6	2.54999	0.00262	-0.00331	0.00000	-0.00328	2.54671
R7	2.70727	-0.00151	-0.00450	0.00000	-0.00450	2.70277
R8	2.52099	-0.00225	-0.00059	0.00000	-0.00056	2.52042
R9	2.08342	0.00282	0.00694	0.00000	0.00694	2.09036
R10	2.77318	0.00471	0.00592	0.00000	0.00595	2.77914
R11	2.89570	-0.00203	0.00198	0.00000	0.00185	2.89755
R12	2.05955	-0.01051	0.00035	0.00000	0.00035	2.05990
R13	2.06402	0.00062	-0.00179	0.00000	-0.00179	2.06223
R14	2.07139	0.00029	-0.00096	0.00000	-0.00096	2.07044
R15	2.08652	-0.00096	-0.00366	0.00000	-0.00366	2.08286
R16	2.74348	0.02318	0.00447	0.00000	0.00451	2.74799
R17	4.32018	0.00208	-0.06088	0.00000	-0.06088	4.25930
R18	2.50499	0.00113	0.00074	0.00000	0.00074	2.50573
R19	2.06309	-0.00152	-0.00348	0.00000	-0.00348	2.05961
R20	2.04398	0.00001	-0.00026	0.00000	-0.00026	2.04372
R21	2.04737	-0.00007	-0.00014	0.00000	-0.00014	2.04723
R22	1.91575	-0.00026	-0.00076	0.00000	-0.00076	1.91500
R23	1.93422	0.03190	-0.00477	0.00000	-0.00992	1.92430
R24	4.08395	0.01264	-0.07512	0.00000	-0.07265	4.01130
R25	2.63214	0.05132	0.07822	0.00000	0.10276	2.73491

R26	2.77780	-0.00221	-0.03013	0.00000	-0.04051	2.73729
R27	2.05555	-0.00048	-0.00006	0.00000	-0.00006	2.05550
R28	2.05246	0.00147	0.00053	0.00000	0.00053	2.05299
R29	2.82532	-0.00691	-0.04235	0.00000	-0.05633	2.76899
R30	2.05466	0.00313	0.00159	0.00000	0.00159	2.05625
R31	2.84486	-0.00285	-0.00172	0.00000	-0.00172	2.84314
R32	2.06756	-0.00115	-0.00050	0.00000	-0.00050	2.06706
R33	2.06775	0.00043	-0.00011	0.00000	-0.00011	2.06765
R34	2.06432	0.00020	0.00052	0.00000	0.00052	2.06484
A1	1.86910	0.00085	0.00170	0.00000	0.00174	1.87084
A2	2.28410	-0.00065	-0.00218	0.00000	-0.00220	2.28190
A3	2.12993	-0.00020	0.00051	0.00000	0.00049	2.13042
A4	1.87128	-0.00091	-0.00351	0.00000	-0.00340	1.86788
A5	2.26722	0.00106	0.00466	0.00000	0.00465	2.27186
A6	2.14432	-0.00011	-0.00095	0.00000	-0.00095	2.14337
A7	1.89208	-0.00062	0.00266	0.00000	0.00273	1.89481
A8	2.25203	-0.00387	0.00120	0.00000	0.00118	2.25321
A9	2.13900	0.00451	-0.00383	0.00000	-0.00386	2.13515
A10	1.89028	0.00032	-0.00005	0.00000	0.00015	1.89042
A11	2.10536	0.01346	0.02034	0.00000	0.02040	2.12576
A12	2.28741	-0.01375	-0.02053	0.00000	-0.02048	2.26694
A13	1.89963	0.00061	0.00050	0.00000	0.00055	1.90018
A14	2.20191	0.00632	0.00356	0.00000	0.00361	2.20552
A15	2.17804	-0.00692	-0.00324	0.00000	-0.00331	2.17474
A16	1.95992	-0.00949	-0.00066	0.00000	-0.00138	1.95854
A17	1.86595	-0.00009	0.00548	0.00000	0.00566	1.87161
A18	1.90270	0.00332	-0.00637	0.00000	-0.00608	1.89661
A19	1.90722	0.00504	0.00443	0.00000	0.00458	1.91181
A20	1.92816	0.00201	0.00010	0.00000	0.00035	1.92851
A21	1.89801	-0.00067	-0.00300	0.00000	-0.00310	1.89491
A22	1.91518	-0.02750	-0.00386	0.00000	-0.00397	1.91121
A23	1.88566	-0.00359	0.00373	0.00000	0.00336	1.88902
A24	1.87717	0.05488	0.00318	0.00000	0.00408	1.88125
A25	1.87259	0.00712	0.00104	0.00000	0.00115	1.87373
A26	1.88642	-0.01332	0.00996	0.00000	0.00976	1.89618
A27	2.02552	-0.01983	-0.01402	0.00000	-0.01435	2.01117
A28	2.14895	0.00072	0.00636	0.00000	0.00637	2.15532
A29	1.94136	0.00095	0.00226	0.00000	0.00227	1.94363
A30	2.19269	-0.00166	-0.00852	0.00000	-0.00851	2.18418
A31	2.07091	0.00033	0.00201	0.00000	0.00201	2.07292
A32	2.16786	-0.00030	-0.00256	0.00000	-0.00256	2.16530
A33	2.04436	-0.00003	0.00058	0.00000	0.00059	2.04495
A34	1.97399	-0.05714	-0.01880	0.00000	-0.02785	1.94614
A35	1.91090	0.09002	0.00466	0.00000	0.00106	1.91196

A36	1.87384	-0.02923	0.00664	0.00000	0.01025	1.88409
A37	2.14523	0.01021	-0.03084	0.00000	-0.04712	2.09811
A38	2.01188	-0.00491	0.04015	0.00000	0.05802	2.06990
A39	1.95048	0.00997	0.02707	0.00000	0.03626	1.98674
A40	2.03468	-0.00358	-0.01432	0.00000	-0.01955	2.01513
A41	2.02596	-0.00229	-0.00412	0.00000	-0.00473	2.02122
A42	1.93309	-0.00131	0.06145	0.00000	0.07837	2.01146
A43	2.22209	0.00581	-0.05207	0.00000	-0.06860	2.15348
A44	2.00147	-0.00421	-0.01425	0.00000	-0.01958	1.98189
A45	1.97729	0.00989	0.02765	0.00000	0.03674	2.01403
A46	2.04196	-0.00317	-0.00819	0.00000	-0.00922	2.03274
A47	2.50386	-0.00195	0.06809	0.00000	0.11934	2.62320
A48	2.44936	-0.00260	0.07419	0.00000	0.12675	2.57612
A49	1.93620	-0.00217	-0.00347	0.00000	-0.00347	1.93273
A50	1.90970	0.00177	0.00256	0.00000	0.00256	1.91226
A51	1.94353	-0.00035	0.00020	0.00000	0.00020	1.94374
A52	1.87736	0.00017	0.00033	0.00000	0.00033	1.87769
A53	1.89792	0.00106	-0.00053	0.00000	-0.00052	1.89739
A54	1.89755	-0.00044	0.00096	0.00000	0.00097	1.89851
A55	3.56158	-0.01335	-0.10331	0.00000	-0.10331	3.45827
A56	2.37193	0.08389	0.23134	0.00000	0.25346	2.62539
A57	2.90000	0.00467	-0.04022	0.00000	-0.04022	2.85978
A58	3.01316	0.04352	0.07410	0.00000	0.07998	3.09314
D1	-0.01012	0.00064	0.00797	0.00000	0.00794	-0.00219
D2	-3.12282	-0.00077	-0.00781	0.00000	-0.00780	-3.13062
D3	3.12008	0.00145	0.01153	0.00000	0.01159	3.13167
D4	0.00738	0.00005	-0.00424	0.00000	-0.00415	0.00324
D5	-0.03084	0.00142	0.01207	0.00000	0.01214	-0.01869
D6	-3.08446	0.00172	0.00100	0.00000	0.00122	-3.08323
D7	3.12091	0.00069	0.00889	0.00000	0.00890	3.12982
D8	0.06730	0.00099	-0.00217	0.00000	-0.00202	0.06528
D9	0.04711	-0.00254	-0.02504	0.00000	-0.02502	0.02208
D10	-3.10718	-0.00111	-0.01896	0.00000	-0.01890	-3.12608
D11	-3.12088	-0.00123	-0.01063	0.00000	-0.01060	-3.13148
D12	0.00802	0.00020	-0.00455	0.00000	-0.00448	0.00354
D13	-0.06673	0.00341	0.03276	0.00000	0.03277	-0.03396
D14	3.09099	0.00165	0.00501	0.00000	0.00534	3.09633
D15	3.08656	0.00217	0.02716	0.00000	0.02711	3.11367
D16	-0.03890	0.00041	-0.00059	0.00000	-0.00032	-0.03923
D17	0.04957	-0.00045	0.02554	0.00000	0.02549	0.07506
D18	-3.07220	-0.00137	0.01642	0.00000	0.01640	-3.05580
D19	-3.10631	0.00111	0.03239	0.00000	0.03241	-3.07390
D20	0.05510	0.00019	0.02327	0.00000	0.02332	0.07842
D21	0.06051	-0.00299	-0.02783	0.00000	-0.02789	0.03262

D22	3.11561	-0.00247	-0.01662	0.00000	-0.01678	3.09883
D23	-3.09949	-0.00062	0.00272	0.00000	0.00304	-3.09645
D24	-0.04439	-0.00010	0.01392	0.00000	0.01415	-0.03024
D25	1.03661	-0.00013	0.22269	0.00000	0.22272	1.25933
D26	3.12821	0.00045	0.23137	0.00000	0.23124	-2.92374
D27	-1.10606	0.00134	0.22747	0.00000	0.22748	-0.87858
D28	-2.00355	-0.00030	0.20974	0.00000	0.20990	-1.79365
D29	0.08805	0.00029	0.21841	0.00000	0.21841	0.30646
D30	2.13696	0.00118	0.21451	0.00000	0.21466	2.35162
D31	-1.10527	0.00170	0.00456	0.00000	0.00456	-1.10071
D32	0.93108	-0.00681	0.00579	0.00000	0.00565	0.93674
D33	3.12987	0.00134	-0.00704	0.00000	-0.00725	3.12262
D34	3.11050	0.00438	-0.00483	0.00000	-0.00466	3.10583
D35	-1.13634	-0.00413	-0.00360	0.00000	-0.00357	-1.13991
D36	1.06245	0.00403	-0.01643	0.00000	-0.01647	1.04597
D37	1.02298	0.00080	-0.00399	0.00000	-0.00395	1.01903
D38	3.05933	-0.00771	-0.00276	0.00000	-0.00286	3.05647
D39	-1.02508	0.00045	-0.01559	0.00000	-0.01576	-1.04083
D40	-3.07397	-0.01839	-0.16324	0.00000	-0.16127	3.04795
D41	-0.98523	-0.03024	-0.16387	0.00000	-0.16550	-1.15073
D42	1.14254	-0.00853	-0.16587	0.00000	-0.16410	0.97844
D43	-3.05190	-0.02038	-0.16650	0.00000	-0.16834	3.06295
D44	-0.96075	0.00558	-0.16528	0.00000	-0.16335	-1.12410
D45	1.12799	-0.00626	-0.16592	0.00000	-0.16758	0.96041
D46	-3.11777	-0.00114	-0.00807	0.00000	-0.00808	-3.12586
D47	0.01331	-0.00034	-0.00132	0.00000	-0.00133	0.01198
D48	0.00108	-0.00005	0.00242	0.00000	0.00243	0.00351
D49	3.13216	0.00074	0.00917	0.00000	0.00918	3.14135
D50	2.23505	-0.00022	-0.30543	0.00000	-0.32156	1.91349
D51	-1.70745	-0.02589	0.49062	0.00000	0.49780	-1.20965
D52	-2.08112	0.02682	-0.25395	0.00000	-0.26087	-2.34198
D53	0.25957	0.00114	0.54211	0.00000	0.55850	0.81806
D54	-2.67077	-0.00556	-0.01942	0.00000	-0.02101	-2.69178
D55	0.01817	-0.00341	-0.01533	0.00000	-0.01724	0.00092
D56	-0.01425	0.00029	-0.00763	0.00000	-0.00673	-0.02098
D57	2.67468	0.00244	-0.00354	0.00000	-0.00296	2.67173
D58	0.23736	0.01661	0.62308	0.00000	0.61089	0.84825
D59	-2.15013	0.01271	0.61437	0.00000	0.59836	-1.55177
D60	2.16591	-0.01656	-0.59614	0.00000	-0.57944	1.58647
D61	-0.24038	-0.01815	-0.59861	0.00000	-0.58472	-0.82510
D62	2.59657	-0.00263	-0.02217	0.00000	-0.02472	2.57185
D63	-1.61805	-0.00264	-0.02228	0.00000	-0.02483	-1.64288
D64	0.48011	-0.00225	-0.01926	0.00000	-0.02181	0.45830
D65	1.36638	0.00159	-0.00198	0.00000	-0.00013	1.36624

D66	-2.84824	0.00158	-0.00210	0.00000	-0.00025	-2.84849
D67	-0.75009	0.00197	0.00093	0.00000	0.00278	-0.74731
D68	-1.02186	0.00023	-0.00247	0.00000	-0.00177	-1.02363
D69	1.04670	0.00023	-0.00258	0.00000	-0.00188	1.04483
D70	-3.13833	0.00062	0.00045	0.00000	0.00115	-3.13718

Item	Value	Threshold	Converged?
Maximum Force	0.090024	0.000450	NO
RMS Force	0.014899	0.000300	NO
Maximum Displacement	1.009735	0.001800	NO
RMS Displacement	0.259707	0.001200	NO

Predicted change in Energy=-2.369415D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.622105	2.076205	-0.239330
2	6	0	-3.521833	1.108623	0.070643
3	7	0	-2.823918	-0.089026	0.136519
4	6	0	-1.521128	0.159875	-0.102176
5	7	0	-1.383042	1.461735	-0.357098
6	6	0	-0.099017	2.130579	-0.615466
7	6	0	0.399856	2.917924	0.602021
8	1	0	-2.752148	3.133784	-0.391118
9	1	0	-4.581886	1.174658	0.235114
10	1	0	0.623781	1.355099	-0.869262
11	1	0	-0.216309	2.791397	-1.475965
12	1	0	-0.309031	3.720394	0.834230
13	1	0	0.420731	2.236758	1.468292
14	35	0	0.090289	-2.698674	0.287655
15	1	0	-0.757874	-0.639719	-0.060904
16	6	0	-3.313562	-1.404401	0.411547
17	6	0	-4.598525	-1.687245	0.576114
18	1	0	-2.499052	-2.125656	0.476668
19	1	0	-4.882966	-2.707213	0.796067
20	1	0	-5.394504	-0.955552	0.507649
21	7	0	1.678884	3.514508	0.251601
22	1	0	2.019872	4.121495	0.987955
23	1	0	2.368874	2.779973	0.105672
24	6	0	3.347539	-0.274642	-1.181604
25	6	0	3.293325	-0.541566	0.239784
26	8	0	2.844691	0.749278	-0.288901

27	1	0	4.293033	-0.019390	-1.654920
28	1	0	2.605675	-0.737554	-1.826281
29	1	0	2.478171	-1.187318	0.559996
30	6	0	4.498348	-0.486914	1.138968
31	1	0	4.218827	-0.149096	2.141081
32	1	0	4.928962	-1.488096	1.235789
33	1	0	5.261157	0.187144	0.741874

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357133	0.000000			
3	N	2.206857	1.387727	0.000000		
4	C	2.214335	2.220992	1.347661	0.000000	
5	N	1.388063	2.209542	2.173624	1.333751	0.000000
6	C	2.551550	3.637418	3.594053	2.483856	1.470655
7	C	3.247862	4.351503	4.432963	3.434080	2.493817
8	H	1.076301	2.215156	3.266505	3.231567	2.161332
9	H	2.208762	1.074767	2.167272	3.242189	3.265843
10	H	3.384166	4.257967	3.870881	2.572473	2.073891
11	H	2.797967	4.018733	4.206729	3.242647	2.093115
12	H	3.034171	4.210286	4.617698	3.875994	2.770253
13	H	3.492936	4.332427	4.208401	3.248174	2.680730
14	Br	5.516726	5.252621	3.914806	3.304533	4.460427
15	H	3.299005	3.273144	2.147272	1.106170	2.212391
16	C	3.607821	2.544579	1.430246	2.433863	3.540121
17	C	4.328365	3.038362	2.428328	3.652712	4.596334
18	H	4.264204	3.416357	2.090240	2.552460	3.848379
19	H	5.391163	4.115766	3.395525	4.508769	5.564116
20	H	4.175611	2.821115	2.737977	4.076654	4.762656
21	N	4.561604	5.733104	5.768356	4.649602	3.736280
22	H	5.218945	6.374116	6.474236	5.424159	4.523640
23	H	5.052146	6.123321	5.932722	4.694702	4.003596
24	C	6.484675	7.118273	6.313381	5.005785	5.106193
25	C	6.486493	7.014136	6.134829	4.877286	5.122294
26	O	5.625749	6.386785	5.746030	4.409381	4.287887
27	H	7.363052	8.082209	7.339284	6.020599	6.007986
28	H	6.145351	6.674807	5.809790	4.561625	4.785942
29	H	6.107562	6.442892	5.431181	4.271744	4.771531
30	C	7.692212	8.246839	7.401270	6.180037	6.373868
31	H	7.577378	8.110880	7.322713	6.170474	6.341657
32	H	8.479318	8.917200	7.954430	6.790407	7.147041
33	H	8.165606	8.856669	8.112408	6.834658	6.854028

	6	7	8	9	10

6	C	0.000000				
7	C	1.533316	0.000000			
8	H	2.845322	3.311804	0.000000		
9	H	4.661908	5.290685	2.752868	0.000000	
10	H	1.090054	2.158063	3.845678	5.324582	0.000000
11	H	1.091282	2.171104	2.779317	4.959829	1.771099
12	H	2.161767	1.095627	2.795427	5.009691	3.060497
13	H	2.150223	1.102202	3.785396	5.260700	2.506534
14	Br	4.916620	5.633900	6.523630	6.069158	4.249252
15	H	2.901066	3.799557	4.280829	4.242954	2.557677
16	C	4.887140	5.701600	4.642691	2.879465	4.975739
17	C	6.020068	6.796474	5.252329	2.882194	6.214294
18	H	5.006842	5.818684	5.336555	3.910066	4.866135
19	H	6.948585	7.719329	6.329853	3.933731	7.042725
20	H	6.231194	6.970462	4.951009	2.296175	6.592022
21	N	2.414124	1.454173	4.493560	6.683742	2.651909
22	H	3.320300	2.054746	5.064543	7.268688	3.612654
23	H	2.651836	2.035294	5.157213	7.134904	2.454813
24	C	4.240795	4.697088	7.031957	8.184335	3.189431
25	C	4.402249	4.524539	7.103097	8.060049	3.457425
26	O	3.268035	3.387328	6.084482	7.457184	2.374085
27	H	4.999293	5.373865	7.821399	9.152167	3.996234
28	H	4.124030	4.911702	6.764113	7.717963	3.036938
29	H	4.362573	4.601540	6.850750	7.451771	3.456215
30	C	5.573604	5.355266	8.247442	9.275150	4.736904
31	H	5.607070	5.134185	8.110723	9.101515	4.924339
32	H	6.465488	6.350393	9.110876	9.927127	5.572215
33	H	5.860953	5.577541	8.612747	9.905427	5.046299

		11	12	13	14	15
11	H	0.000000				
12	H	2.491713	0.000000			
13	H	3.063020	1.770809	0.000000		
14	Br	5.774534	6.454660	5.085429	0.000000	
15	H	3.750767	4.473624	3.464344	2.253923	0.000000
16	C	5.546206	5.955618	5.321625	3.643719	2.709149
17	C	6.593412	6.907165	6.433250	4.805327	4.031588
18	H	5.762041	6.253027	5.342201	2.658714	2.351318
19	H	7.561385	7.889009	7.281754	4.999182	4.693114
20	H	6.692389	6.916152	6.703033	5.759325	4.682023
21	N	2.664419	2.081743	2.167009	6.413156	4.826288
22	H	3.583373	2.368186	2.517977	7.122388	5.611162
23	H	3.030656	2.930250	2.438662	5.936382	4.636657
24	C	4.710441	5.778789	4.679240	4.317908	4.271261
25	C	5.135170	5.612009	4.180923	3.861974	4.063529

26	O	3.866405	4.476038	3.343039	4.450564	3.867786
27	H	5.316645	6.431240	5.462543	5.349319	5.332669
28	H	4.532087	5.953750	4.947194	3.826472	3.799947
29	H	5.218767	5.650605	4.096628	2.839075	3.340265
30	C	6.309769	6.395717	4.914652	5.004757	5.393599
31	H	6.434279	6.097730	4.535468	5.194262	5.464156
32	H	7.220907	7.397716	5.852585	5.077127	5.894172
33	H	6.457830	6.596922	5.306442	5.939035	6.128368

		16	17	18	19	20
16	C	0.000000				
17	C	1.325976	0.000000			
18	H	1.089897	2.147063	0.000000		
19	H	2.075622	1.081490	2.474524	0.000000	
20	H	2.130968	1.083349	3.123099	1.847477	0.000000
21	N	7.010404	8.159007	7.022625	9.058926	8.371369
22	H	7.701512	8.815568	7.727159	9.711707	8.998893
23	H	7.063470	8.289872	6.920949	9.120035	8.624718
24	C	6.941523	8.259840	6.352854	8.807372	8.929756
25	C	6.665204	7.981666	6.009750	8.476510	8.701811
26	O	6.561481	7.879489	6.116121	8.534704	8.451348
27	H	8.003051	9.317674	7.423775	9.870699	9.970029
28	H	6.363170	7.653360	5.769632	8.175330	8.336524
29	H	5.797701	7.094351	5.065587	7.520117	7.876260
30	C	7.899167	9.192969	7.217182	9.646572	9.924047
31	H	7.829684	9.086292	7.197705	9.549642	9.784406
32	H	8.284056	9.552374	7.493874	9.897148	10.362806
33	H	8.727424	10.037636	8.101865	10.549098	10.719316

		21	22	23	24	25
21	N	0.000000				
22	H	1.013372	0.000000			
23	H	1.018295	1.643140	0.000000		
24	C	4.381340	5.078947	3.456231	0.000000	
25	C	4.365581	4.891378	3.450393	1.447250	0.000000
26	O	3.049221	3.698991	2.122690	1.448512	1.465285
27	H	4.791350	5.412853	3.826030	1.087722	2.204991
28	H	4.822507	5.645658	4.020139	1.086397	2.186298
29	H	4.779240	5.345716	3.994715	2.149872	1.088121
30	C	4.974754	5.234795	4.034217	2.598937	1.504526
31	H	4.841842	4.939944	4.018041	3.437316	2.150701
32	H	6.046296	6.323903	5.103688	3.133235	2.136178
33	H	4.913695	5.103489	3.936091	2.752263	2.157655

		26	27	28	29	30
26	O	0.000000				
27	H	2.134139	0.000000			

28	H	2.152054	1.841820	0.000000		
29	H	2.146011	3.092511	2.431638	0.000000	
30	C	2.510291	2.840165	3.526717	2.215149	0.000000
31	H	2.932599	3.798940	4.323020	2.570528	1.093839
32	H	3.416828	3.304195	3.916280	2.559989	1.094152
33	H	2.686596	2.593172	3.808158	3.109217	1.092664

		31	32	33
31	H	0.000000		
32	H	1.765437	0.000000	
33	H	1.776876	1.777846	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.268029	2.523879	-0.219035
2	6	0	-3.282233	1.655378	0.023672
3	7	0	-2.736262	0.379622	0.011475
4	6	0	-1.410393	0.482411	-0.206916
5	7	0	-1.111940	1.771513	-0.374346
6	6	0	0.246708	2.293764	-0.584481
7	6	0	0.824926	2.932451	0.683904
8	1	0	-2.266563	3.597093	-0.300471
9	1	0	-4.328011	1.839654	0.189549
10	1	0	0.872224	1.454047	-0.887503
11	1	0	0.219965	3.019070	-1.399413
12	1	0	0.216735	3.798613	0.967217
13	1	0	0.753436	2.198410	1.503004
14	35	0	-0.163689	-2.571198	-0.004081
15	1	0	-0.750788	-0.405525	-0.217027
16	6	0	-3.385491	-0.881177	0.197198
17	6	0	-4.697020	-1.014890	0.339412
18	1	0	-2.665718	-1.699370	0.216220
19	1	0	-5.105994	-2.004629	0.490337
20	1	0	-5.397095	-0.188407	0.317793
21	7	0	2.170780	3.389802	0.377103
22	1	0	2.575406	3.900807	1.153037
23	1	0	2.767584	2.587558	0.184351

24	6	0	3.380143	-0.472607	-1.300809
25	6	0	3.278750	-0.823708	0.099541
26	8	0	2.996446	0.544254	-0.343229
27	1	0	4.354659	-0.304400	-1.753760
28	1	0	2.594246	-0.797914	-1.976679
29	1	0	2.387610	-1.384516	0.374079
30	6	0	4.471860	-0.976091	1.003347
31	1	0	4.225014	-0.673195	2.025014
32	1	0	4.776163	-2.026617	1.034431
33	1	0	5.315313	-0.375795	0.653851

Rotational constants (GHZ): 0.4188060 0.2901875 0.1801801

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1308.6593068680 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 3.64D-06 NBF= 482

NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482

Lowest energy guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999202 0.010789 -0.002635 0.038362 Ang= 4.58 deg.

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.991861 -0.007953 0.003199 -0.127036 Ang= -14.63 deg.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3205.64724950 A.U. after 12 cycles

NFock= 12 Conv=0.69D-08 -V/T= 2.0018

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z

1	6	0.000651025	-0.000654896	-0.000801301
2	6	-0.001693760	0.000444569	-0.001800315
3	7	0.001528001	0.000968423	0.001956263
4	6	-0.003765859	-0.002412079	-0.001700970
5	7	-0.000017299	-0.000150866	0.003284316
6	6	0.000919774	0.000992330	-0.000655557
7	6	-0.002527470	-0.000281046	0.000187799
8	1	-0.000119959	-0.000095039	-0.000006317
9	1	0.000025315	-0.000189873	-0.000073802
10	1	0.000320177	0.000149883	0.000454229
11	1	-0.000560643	0.000158807	0.000256923
12	1	-0.000183378	-0.000223878	0.000527555
13	1	0.000830918	0.000393213	-0.000459970
14	35	0.001013451	0.000147668	-0.000101231
15	1	0.001669287	0.000825380	-0.001342280
16	6	0.000689109	0.001773846	0.001321566
17	6	-0.000192635	-0.000630811	0.000330907
18	1	-0.000814978	-0.000114557	-0.000477474
19	1	-0.000112371	-0.000029808	-0.000313691
20	1	0.000008187	-0.000021327	-0.000122690
21	7	0.002380684	-0.000759998	-0.000659175
22	1	-0.000793174	0.000419780	0.000073964
23	1	0.000618204	0.000531681	0.000288305
24	6	0.004146626	0.004212666	-0.009909283
25	6	0.000724426	0.001032912	0.010728907
26	8	-0.002853040	-0.006993809	-0.000600051
27	1	0.000080608	-0.000604235	-0.000015775
28	1	-0.000547615	0.000884692	-0.000298071
29	1	-0.001660882	0.001586101	0.001563002
30	6	-0.000007579	-0.001451110	-0.001297635
31	1	-0.000232947	0.000118184	-0.000417010
32	1	0.000398677	-0.000026609	0.000235618
33	1	0.000079119	-0.000000190	-0.000156757

Cartesian Forces: Max 0.010728907 RMS 0.002014816

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.009748918 RMS 0.001327523
Search for a local minimum.
Step number 25 out of a maximum of 172

All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 19 20 22 25 23
ITU= 0 -1 1 -1 1 1 1 1 1 1 1 1 1 0 -1 -1 1 1 1 -1
ITU= 1 0 0 -1 0
Use linear search instead of GDIIS.
Energy rises -- skip Quadratic/GDIIS search.
Quartic linear search produced a step of -0.45594.
Iteration 1 RMS(Cart)= 0.07486364 RMS(Int)= 0.00440451
Iteration 2 RMS(Cart)= 0.00912038 RMS(Int)= 0.00143169
Iteration 3 RMS(Cart)= 0.00009294 RMS(Int)= 0.00143142
Iteration 4 RMS(Cart)= 0.00000039 RMS(Int)= 0.00143142

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56461	0.00009	0.00025	0.00000	0.00026	2.56487
R2	2.62306	-0.00042	-0.00040	0.00000	-0.00040	2.62266
R3	2.03391	-0.00008	0.00002	0.00000	0.00002	2.03393
R4	2.62242	0.00075	0.00114	0.00000	0.00115	2.62357
R5	2.03102	-0.00005	-0.00009	0.00000	-0.00009	2.03092
R6	2.54671	-0.00005	-0.00122	0.00000	-0.00121	2.54550
R7	2.70277	-0.00061	-0.00164	0.00000	-0.00164	2.70113
R8	2.52042	-0.00076	-0.00023	0.00000	-0.00022	2.52020
R9	2.09036	0.00113	0.00253	0.00000	0.00253	2.09289
R10	2.77914	0.00108	0.00215	0.00000	0.00216	2.78129
R11	2.89755	-0.00069	0.00078	0.00000	0.00076	2.89831
R12	2.05990	0.00000	0.00013	0.00000	0.00013	2.06003
R13	2.06223	-0.00005	-0.00065	0.00000	-0.00065	2.06157
R14	2.07044	0.00007	-0.00035	0.00000	-0.00035	2.07009
R15	2.08286	-0.00059	-0.00134	0.00000	-0.00134	2.08152
R16	2.74799	0.00175	0.00161	0.00000	0.00162	2.74961
R17	4.25930	0.00023	-0.02225	0.00000	-0.02225	4.23705
R18	2.50573	0.00042	0.00027	0.00000	0.00027	2.50600
R19	2.05961	-0.00056	-0.00127	0.00000	-0.00127	2.05834
R20	2.04372	0.00000	-0.00009	0.00000	-0.00009	2.04363
R21	2.04723	-0.00001	-0.00005	0.00000	-0.00005	2.04718
R22	1.91500	0.00004	-0.00028	0.00000	-0.00028	1.91472
R23	1.92430	0.00155	0.00061	0.00000	-0.00004	1.92425
R24	4.01130	0.00097	-0.02858	0.00000	-0.02826	3.98304
R25	2.73491	0.00975	0.01739	0.00000	0.02209	2.75700
R26	2.73729	-0.00023	-0.00628	0.00000	-0.00820	2.72909
R27	2.05550	-0.00006	-0.00002	0.00000	-0.00002	2.05548
R28	2.05299	0.00017	0.00019	0.00000	0.00019	2.05319
R29	2.76899	-0.00254	-0.00910	0.00000	-0.01190	2.75708
R30	2.05625	0.00076	0.00058	0.00000	0.00058	2.05683

R31	2.84314	-0.00083	-0.00063	0.00000	-0.00063	2.84251
R32	2.06706	-0.00028	-0.00018	0.00000	-0.00018	2.06687
R33	2.06765	0.00020	-0.00004	0.00000	-0.00004	2.06761
R34	2.06484	0.00011	0.00019	0.00000	0.00019	2.06502
A1	1.87084	0.00005	0.00060	0.00000	0.00061	1.87145
A2	2.28190	-0.00015	-0.00079	0.00000	-0.00079	2.28110
A3	2.13042	0.00010	0.00019	0.00000	0.00019	2.13061
A4	1.86788	-0.00051	-0.00133	0.00000	-0.00131	1.86657
A5	2.27186	0.00044	0.00170	0.00000	0.00170	2.27357
A6	2.14337	0.00007	-0.00034	0.00000	-0.00034	2.14302
A7	1.89481	0.00016	0.00094	0.00000	0.00096	1.89577
A8	2.25321	-0.00105	0.00045	0.00000	0.00045	2.25366
A9	2.13515	0.00089	-0.00139	0.00000	-0.00139	2.13375
A10	1.89042	-0.00021	-0.00011	0.00000	-0.00007	1.89035
A11	2.12576	0.00513	0.00740	0.00000	0.00742	2.13317
A12	2.26694	-0.00493	-0.00753	0.00000	-0.00752	2.25942
A13	1.90018	0.00056	0.00016	0.00000	0.00017	1.90035
A14	2.20552	0.00124	0.00128	0.00000	0.00129	2.20680
A15	2.17474	-0.00176	-0.00116	0.00000	-0.00117	2.17357
A16	1.95854	0.00074	0.00009	0.00000	-0.00004	1.95850
A17	1.87161	-0.00021	0.00193	0.00000	0.00196	1.87357
A18	1.89661	-0.00019	-0.00246	0.00000	-0.00241	1.89420
A19	1.91181	-0.00070	0.00155	0.00000	0.00158	1.91339
A20	1.92851	-0.00004	-0.00008	0.00000	-0.00003	1.92847
A21	1.89491	0.00039	-0.00105	0.00000	-0.00107	1.89384
A22	1.91121	-0.00033	-0.00136	0.00000	-0.00138	1.90982
A23	1.88902	0.00078	0.00153	0.00000	0.00147	1.89049
A24	1.88125	-0.00008	0.00076	0.00000	0.00092	1.88217
A25	1.87373	-0.00007	0.00034	0.00000	0.00035	1.87409
A26	1.89618	0.00087	0.00373	0.00000	0.00369	1.89987
A27	2.01117	-0.00116	-0.00497	0.00000	-0.00503	2.00614
A28	2.15532	0.00047	0.00232	0.00000	0.00232	2.15764
A29	1.94363	0.00032	0.00082	0.00000	0.00082	1.94446
A30	2.18418	-0.00078	-0.00312	0.00000	-0.00312	2.18106
A31	2.07292	0.00013	0.00073	0.00000	0.00073	2.07365
A32	2.16530	-0.00008	-0.00094	0.00000	-0.00094	2.16437
A33	2.04495	-0.00005	0.00021	0.00000	0.00021	2.04516
A34	1.94614	-0.00035	-0.00274	0.00000	-0.00405	1.94209
A35	1.91196	0.00053	0.00334	0.00000	0.00287	1.91482
A36	1.88409	-0.00015	0.00078	0.00000	0.00126	1.88535
A37	2.09811	-0.00035	-0.00384	0.00000	-0.00568	2.09243
A38	2.06990	0.00124	0.00652	0.00000	0.00874	2.07863
A39	1.98674	0.00343	0.00570	0.00000	0.00712	1.99385
A40	2.01513	-0.00195	-0.00285	0.00000	-0.00336	2.01177

A41	2.02122	-0.00031	-0.00122	0.00000	-0.00134	2.01988
A42	2.01146	0.00159	0.01474	0.00000	0.01692	2.02838
A43	2.15348	-0.00152	-0.01148	0.00000	-0.01340	2.14008
A44	1.98189	-0.00244	-0.00278	0.00000	-0.00341	1.97848
A45	2.01403	0.00314	0.00596	0.00000	0.00740	2.02143
A46	2.03274	0.00005	-0.00252	0.00000	-0.00278	2.02996
A47	2.62320	-0.00245	0.00151	0.00000	0.01210	2.63529
A48	2.57612	-0.00270	0.00314	0.00000	0.01398	2.59010
A49	1.93273	-0.00060	-0.00127	0.00000	-0.00127	1.93146
A50	1.91226	0.00075	0.00093	0.00000	0.00093	1.91319
A51	1.94374	-0.00016	0.00007	0.00000	0.00007	1.94381
A52	1.87769	0.00002	0.00012	0.00000	0.00012	1.87781
A53	1.89739	0.00023	-0.00019	0.00000	-0.00019	1.89720
A54	1.89851	-0.00024	0.00035	0.00000	0.00035	1.89887
A55	3.45827	-0.00362	-0.03775	0.00000	-0.03775	3.42052
A56	2.62539	-0.00201	0.07445	0.00000	0.07792	2.70331
A57	2.85978	0.00159	-0.01470	0.00000	-0.01470	2.84508
A58	3.09314	0.00102	0.02439	0.00000	0.02538	3.11852
D1	-0.00219	0.00030	0.00292	0.00000	0.00292	0.00073
D2	-3.13062	-0.00022	-0.00286	0.00000	-0.00285	-3.13347
D3	3.13167	0.00041	0.00419	0.00000	0.00420	3.13587
D4	0.00324	-0.00011	-0.00159	0.00000	-0.00157	0.00167
D5	-0.01869	0.00052	0.00438	0.00000	0.00439	-0.01431
D6	-3.08323	0.00009	0.00026	0.00000	0.00031	-3.08293
D7	3.12982	0.00042	0.00325	0.00000	0.00325	3.13306
D8	0.06528	-0.00001	-0.00086	0.00000	-0.00083	0.06444
D9	0.02208	-0.00101	-0.00916	0.00000	-0.00915	0.01293
D10	-3.12608	-0.00045	-0.00695	0.00000	-0.00694	-3.13302
D11	-3.13148	-0.00054	-0.00390	0.00000	-0.00389	-3.13537
D12	0.00354	0.00002	-0.00170	0.00000	-0.00168	0.00186
D13	-0.03396	0.00135	0.01197	0.00000	0.01197	-0.02199
D14	3.09633	0.00072	0.00168	0.00000	0.00175	3.09808
D15	3.11367	0.00084	0.00994	0.00000	0.00993	3.12360
D16	-0.03923	0.00021	-0.00034	0.00000	-0.00029	-0.03951
D17	0.07506	-0.00017	0.00936	0.00000	0.00935	0.08441
D18	-3.05580	-0.00064	0.00601	0.00000	0.00601	-3.04979
D19	-3.07390	0.00045	0.01183	0.00000	0.01183	-3.06207
D20	0.07842	-0.00002	0.00848	0.00000	0.00849	0.08691
D21	0.03262	-0.00115	-0.01014	0.00000	-0.01015	0.02247
D22	3.09883	-0.00057	-0.00600	0.00000	-0.00603	3.09280
D23	-3.09645	-0.00055	0.00085	0.00000	0.00091	-3.09554
D24	-0.03024	0.00003	0.00499	0.00000	0.00503	-0.02521
D25	1.25933	0.00065	0.08136	0.00000	0.08136	1.34069
D26	-2.92374	0.00009	0.08460	0.00000	0.08458	-2.83916

D27	-0.87858	0.00034	0.08311	0.00000	0.08312	-0.79546
D28	-1.79365	0.00003	0.07656	0.00000	0.07659	-1.71706
D29	0.30646	-0.00053	0.07981	0.00000	0.07981	0.38627
D30	2.35162	-0.00028	0.07832	0.00000	0.07835	2.42997
D31	-1.10071	-0.00026	0.00166	0.00000	0.00167	-1.09904
D32	0.93674	-0.00009	0.00218	0.00000	0.00216	0.93889
D33	3.12262	-0.00107	-0.00248	0.00000	-0.00251	3.12011
D34	3.10583	-0.00001	-0.00184	0.00000	-0.00181	3.10402
D35	-1.13991	0.00017	-0.00133	0.00000	-0.00132	-1.14123
D36	1.04597	-0.00082	-0.00598	0.00000	-0.00599	1.03999
D37	1.01903	-0.00002	-0.00148	0.00000	-0.00147	1.01756
D38	3.05647	0.00015	-0.00096	0.00000	-0.00098	3.05549
D39	-1.04083	-0.00084	-0.00562	0.00000	-0.00565	-1.04648
D40	3.04795	-0.00056	-0.06055	0.00000	-0.06025	2.98769
D41	-1.15073	-0.00061	-0.05914	0.00000	-0.05938	-1.21011
D42	0.97844	-0.00060	-0.06142	0.00000	-0.06116	0.91728
D43	3.06295	-0.00066	-0.06000	0.00000	-0.06028	3.00267
D44	-1.12410	-0.00038	-0.06128	0.00000	-0.06099	-1.18509
D45	0.96041	-0.00043	-0.05987	0.00000	-0.06011	0.90030
D46	-3.12586	-0.00056	-0.00294	0.00000	-0.00295	-3.12881
D47	0.01198	-0.00017	-0.00048	0.00000	-0.00048	0.01150
D48	0.00351	-0.00002	0.00088	0.00000	0.00088	0.00439
D49	3.14135	0.00038	0.00334	0.00000	0.00335	-3.13849
D50	1.91349	0.00194	-0.10425	0.00000	-0.10671	1.80678
D51	-1.20965	-0.00060	0.17601	0.00000	0.17722	-1.03243
D52	-2.34198	0.00089	-0.08964	0.00000	-0.09077	-2.43275
D53	0.81806	-0.00165	0.19062	0.00000	0.19316	1.01122
D54	-2.69178	-0.00131	-0.00637	0.00000	-0.00680	-2.69858
D55	0.00092	-0.00094	-0.00473	0.00000	-0.00508	-0.00415
D56	-0.02098	-0.00004	-0.00320	0.00000	-0.00306	-0.02404
D57	2.67173	0.00034	-0.00156	0.00000	-0.00134	2.67039
D58	0.84825	0.00128	0.23323	0.00000	0.23205	1.08030
D59	-1.55177	0.00000	0.23179	0.00000	0.22972	-1.32205
D60	1.58647	-0.00138	-0.22545	0.00000	-0.22318	1.36329
D61	-0.82510	-0.00226	-0.22507	0.00000	-0.22335	-1.04844
D62	2.57185	-0.00063	-0.00694	0.00000	-0.00750	2.56435
D63	-1.64288	-0.00050	-0.00698	0.00000	-0.00754	-1.65042
D64	0.45830	-0.00040	-0.00587	0.00000	-0.00644	0.45186
D65	1.36624	0.00001	-0.00157	0.00000	-0.00107	1.36517
D66	-2.84849	0.00014	-0.00161	0.00000	-0.00112	-2.84961
D67	-0.74731	0.00024	-0.00050	0.00000	-0.00001	-0.74732
D68	-1.02363	0.00010	-0.00122	0.00000	-0.00115	-1.02478
D69	1.04483	0.00023	-0.00126	0.00000	-0.00119	1.04363
D70	-3.13718	0.00033	-0.00016	0.00000	-0.00009	-3.13727

Item	Value	Threshold	Converged?
Maximum Force	0.009749	0.000450	NO
RMS Force	0.001328	0.000300	NO
Maximum Displacement	0.317610	0.001800	NO
RMS Displacement	0.081258	0.001200	NO

Predicted change in Energy=-5.568426D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.694656	2.089504	-0.265152
2	6	0	-3.588149	1.119755	0.056463
3	7	0	-2.880086	-0.071576	0.139200
4	6	0	-1.581199	0.181763	-0.112137
5	7	0	-1.451591	1.482467	-0.376612
6	6	0	-0.170460	2.156135	-0.643183
7	6	0	0.381156	2.865704	0.599607
8	1	0	-2.832175	3.144514	-0.427912
9	1	0	-4.648155	1.179532	0.223293
10	1	0	0.535308	1.393581	-0.972988
11	1	0	-0.315948	2.868388	-1.456613
12	1	0	-0.312262	3.656705	0.905354
13	1	0	0.430033	2.134946	1.422344
14	35	0	0.119400	-2.605255	0.359900
15	1	0	-0.805709	-0.607517	-0.064900
16	6	0	-3.357075	-1.385411	0.438256
17	6	0	-4.639132	-1.681135	0.603997
18	1	0	-2.536845	-2.097681	0.517655
19	1	0	-4.912568	-2.700403	0.840300
20	1	0	-5.443214	-0.960195	0.518640
21	7	0	1.654701	3.470191	0.239339
22	1	0	1.997552	4.073006	0.978050
23	1	0	2.347915	2.741508	0.080117
24	6	0	3.489895	-0.247572	-1.190153
25	6	0	3.380906	-0.532347	0.236570
26	8	0	2.992027	0.769827	-0.294238
27	1	0	4.461105	-0.022945	-1.625365
28	1	0	2.753813	-0.667026	-1.870390
29	1	0	2.534124	-1.144482	0.541410
30	6	0	4.571466	-0.536082	1.155890
31	1	0	4.289043	-0.190934	2.154580

32	1	0	4.955970	-1.555634	1.254852
33	1	0	5.369925	0.106034	0.776043

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357269	0.000000			
3	N	2.206389	1.388333	0.000000		
4	C	2.214198	2.221735	1.347018	0.000000	
5	N	1.387850	2.209977	2.172950	1.333632	0.000000
6	C	2.553216	3.639257	3.594008	2.484016	1.471796
7	C	3.287995	4.370209	4.413081	3.400140	2.495056
8	H	1.076312	2.214895	3.266059	3.231493	2.161260
9	H	2.209703	1.074717	2.167581	3.242572	3.266447
10	H	3.379054	4.258832	3.879248	2.586343	2.076374
11	H	2.772092	4.006797	4.214833	3.259821	2.092096
12	H	3.082532	4.229441	4.591382	3.836758	2.769263
13	H	3.551533	4.363718	4.179962	3.196031	2.683743
14	Br	5.509116	5.264380	3.932576	3.298837	4.440713
15	H	3.298810	3.277220	2.152192	1.107511	2.209607
16	C	3.606746	2.544606	1.429376	2.431605	3.538305
17	C	4.330604	3.041273	2.429189	3.651601	4.596780
18	H	4.262653	3.416114	2.089532	2.550640	3.846421
19	H	5.392993	4.118507	3.396065	4.506888	5.563780
20	H	4.179662	2.825078	2.739205	4.076409	4.764571
21	N	4.591047	5.748519	5.754862	4.626915	3.738916
22	H	5.243724	6.385223	6.455430	5.397939	4.521348
23	H	5.096257	6.153658	5.937081	4.693313	4.028651
24	C	6.675794	7.315897	6.509594	5.202158	5.298412
25	C	6.636134	7.164468	6.278679	5.025339	5.271479
26	O	5.837872	6.598800	5.947902	4.614475	4.501153
27	H	7.584031	8.302096	7.550440	6.232271	6.227810
28	H	6.313562	6.864826	6.011143	4.754390	4.953496
29	H	6.200754	6.545546	5.534128	4.372864	4.861023
30	C	7.855545	8.398206	7.534922	6.322854	6.534548
31	H	7.734827	8.256522	7.447980	6.303701	6.493233
32	H	8.609851	9.033041	8.053005	6.900855	7.276577
33	H	8.369928	9.043922	8.276460	7.008047	7.053811

		6	7	8	9	10
6	C	0.000000				
7	C	1.533719	0.000000			
8	H	2.847449	3.385118	0.000000		
9	H	4.664149	5.317777	2.753725	0.000000	
10	H	1.090122	2.159621	3.834425	5.324020	0.000000

11	H	1.090936	2.171175	2.732375	4.943919	1.770193
12	H	2.160969	1.095442	2.896533	5.039996	3.060764
13	H	2.151148	1.101495	3.883899	5.304576	2.509645
14	Br	4.874528	5.482460	6.510936	6.088748	4.235594
15	H	2.894084	3.730078	4.279729	4.247469	2.574363
16	C	4.885342	5.663248	4.641765	2.879588	4.986487
17	C	6.020725	6.773260	5.255170	2.885902	6.222185
18	H	5.004226	5.758180	5.334972	3.909527	4.883549
19	H	6.947969	7.685245	6.332413	3.937577	7.051814
20	H	6.234042	6.969028	4.956018	2.301691	6.596055
21	N	2.415947	1.455031	4.547895	6.706219	2.652374
22	H	3.317087	2.052690	5.115183	7.287474	3.622710
23	H	2.684778	2.037998	5.220521	7.169746	2.492284
24	C	4.413070	4.749736	7.214973	8.382262	3.386759
25	C	4.540274	4.547202	7.250049	8.209538	3.642754
26	O	3.470581	3.465300	6.291132	7.668642	2.623974
27	H	5.211954	5.471816	8.041059	9.372412	4.224219
28	H	4.245898	4.920423	6.914611	7.910905	3.158037
29	H	4.428555	4.551950	6.937740	7.555618	3.567973
30	C	5.741999	5.425891	8.418380	9.424143	4.954422
31	H	5.763971	5.199284	8.276848	9.245623	5.136428
32	H	6.607575	6.395819	9.250854	10.039147	5.762239
33	H	6.075605	5.703922	8.829287	10.090582	5.300039

		11	12	13	14	15
11	H	0.000000				
12	H	2.490050	0.000000			
13	H	3.063139	1.770319	0.000000		
14	Br	5.783599	6.300476	4.867729	0.000000	
15	H	3.776063	4.400963	3.355601	2.242150	0.000000
16	C	5.561815	5.908638	5.263414	3.685110	2.714360
17	C	6.605619	6.877875	6.397546	4.853577	4.036732
18	H	5.787224	6.181589	5.247472	2.708903	2.357285
19	H	7.577346	7.847285	7.229299	5.055743	4.697430
20	H	6.696905	6.913175	6.700120	5.802939	4.687361
21	N	2.668685	2.085020	2.163837	6.267593	4.772199
22	H	3.568049	2.348155	2.531914	6.964821	5.554576
23	H	3.077954	2.931748	2.418215	5.799347	4.602428
24	C	4.925916	5.838744	4.675927	4.395630	4.455106
25	C	5.300810	5.624493	4.150682	3.866468	4.198128
26	O	4.086291	4.548782	3.372539	4.480073	4.046291
27	H	5.586458	6.536773	5.494958	5.427707	5.524139
28	H	4.700404	5.983329	4.908472	3.958668	3.991683
29	H	5.312074	5.593368	3.994733	2.828020	3.436630
30	C	6.504030	6.441508	4.935267	4.973527	5.514476

31	H	6.603492	6.126736	4.564849	5.141570	5.572802
32	H	7.397103	7.419225	5.842307	5.029419	5.986453
33	H	6.704066	6.701584	5.379286	5.923873	6.273340

		16	17	18	19	20
16	C	0.000000				
17	C	1.326120	0.000000			
18	H	1.089224	2.144895	0.000000		
19	H	2.076151	1.081441	2.472131	0.000000	
20	H	2.130551	1.083323	3.121035	1.847532	0.000000
21	N	6.980998	8.141343	6.974792	9.031413	8.371782
22	H	7.665359	8.791793	7.671382	9.677180	8.994953
23	H	7.050293	8.285713	6.889853	9.105322	8.636932
24	C	7.129333	8.447198	6.531547	8.985572	9.122952
25	C	6.794761	8.110223	6.127728	8.593408	8.838988
26	O	6.744827	8.065273	6.280939	8.707026	8.649106
27	H	8.199925	9.514934	7.607126	10.055548	10.176971
28	H	6.571824	7.861720	5.978344	8.381877	8.543107
29	H	5.897025	7.193575	5.159833	7.613373	7.979499
30	C	8.006130	9.297895	7.305753	9.732974	10.043893
31	H	7.926894	9.183535	7.273785	9.627794	9.898732
32	H	8.354790	9.617970	7.548480	9.943360	10.442203
33	H	8.859968	10.168815	8.212194	10.658794	10.868628

		21	22	23	24	25
21	N	0.000000				
22	H	1.013226	0.000000			
23	H	1.018272	1.643754	0.000000		
24	C	4.385562	5.059209	3.442717	0.000000	
25	C	4.358910	4.865464	3.436520	1.458942	0.000000
26	O	3.060247	3.676777	2.107735	1.444174	1.458986
27	H	4.853352	5.442764	3.875105	1.087711	2.212041
28	H	4.772376	5.581527	3.948079	1.086499	2.202422
29	H	4.707424	5.263150	3.917701	2.171694	1.088428
30	C	5.039623	5.282079	4.104151	2.599413	1.504193
31	H	4.900177	4.981600	4.082963	3.439343	2.149427
32	H	6.098243	6.364782	5.162110	3.136630	2.136550
33	H	5.040683	5.210621	4.069714	2.743260	2.157489

		26	27	28	29	30
26	O	0.000000				
27	H	2.135082	0.000000			
28	H	2.146054	1.841120	0.000000		
29	H	2.138355	3.109022	2.468401	0.000000	
30	C	2.510557	2.830348	3.532616	2.213255	0.000000
31	H	2.932920	3.787586	4.334048	2.567355	1.093742
32	H	3.415337	3.299952	3.925080	2.558004	1.094132

33	H	2.690822	2.570866	3.800693	3.108152	1.092764

	31	32	33
31	H	0.000000	
32	H	1.765421	0.000000
33	H	1.776755	1.778134	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.444427	2.435023	-0.214220
2	6	0	-3.417870	1.518251	0.018413
3	7	0	-2.811080	0.269706	-0.001806
4	6	0	-1.493282	0.435560	-0.226213
5	7	0	-1.254448	1.739165	-0.375031
6	6	0	0.080386	2.325093	-0.577738
7	6	0	0.675914	2.875305	0.724148
8	1	0	-2.493042	3.507966	-0.284062
9	1	0	-4.470998	1.650829	0.186827
10	1	0	0.724330	1.538419	-0.971244
11	1	0	0.002211	3.115242	-1.325866
12	1	0	0.046861	3.691299	1.096222
13	1	0	0.656194	2.073977	1.479645
14	35	0	-0.032569	-2.513277	0.004013
15	1	0	-0.785865	-0.416343	-0.246284
16	6	0	-3.397528	-1.021181	0.179315
17	6	0	-4.701176	-1.223032	0.314781
18	1	0	-2.639515	-1.803147	0.198174
19	1	0	-5.059907	-2.232875	0.459850
20	1	0	-5.442324	-0.433277	0.290795
21	7	0	1.998444	3.401365	0.422008
22	1	0	2.382238	3.906903	1.211793
23	1	0	2.630940	2.634460	0.201365
24	6	0	3.535943	-0.316577	-1.323316
25	6	0	3.389483	-0.714822	0.072558
26	8	0	3.114426	0.656443	-0.342912
27	1	0	4.526688	-0.136030	-1.734342
28	1	0	2.774764	-0.612620	-2.039866

29	1	0	2.492179	-1.278984	0.320030
30	6	0	4.566349	-0.897412	0.991386
31	1	0	4.303196	-0.618576	2.015726
32	1	0	4.864660	-1.950043	1.001496
33	1	0	5.418721	-0.292935	0.671694

Rotational constants (GHZ): 0.4300776 0.2787576 0.1778572

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1303.3155608166 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 3.75D-06 NBF= 482

NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482

Lowest energy guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999827 0.006416 -0.001390 0.017381 Ang= 2.13 deg.

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999769 -0.004423 0.001181 -0.020989 Ang= -2.46 deg.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3205.64769885 A.U. after 10 cycles

NFock= 10 Conv=0.89D-08 -V/T= 2.0018

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000484883	-0.000297775	-0.000521967
2	6	-0.000990936	0.000256408	-0.001053099
3	7	0.001124322	0.000740741	0.001106649
4	6	-0.002614211	-0.001925857	-0.000834124

5	7	0.000193553	-0.000342137	0.001868894
6	6	0.000942929	0.000883509	-0.000121040
7	6	-0.001601110	-0.000180432	0.000339891
8	1	-0.000092268	-0.000023946	-0.000036378
9	1	-0.000003018	-0.000074637	-0.000064713
10	1	0.000278638	-0.000150306	0.000286653
11	1	-0.000311726	-0.000000398	0.000164942
12	1	-0.000044769	-0.000165503	0.000235205
13	1	0.000446301	0.000233263	-0.000356337
14	35	0.000403683	0.000126608	-0.000063845
15	1	0.001206838	0.000507860	-0.000899038
16	6	0.000468717	0.001074074	0.000827727
17	6	-0.000097855	-0.000380556	0.000215730
18	1	-0.000452070	-0.000059161	-0.000308467
19	1	-0.000070290	-0.000015963	-0.000196416
20	1	0.000031111	-0.000014197	-0.000080415
21	7	0.001122987	-0.000255416	-0.000477113
22	1	-0.000378272	0.000297033	0.000033940
23	1	0.000649306	0.000261879	0.000179481
24	6	0.002051083	0.001303330	-0.003598195
25	6	0.000898367	0.000499622	0.004217316
26	8	-0.002533535	-0.002685876	-0.000354467
27	1	0.000068118	-0.000239677	0.000121997
28	1	-0.000298101	0.000336564	0.000076872
29	1	-0.001076806	0.000835995	0.000064156
30	6	-0.000077291	-0.000686583	-0.000683397
31	1	-0.000065798	0.000155343	-0.000170725
32	1	0.000276966	-0.000021159	0.000122072
33	1	0.000060255	0.000007349	-0.000041789

Cartesian Forces: Max 0.004217316 RMS 0.000943845

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.003299743 RMS 0.000652114
Search for a local minimum.
Step number 26 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Update second derivatives using D2CorX and points 21 23 26
ITU= 0 0 -1 1 -1 1 1 1 1 1 1 1 1 0 -1 -1 1 1 1

ITU= -1 1 0 0 -1 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00042	0.00123	0.00241	0.00416	0.00687
Eigenvalues ---	0.00726	0.00799	0.01289	0.01579	0.01858
Eigenvalues ---	0.01964	0.02140	0.02306	0.02326	0.02388
Eigenvalues ---	0.02647	0.02838	0.03010	0.03084	0.03132
Eigenvalues ---	0.03267	0.03521	0.03668	0.03958	0.04058
Eigenvalues ---	0.04303	0.04509	0.05251	0.05440	0.05737
Eigenvalues ---	0.05816	0.05950	0.06717	0.07537	0.08662
Eigenvalues ---	0.09318	0.09691	0.10828	0.12114	0.12479
Eigenvalues ---	0.12763	0.13168	0.14579	0.15794	0.15982
Eigenvalues ---	0.15999	0.16001	0.16006	0.16021	0.16072
Eigenvalues ---	0.16186	0.16763	0.19007	0.22024	0.22174
Eigenvalues ---	0.22847	0.23354	0.24693	0.25932	0.27593
Eigenvalues ---	0.29148	0.29924	0.31661	0.32245	0.32637
Eigenvalues ---	0.33808	0.34280	0.34338	0.34357	0.34550
Eigenvalues ---	0.34681	0.34730	0.35064	0.35179	0.35315
Eigenvalues ---	0.35515	0.35644	0.35888	0.35986	0.36419
Eigenvalues ---	0.36629	0.38743	0.41576	0.42118	0.43216
Eigenvalues ---	0.45475	0.46197	0.47367	0.49386	0.54809
Eigenvalues ---	0.58203	0.60602	1.30416		

RFO step: Lambda=-2.27429776D-04 EMin= 4.23981144D-04

Quartic linear search produced a step of -0.02650.

Iteration 1 RMS(Cart)= 0.03443882 RMS(Int)= 0.00050477

Iteration 2 RMS(Cart)= 0.00148199 RMS(Int)= 0.00022172

Iteration 3 RMS(Cart)= 0.00000116 RMS(Int)= 0.00022172

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00022172

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56487	-0.00002	0.00001	-0.00021	-0.00020	2.56467
R2	2.62266	-0.00029	-0.00001	-0.00045	-0.00046	2.62220
R3	2.03393	-0.00001	0.00000	0.00007	0.00007	2.03401
R4	2.62357	0.00048	0.00004	-0.00003	0.00000	2.62357
R5	2.03092	-0.00001	0.00000	-0.00003	-0.00003	2.03089
R6	2.54550	-0.00035	-0.00004	-0.00027	-0.00031	2.54519
R7	2.70113	-0.00041	-0.00005	0.00016	0.00011	2.70124
R8	2.52020	-0.00021	-0.00001	0.00086	0.00085	2.52105
R9	2.09289	0.00065	0.00008	-0.00057	-0.00049	2.09240
R10	2.78129	0.00054	0.00007	0.00008	0.00015	2.78144
R11	2.89831	-0.00057	0.00003	-0.00156	-0.00153	2.89678
R12	2.06003	0.00020	0.00000	0.00008	0.00009	2.06012
R13	2.06157	-0.00008	-0.00002	0.00032	0.00029	2.06186
R14	2.07009	-0.00002	-0.00001	-0.00003	-0.00005	2.07004
R15	2.08152	-0.00040	-0.00004	0.00019	0.00014	2.08167

R16	2.74961	0.00066	0.00005	0.00034	0.00039	2.75000
R17	4.23705	0.00004	-0.00070	0.00175	0.00104	4.23809
R18	2.50600	0.00022	0.00001	-0.00006	-0.00005	2.50595
R19	2.05834	-0.00032	-0.00004	-0.00017	-0.00021	2.05812
R20	2.04363	-0.00001	0.00000	-0.00003	-0.00003	2.04360
R21	2.04718	-0.00003	0.00000	-0.00010	-0.00010	2.04708
R22	1.91472	0.00007	-0.00001	0.00019	0.00018	1.91490
R23	1.92425	0.00023	0.00004	-0.00150	-0.00134	1.92291
R24	3.98304	0.00024	-0.00091	0.01679	0.01583	3.99887
R25	2.75700	0.00330	0.00043	-0.00424	-0.00451	2.75249
R26	2.72909	0.00009	-0.00015	0.00312	0.00324	2.73233
R27	2.05548	-0.00004	0.00000	-0.00022	-0.00022	2.05525
R28	2.05319	0.00002	0.00001	-0.00017	-0.00016	2.05302
R29	2.75708	-0.00109	-0.00021	0.00136	0.00157	2.75866
R30	2.05683	0.00038	0.00002	-0.00019	-0.00017	2.05666
R31	2.84251	-0.00032	-0.00002	0.00012	0.00010	2.84261
R32	2.06687	-0.00009	-0.00001	0.00019	0.00018	2.06705
R33	2.06761	0.00013	0.00000	0.00026	0.00026	2.06787
R34	2.06502	0.00006	0.00001	-0.00011	-0.00011	2.06492
A1	1.87145	0.00000	0.00002	-0.00022	-0.00020	1.87125
A2	2.28110	-0.00009	-0.00002	0.00032	0.00029	2.28139
A3	2.13061	0.00009	0.00001	-0.00010	-0.00009	2.13052
A4	1.86657	-0.00033	-0.00004	0.00023	0.00019	1.86676
A5	2.27357	0.00023	0.00005	-0.00096	-0.00090	2.27266
A6	2.14302	0.00010	-0.00001	0.00070	0.00069	2.14371
A7	1.89577	0.00023	0.00003	0.00019	0.00023	1.89599
A8	2.25366	-0.00050	0.00001	-0.00041	-0.00039	2.25327
A9	2.13375	0.00027	-0.00004	0.00021	0.00017	2.13392
A10	1.89035	-0.00023	0.00000	-0.00053	-0.00054	1.88981
A11	2.13317	0.00283	0.00023	0.00374	0.00397	2.13714
A12	2.25942	-0.00261	-0.00024	-0.00309	-0.00333	2.25608
A13	1.90035	0.00034	0.00000	0.00038	0.00038	1.90073
A14	2.20680	0.00020	0.00004	-0.00265	-0.00262	2.20418
A15	2.17357	-0.00052	-0.00004	0.00254	0.00251	2.17608
A16	1.95850	0.00070	0.00001	0.00139	0.00142	1.95992
A17	1.87357	-0.00024	0.00006	-0.00255	-0.00250	1.87107
A18	1.89420	-0.00022	-0.00008	-0.00078	-0.00087	1.89334
A19	1.91339	-0.00048	0.00005	-0.00112	-0.00108	1.91231
A20	1.92847	-0.00005	0.00000	0.00099	0.00098	1.92945
A21	1.89384	0.00028	-0.00003	0.00203	0.00200	1.89584
A22	1.90982	0.00046	-0.00004	0.00208	0.00204	1.91186
A23	1.89049	0.00044	0.00005	-0.00030	-0.00024	1.89025
A24	1.88217	-0.00121	0.00002	-0.00271	-0.00272	1.87946
A25	1.87409	-0.00017	0.00001	0.00097	0.00097	1.87506

A26	1.89987	0.00077	0.00012	-0.00159	-0.00147	1.89840
A27	2.00614	-0.00024	-0.00016	0.00169	0.00155	2.00768
A28	2.15764	0.00029	0.00007	0.00009	0.00016	2.15781
A29	1.94446	0.00014	0.00003	0.00014	0.00017	1.94462
A30	2.18106	-0.00043	-0.00010	-0.00023	-0.00033	2.18073
A31	2.07365	0.00010	0.00002	0.00018	0.00020	2.07386
A32	2.16437	-0.00007	-0.00003	0.00009	0.00006	2.16443
A33	2.04516	-0.00002	0.00001	-0.00027	-0.00026	2.04490
A34	1.94209	0.00054	-0.00005	-0.00303	-0.00284	1.93925
A35	1.91482	-0.00175	0.00012	-0.00336	-0.00315	1.91168
A36	1.88535	0.00080	0.00001	0.00175	0.00166	1.88701
A37	2.09243	-0.00067	-0.00007	-0.01533	-0.01518	2.07725
A38	2.07863	0.00083	0.00015	0.01089	0.01079	2.08942
A39	1.99385	0.00160	0.00014	0.00460	0.00447	1.99833
A40	2.01177	-0.00111	-0.00008	-0.00544	-0.00535	2.00641
A41	2.01988	0.00005	-0.00004	0.00327	0.00325	2.02313
A42	2.02838	0.00058	0.00041	-0.00178	-0.00192	2.02646
A43	2.14008	-0.00110	-0.00031	-0.00593	-0.00572	2.13436
A44	1.97848	-0.00155	-0.00007	-0.00925	-0.00924	1.96924
A45	2.02143	0.00142	0.00015	0.00587	0.00581	2.02725
A46	2.02996	0.00054	-0.00007	0.00642	0.00638	2.03635
A47	2.63529	-0.00051	-0.00023	-0.00083	-0.00271	2.63258
A48	2.59010	-0.00124	-0.00019	-0.00626	-0.00789	2.58221
A49	1.93146	-0.00025	-0.00004	-0.00009	-0.00013	1.93133
A50	1.91319	0.00045	0.00003	0.00173	0.00176	1.91495
A51	1.94381	-0.00007	0.00000	-0.00064	-0.00064	1.94317
A52	1.87781	0.00000	0.00000	0.00070	0.00070	1.87851
A53	1.89720	0.00005	-0.00001	-0.00080	-0.00080	1.89639
A54	1.89887	-0.00018	0.00001	-0.00089	-0.00088	1.89799
A55	3.42052	-0.00149	-0.00119	0.01898	0.01778	3.43830
A56	2.70331	-0.00258	0.00226	-0.03676	-0.03505	2.66826
A57	2.84508	0.00077	-0.00046	0.02461	0.02415	2.86923
A58	3.11852	-0.00031	0.00075	-0.02251	-0.02193	3.09660
D1	0.00073	0.00016	0.00009	-0.00275	-0.00265	-0.00192
D2	-3.13347	-0.00013	-0.00009	0.00087	0.00078	-3.13270
D3	3.13587	0.00022	0.00013	-0.00363	-0.00350	3.13237
D4	0.00167	-0.00007	-0.00005	-0.00002	-0.00007	0.00160
D5	-0.01431	0.00034	0.00014	0.00345	0.00359	-0.01072
D6	-3.08293	0.00003	0.00001	-0.00060	-0.00058	-3.08351
D7	3.13306	0.00029	0.00010	0.00424	0.00434	3.13740
D8	0.06444	-0.00002	-0.00003	0.00019	0.00017	0.06461
D9	0.01293	-0.00060	-0.00029	0.00114	0.00085	0.01378
D10	-3.13302	-0.00027	-0.00022	0.00123	0.00102	-3.13200
D11	-3.13537	-0.00034	-0.00012	-0.00215	-0.00227	-3.13764

D12	0.00186	-0.00001	-0.00005	-0.00205	-0.00211	-0.00025
D13	-0.02199	0.00082	0.00038	0.00102	0.00140	-0.02060
D14	3.09808	0.00044	0.00005	0.00618	0.00625	3.10433
D15	3.12360	0.00052	0.00031	0.00094	0.00124	3.12485
D16	-0.03951	0.00015	-0.00001	0.00609	0.00610	-0.03342
D17	0.08441	-0.00009	0.00030	-0.01349	-0.01320	0.07121
D18	-3.04979	-0.00039	0.00019	-0.01408	-0.01389	-3.06368
D19	-3.06207	0.00027	0.00037	-0.01339	-0.01301	-3.07508
D20	0.08691	-0.00002	0.00027	-0.01398	-0.01371	0.07321
D21	0.02247	-0.00072	-0.00032	-0.00275	-0.00307	0.01940
D22	3.09280	-0.00038	-0.00019	0.00094	0.00076	3.09356
D23	-3.09554	-0.00040	0.00003	-0.00852	-0.00848	-3.10402
D24	-0.02521	-0.00006	0.00016	-0.00483	-0.00465	-0.02986
D25	1.34069	0.00039	0.00257	-0.03831	-0.03574	1.30495
D26	-2.83916	0.00007	0.00268	-0.04054	-0.03786	-2.87703
D27	-0.79546	0.00015	0.00263	-0.03993	-0.03730	-0.83277
D28	-1.71706	0.00000	0.00242	-0.04283	-0.04041	-1.75747
D29	0.38627	-0.00033	0.00252	-0.04506	-0.04253	0.34374
D30	2.42997	-0.00024	0.00248	-0.04444	-0.04197	2.38800
D31	-1.09904	-0.00021	0.00005	0.00233	0.00238	-1.09666
D32	0.93889	0.00009	0.00007	0.00446	0.00453	0.94342
D33	3.12011	-0.00069	-0.00008	0.00464	0.00457	3.12468
D34	3.10402	-0.00003	-0.00006	0.00539	0.00533	3.10935
D35	-1.14123	0.00027	-0.00004	0.00752	0.00748	-1.13376
D36	1.03999	-0.00052	-0.00019	0.00770	0.00751	1.04750
D37	1.01756	-0.00004	-0.00005	0.00298	0.00293	1.02049
D38	3.05549	0.00025	-0.00003	0.00511	0.00508	3.06057
D39	-1.04648	-0.00053	-0.00018	0.00529	0.00512	-1.04136
D40	2.98769	0.00018	-0.00192	0.02191	0.01993	3.00762
D41	-1.21011	0.00037	-0.00186	0.01999	0.01818	-1.19193
D42	0.91728	-0.00012	-0.00195	0.02184	0.01984	0.93712
D43	3.00267	0.00007	-0.00189	0.01993	0.01809	3.02076
D44	-1.18509	-0.00031	-0.00195	0.02064	0.01864	-1.16645
D45	0.90030	-0.00012	-0.00189	0.01873	0.01689	0.91719
D46	-3.12881	-0.00035	-0.00009	-0.00164	-0.00173	-3.13054
D47	0.01150	-0.00010	-0.00001	-0.00150	-0.00152	0.00998
D48	0.00439	-0.00001	0.00003	-0.00097	-0.00094	0.00345
D49	-3.13849	0.00024	0.00011	-0.00083	-0.00072	-3.13921
D50	1.80678	0.00076	-0.00323	0.06082	0.05801	1.86479
D51	-1.03243	0.00031	0.00553	-0.07876	-0.07340	-1.10583
D52	-2.43275	-0.00006	-0.00281	0.05114	0.04850	-2.38425
D53	1.01122	-0.00052	0.00596	-0.08844	-0.08291	0.92831
D54	-2.69858	-0.00059	-0.00019	0.00336	0.00326	-2.69533
D55	-0.00415	-0.00036	-0.00014	0.00185	0.00181	-0.00234

D56	-0.02404	-0.00008	-0.00010	0.00149	0.00140	-0.02264
D57	2.67039	0.00014	-0.00006	-0.00003	-0.00004	2.67035
D58	1.08030	0.00020	0.00741	-0.09217	-0.08466	0.99563
D59	-1.32205	-0.00047	0.00739	-0.09650	-0.08892	-1.41097
D60	1.36329	0.00003	-0.00719	0.09985	0.09207	1.45536
D61	-1.04844	-0.00067	-0.00716	0.09360	0.08596	-0.96249
D62	2.56435	-0.00024	-0.00020	-0.00038	-0.00048	2.56387
D63	-1.65042	-0.00011	-0.00021	0.00150	0.00140	-1.64902
D64	0.45186	-0.00007	-0.00017	0.00112	0.00106	0.45292
D65	1.36517	-0.00014	-0.00006	-0.00402	-0.00415	1.36102
D66	-2.84961	-0.00002	-0.00006	-0.00213	-0.00227	-2.85187
D67	-0.74732	0.00002	-0.00003	-0.00251	-0.00261	-0.74993
D68	-1.02478	0.00000	-0.00004	-0.00385	-0.00392	-1.02870
D69	1.04363	0.00013	-0.00004	-0.00196	-0.00203	1.04160
D70	-3.13727	0.00016	-0.00001	-0.00234	-0.00238	-3.13965

Item	Value	Threshold	Converged?
Maximum Force	0.003300	0.000450	NO
RMS Force	0.000652	0.000300	NO
Maximum Displacement	0.141079	0.001800	NO
RMS Displacement	0.034849	0.001200	NO

Predicted change in Energy=-1.178546D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.663413	2.081051	-0.259313
2	6	0	-3.562183	1.114561	0.056916
3	7	0	-2.860262	-0.080582	0.136996
4	6	0	-1.559504	0.166982	-0.109498
5	7	0	-1.422795	1.468864	-0.366763
6	6	0	-0.139479	2.140728	-0.627748
7	6	0	0.385643	2.889572	0.602413
8	1	0	-2.795662	3.136867	-0.421455
9	1	0	-4.622649	1.179331	0.218776
10	1	0	0.574699	1.370074	-0.918453
11	1	0	-0.272347	2.826638	-1.465814
12	1	0	-0.316391	3.685292	0.874291
13	1	0	0.426332	2.182792	1.446373
14	35	0	0.122408	-2.643914	0.285244
15	1	0	-0.786197	-0.624487	-0.069815
16	6	0	-3.345181	-1.393086	0.429350

17	6	0	-4.627971	-1.680117	0.604221
18	1	0	-2.530326	-2.112743	0.494703
19	1	0	-4.907697	-2.699416	0.832835
20	1	0	-5.426929	-0.952008	0.533559
21	7	0	1.660182	3.492495	0.242197
22	1	0	1.994975	4.104691	0.977010
23	1	0	2.353669	2.761816	0.098613
24	6	0	3.434158	-0.255784	-1.181505
25	6	0	3.342326	-0.531585	0.245748
26	8	0	2.927093	0.761987	-0.288408
27	1	0	4.406645	-0.032272	-1.614137
28	1	0	2.698349	-0.678216	-1.860054
29	1	0	2.502330	-1.147380	0.561469
30	6	0	4.547877	-0.521357	1.145358
31	1	0	4.279681	-0.170283	2.146007
32	1	0	4.942663	-1.537034	1.245219
33	1	0	5.335072	0.123891	0.747879

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357163	0.000000			
3	N	2.206460	1.388334	0.000000		
4	C	2.214660	2.221783	1.346855	0.000000	
5	N	1.387606	2.209528	2.172756	1.334081	0.000000
6	C	2.551381	3.638226	3.594678	2.486108	1.471875
7	C	3.270019	4.362747	4.424288	3.420952	2.495629
8	H	1.076350	2.214976	3.266193	3.231969	2.161016
9	H	2.209134	1.074701	2.167966	3.242756	3.265846
10	H	3.380137	4.257984	3.875221	2.580051	2.074634
11	H	2.780062	4.009107	4.209303	3.251175	2.091649
12	H	3.060581	4.220417	4.603986	3.858973	2.770721
13	H	3.530756	4.356600	4.199885	3.229206	2.686341
14	Br	5.512044	5.268252	3.935604	3.299362	4.441589
15	H	3.298452	3.278177	2.154148	1.107250	2.208066
16	C	3.606756	2.544423	1.429435	2.431627	3.538379
17	C	4.330308	3.040670	2.429323	3.651939	4.596961
18	H	4.263116	3.416412	2.089615	2.550431	3.846642
19	H	5.392815	4.118115	3.396244	4.507174	5.564003
20	H	4.179128	2.824035	2.739420	4.077086	4.764902
21	N	4.575714	5.741254	5.763017	4.642102	3.737735
22	H	5.227255	6.377261	6.464941	5.414830	4.520450
23	H	5.075693	6.141050	5.938499	4.699936	4.018704
24	C	6.594817	7.236043	6.433418	5.124900	5.218066

25	C	6.568854	7.100542	6.219914	4.964084	5.204166
26	O	5.744086	6.508015	5.863819	4.529414	4.407646
27	H	7.502492	8.222521	7.475074	6.156182	6.147497
28	H	6.238943	6.788452	5.936626	4.680611	4.880952
29	H	6.146653	6.492247	5.484126	4.321602	4.807594
30	C	7.794121	8.344699	7.489433	6.272845	6.472744
31	H	7.685090	8.216444	7.417746	6.268742	6.443528
32	H	8.556082	8.987515	8.014677	6.856902	7.221701
33	H	8.295822	8.978864	8.220613	6.947815	6.979982

		6	7	8	9	10
6	C	0.000000				
7	C	1.532910	0.000000			
8	H	2.844320	3.351144	0.000000		
9	H	4.662585	5.306137	2.753130	0.000000	
10	H	1.090169	2.158158	3.837695	5.323730	0.000000
11	H	1.091092	2.171284	2.748462	4.947382	1.771630
12	H	2.161734	1.095418	2.850703	5.025275	3.060752
13	H	2.150322	1.101572	3.844513	5.292082	2.504980
14	Br	4.878006	5.548816	6.513984	6.094029	4.214920
15	H	2.894123	3.764799	4.278947	4.249166	2.559394
16	C	4.886903	5.682443	4.641802	2.879861	4.981675
17	C	6.021891	6.783686	5.254780	2.885315	6.220127
18	H	5.006802	5.791168	5.335556	3.910461	4.875265
19	H	6.949547	7.701255	6.332151	3.937385	7.048718
20	H	6.234643	6.967674	4.955252	2.299687	6.596965
21	N	2.413060	1.455239	4.519010	6.695165	2.651425
22	H	3.314859	2.051045	5.083561	7.274998	3.617747
23	H	2.670044	2.035500	5.189098	7.154558	2.477116
24	C	4.338295	4.729595	7.134312	8.302559	3.299866
25	C	4.475178	4.535801	7.181754	8.146704	3.554072
26	O	3.379341	3.432076	6.197393	7.578259	2.510076
27	H	5.134407	5.442308	7.958590	9.292776	4.139367
28	H	4.185486	4.913395	6.841679	7.833838	3.097094
29	H	4.382356	4.558401	6.884013	7.503089	3.499072
30	C	5.674673	5.408642	8.352549	9.372803	4.860346
31	H	5.706440	5.187381	8.221288	9.207994	5.048812
32	H	6.546916	6.385488	9.192650	9.996370	5.675549
33	H	5.994221	5.671595	8.749525	10.027467	5.195265

		11	12	13	14	15
11	H	0.000000				
12	H	2.493053	0.000000			
13	H	3.063253	1.770994	0.000000		
14	Br	5.757515	6.371685	4.973699	0.000000	
15	H	3.758074	4.436919	3.413191	2.242703	0.000000

16	C	5.553380	5.929710	5.295805	3.689107	2.718145
17	C	6.600557	6.888416	6.416952	4.857649	4.040781
18	H	5.774044	6.217942	5.300861	2.713488	2.361265
19	H	7.570174	7.864242	7.257014	5.060128	4.701794
20	H	6.696669	6.909287	6.702303	5.806837	4.691239
21	N	2.663707	2.084120	2.165120	6.326304	4.799131
22	H	3.569532	2.351353	2.524804	7.037664	5.585328
23	H	3.057383	2.929796	2.422055	5.851092	4.621058
24	C	4.829113	5.815926	4.679681	4.338457	4.379862
25	C	5.222353	5.618125	4.160813	3.851151	4.141607
26	O	3.985660	4.518602	3.358862	4.449213	3.969712
27	H	5.485283	6.505353	5.487815	5.364980	5.449885
28	H	4.611340	5.967034	4.927462	3.886096	3.917895
29	H	5.253716	5.603370	4.022794	2.824879	3.389151
30	C	6.423539	6.436651	4.938640	4.982953	5.471712
31	H	6.538176	6.132421	4.568889	5.183069	5.547908
32	H	7.320359	7.420776	5.854470	5.038014	5.948268
33	H	6.606695	6.681211	5.368677	5.920020	6.220822

		16	17	18	19	20
16	C	0.000000				
17	C	1.326091	0.000000			
18	H	1.089112	2.144592	0.000000		
19	H	2.076235	1.081425	2.471924	0.000000	
20	H	2.130513	1.083268	3.120757	1.847323	0.000000
21	N	6.996970	8.150328	7.003057	9.045753	8.370522
22	H	7.683928	8.801500	7.705028	9.693479	8.991747
23	H	7.060417	8.290338	6.911702	9.115458	8.632460
24	C	7.060294	8.379468	6.467847	8.922749	9.052350
25	C	6.745268	8.060600	6.086878	8.550265	8.784044
26	O	6.670902	7.989972	6.217777	8.638427	8.567560
27	H	8.131326	9.447793	7.543019	9.992912	10.107309
28	H	6.502051	7.794320	5.911158	8.317982	8.474933
29	H	5.854162	7.150303	5.124843	7.575682	7.931715
30	C	7.973264	9.264543	7.284012	9.708218	10.002826
31	H	7.910795	9.165313	7.271599	9.619191	9.870631
32	H	8.329149	9.593143	7.532615	9.927275	10.410435
33	H	8.817566	10.126071	8.181144	10.625092	10.817770

		21	22	23	24	25
21	N	0.000000				
22	H	1.013322	0.000000			
23	H	1.017561	1.644249	0.000000		
24	C	4.384462	5.073871	3.451387	0.000000	
25	C	4.361518	4.883150	3.441741	1.456555	0.000000
26	O	3.056514	3.693751	2.116109	1.445889	1.459818

27	H	4.838699	5.444690	3.867189	1.087593	2.200287
28	H	4.784566	5.605342	3.973538	1.086413	2.206946
29	H	4.726477	5.292856	3.939308	2.168226	1.088336
30	C	5.026479	5.286394	4.085272	2.593297	1.504246
31	H	4.888988	4.986164	4.061840	3.434320	2.149455
32	H	6.089080	6.371017	5.147592	3.131481	2.137977
33	H	5.010790	5.201491	4.033479	2.734986	2.157040

		26	27	28	29	30
26	O	0.000000				
27	H	2.139504	0.000000			
28	H	2.143963	1.842822	0.000000		
29	H	2.132697	3.098894	2.474331	0.000000	
30	C	2.515869	2.806058	3.532402	2.217452	0.000000
31	H	2.936834	3.764817	4.336719	2.573802	1.093837
32	H	3.420530	3.275292	3.926479	2.564092	1.094270
33	H	2.698040	2.542731	3.794338	3.110515	1.092708

		31	32	33
31	H	0.000000		
32	H	1.766062	0.000000	
33	H	1.776274	1.777640	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.386837	2.455767	-0.228925
2	6	0	-3.375063	1.557881	0.014181
3	7	0	-2.788674	0.299467	0.010577
4	6	0	-1.468083	0.440732	-0.213256
5	7	0	-1.207811	1.739021	-0.375974
6	6	0	0.135191	2.304302	-0.583865
7	6	0	0.715649	2.911114	0.698578
8	1	0	-2.418267	3.528185	-0.315306
9	1	0	-4.426407	1.710239	0.176801
10	1	0	0.777134	1.492650	-0.926791
11	1	0	0.075345	3.057535	-1.370974
12	1	0	0.088324	3.747857	1.024564
13	1	0	0.681714	2.145391	1.489766

14	35	0	-0.060093	-2.536573	-0.015765
15	1	0	-0.772516	-0.420646	-0.227948
16	6	0	-3.396959	-0.979178	0.206392
17	6	0	-4.702633	-1.156227	0.356013
18	1	0	-2.653577	-1.774970	0.222593
19	1	0	-5.078609	-2.158435	0.509966
20	1	0	-5.429346	-0.353155	0.335174
21	7	0	2.044464	3.415818	0.386736
22	1	0	2.427618	3.940044	1.164682
23	1	0	2.668071	2.635339	0.193352
24	6	0	3.474719	-0.371612	-1.296492
25	6	0	3.343277	-0.738416	0.106978
26	8	0	3.056037	0.623135	-0.334318
27	1	0	4.468102	-0.210170	-1.708782
28	1	0	2.709483	-0.673751	-2.006013
29	1	0	2.446326	-1.293529	0.374939
30	6	0	4.535469	-0.905436	1.008943
31	1	0	4.291256	-0.602821	2.031324
32	1	0	4.832646	-1.958209	1.036943
33	1	0	5.383420	-0.310301	0.661376

Rotational constants (GHZ): 0.4257458 0.2831825 0.1787776

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1305.5254000361 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 3.67D-06 NBF= 482

NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999982 0.002510 -0.000414 0.005524 Ang= 0.70 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3205.64781609 A.U. after 11 cycles
NFock= 11 Conv=0.62D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000474024	-0.000422684	-0.000298922
2	6	-0.001173519	0.000317983	-0.001297529
3	7	0.000967685	0.000432039	0.001209819
4	6	-0.002117393	-0.000764211	-0.000733883
5	7	-0.000053457	-0.000269051	0.001875200
6	6	0.000450790	0.000191272	-0.000585996
7	6	-0.001833182	-0.000213985	-0.000130835
8	1	-0.000100602	-0.000059339	0.000078433
9	1	-0.000009954	-0.000182830	-0.000042721
10	1	0.000420494	0.000131260	0.000198969
11	1	-0.000186840	0.000096949	0.000230861
12	1	-0.000143303	-0.000188306	0.000354205
13	1	0.000521682	0.000309624	-0.000280216
14	35	0.000377293	0.000095043	-0.000012019
15	1	0.000906439	0.000222715	-0.000836736
16	6	0.000535691	0.001103451	0.000786944
17	6	-0.000127183	-0.000400759	0.000198395
18	1	-0.000414844	-0.000075783	-0.000359125
19	1	-0.000050409	-0.000024468	-0.000166398
20	1	-0.000003437	0.000005485	-0.000086956
21	7	0.000774679	-0.000033926	0.000129928
22	1	-0.000104417	0.000322397	-0.000106672
23	1	0.001259550	0.000103360	0.000062025

24	6	0.001887956	0.001718113	-0.004488832
25	6	-0.001121225	-0.000576570	0.004665356
26	8	-0.000060686	-0.002535639	-0.000253979
27	1	-0.000331846	0.000750645	-0.000701603
28	1	0.000038335	-0.000406769	0.000493462
29	1	-0.000438513	0.000269044	0.000453447
30	6	-0.000523068	-0.000086312	-0.000139553
31	1	0.000060773	0.000053947	-0.000135090
32	1	0.000005594	0.000044506	-0.000020316
33	1	0.000112895	0.000072798	-0.000059661

Cartesian Forces: Max 0.004665356 RMS 0.000932727

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.004750345 RMS 0.000593233
Search for a local minimum.
Step number 27 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 25 26 27
DE= -1.17D-04 DEPred=-1.18D-04 R= 9.95D-01
TightC=F SS= 1.41D+00 RLast= 2.55D-01 DXNew= 7.0965D-01 7.6649D-01
Trust test= 9.95D-01 RLast= 2.55D-01 DXMaxT set to 7.10D-01
ITU= 1 0 0 -1 1 -1 1 1 1 1 1 1 1 1 0 -1 -1 1 1
ITU= 1 -1 1 0 0 -1 0

Eigenvalues ---	0.00103	0.00123	0.00247	0.00416	0.00679
Eigenvalues ---	0.00727	0.00785	0.01326	0.01557	0.01874
Eigenvalues ---	0.01957	0.02175	0.02355	0.02387	0.02455
Eigenvalues ---	0.02603	0.02908	0.03031	0.03092	0.03136
Eigenvalues ---	0.03336	0.03510	0.03723	0.03961	0.04069
Eigenvalues ---	0.04388	0.04488	0.05148	0.05443	0.05741
Eigenvalues ---	0.05810	0.05936	0.07263	0.08615	0.08890
Eigenvalues ---	0.09257	0.09639	0.10790	0.12201	0.12367
Eigenvalues ---	0.12653	0.13353	0.15240	0.15692	0.15973
Eigenvalues ---	0.16000	0.16002	0.16004	0.16019	0.16082
Eigenvalues ---	0.16323	0.18174	0.20975	0.22071	0.22228
Eigenvalues ---	0.22933	0.23221	0.24865	0.25731	0.27226
Eigenvalues ---	0.29037	0.30148	0.31580	0.31738	0.32748
Eigenvalues ---	0.33675	0.34283	0.34343	0.34365	0.34551

Eigenvalues --- 0.34686 0.34732 0.35076 0.35208 0.35350
Eigenvalues --- 0.35522 0.35588 0.35755 0.35892 0.36419
Eigenvalues --- 0.36625 0.38793 0.41277 0.41989 0.42668
Eigenvalues --- 0.45408 0.45498 0.46567 0.49517 0.54812
Eigenvalues --- 0.58025 0.60601 1.14647
En-DIIS/RFO-DIIS IScMMF= 0 using points: 27 26
RFO step: Lambda=-1.07111597D-04.
DidBck=F Rises=F RFO-DIIS coefs: 0.97842 0.02158
Iteration 1 RMS(Cart)= 0.05934864 RMS(Int)= 0.00137937
Iteration 2 RMS(Cart)= 0.00302897 RMS(Int)= 0.00017517
Iteration 3 RMS(Cart)= 0.00000417 RMS(Int)= 0.00017516
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00017516

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56467	0.00011	0.00000	0.00001	0.00003	2.56469
R2	2.62220	-0.00008	0.00001	-0.00069	-0.00066	2.62153
R3	2.03401	-0.00006	0.00000	-0.00008	-0.00008	2.03392
R4	2.62357	0.00038	0.00000	0.00121	0.00120	2.62477
R5	2.03089	-0.00001	0.00000	-0.00002	-0.00002	2.03087
R6	2.54519	-0.00027	0.00001	-0.00122	-0.00124	2.54395
R7	2.70124	-0.00045	0.00000	-0.00160	-0.00161	2.69964
R8	2.52105	-0.00063	-0.00002	-0.00032	-0.00034	2.52071
R9	2.09240	0.00065	0.00001	0.00056	0.00057	2.09297
R10	2.78144	0.00076	0.00000	0.00288	0.00288	2.78432
R11	2.89678	-0.00031	0.00003	-0.00182	-0.00178	2.89500
R12	2.06012	0.00013	0.00000	0.00040	0.00039	2.06052
R13	2.06186	-0.00009	-0.00001	-0.00030	-0.00030	2.06156
R14	2.07004	0.00004	0.00000	-0.00016	-0.00016	2.06988
R15	2.08167	-0.00039	0.00000	-0.00145	-0.00146	2.08021
R16	2.75000	0.00128	-0.00001	0.00484	0.00483	2.75483
R17	4.23809	0.00007	-0.00002	0.00288	0.00285	4.24095
R18	2.50595	0.00026	0.00000	0.00048	0.00048	2.50643
R19	2.05812	-0.00028	0.00000	-0.00112	-0.00112	2.05701
R20	2.04360	0.00000	0.00000	-0.00002	-0.00002	2.04358
R21	2.04708	0.00001	0.00000	0.00002	0.00002	2.04710
R22	1.91490	0.00008	0.00000	0.00034	0.00034	1.91524
R23	1.92291	0.00103	0.00003	0.00175	0.00195	1.92487
R24	3.99887	0.00058	-0.00034	0.01677	0.01635	4.01521
R25	2.75249	0.00475	0.00010	0.00565	0.00532	2.75781
R26	2.73233	-0.00002	-0.00007	-0.00066	-0.00057	2.73177
R27	2.05525	0.00014	0.00000	0.00030	0.00031	2.05556
R28	2.05302	-0.00018	0.00000	0.00038	0.00038	2.05341
R29	2.75866	-0.00134	-0.00003	0.00237	0.00259	2.76125
R30	2.05666	0.00032	0.00000	0.00058	0.00058	2.05724

R31	2.84261	-0.00049	0.00000	-0.00203	-0.00203	2.84058
R32	2.06705	-0.00012	0.00000	-0.00048	-0.00049	2.06656
R33	2.06787	-0.00004	-0.00001	-0.00019	-0.00020	2.06768
R34	2.06492	0.00015	0.00000	0.00057	0.00057	2.06549
A1	1.87125	0.00013	0.00000	0.00126	0.00126	1.87250
A2	2.28139	-0.00018	-0.00001	-0.00143	-0.00143	2.27996
A3	2.13052	0.00006	0.00000	0.00019	0.00019	2.13071
A4	1.86676	-0.00047	0.00000	-0.00188	-0.00194	1.86482
A5	2.27266	0.00042	0.00002	0.00299	0.00300	2.27566
A6	2.14371	0.00006	-0.00001	-0.00099	-0.00101	2.14270
A7	1.89599	0.00019	0.00000	0.00132	0.00124	1.89723
A8	2.25327	-0.00034	0.00001	-0.00204	-0.00202	2.25125
A9	2.13392	0.00015	0.00000	0.00076	0.00077	2.13469
A10	1.88981	0.00005	0.00001	-0.00012	-0.00017	1.88964
A11	2.13714	0.00213	-0.00009	0.01005	0.00998	2.14713
A12	2.25608	-0.00218	0.00007	-0.01007	-0.00998	2.24610
A13	1.90073	0.00013	-0.00001	-0.00007	-0.00016	1.90057
A14	2.20418	0.00061	0.00006	-0.00351	-0.00352	2.20066
A15	2.17608	-0.00072	-0.00005	0.00492	0.00481	2.18088
A16	1.95992	0.00023	-0.00003	0.00509	0.00509	1.96501
A17	1.87107	0.00015	0.00005	0.00066	0.00071	1.87178
A18	1.89334	-0.00004	0.00002	-0.00369	-0.00368	1.88965
A19	1.91231	-0.00046	0.00002	-0.00117	-0.00116	1.91115
A20	1.92945	-0.00003	-0.00002	-0.00371	-0.00374	1.92571
A21	1.89584	0.00018	-0.00004	0.00294	0.00290	1.89874
A22	1.91186	-0.00005	-0.00004	0.00164	0.00160	1.91346
A23	1.89025	0.00037	0.00001	0.00328	0.00329	1.89354
A24	1.87946	-0.00008	0.00006	-0.00422	-0.00420	1.87525
A25	1.87506	-0.00007	-0.00002	0.00174	0.00171	1.87677
A26	1.89840	0.00050	0.00003	0.00088	0.00093	1.89933
A27	2.00768	-0.00066	-0.00003	-0.00308	-0.00310	2.00458
A28	2.15781	0.00035	0.00000	0.00163	0.00161	2.15941
A29	1.94462	0.00009	0.00000	0.00195	0.00192	1.94655
A30	2.18073	-0.00044	0.00001	-0.00351	-0.00352	2.17721
A31	2.07386	0.00006	0.00000	0.00074	0.00073	2.07459
A32	2.16443	-0.00005	0.00000	-0.00085	-0.00085	2.16358
A33	2.04490	-0.00001	0.00001	0.00012	0.00012	2.04502
A34	1.93925	0.00009	0.00006	-0.00051	-0.00031	1.93894
A35	1.91168	-0.00009	0.00007	0.00243	0.00255	1.91422
A36	1.88701	0.00004	-0.00004	-0.00022	-0.00031	1.88671
A37	2.07725	0.00110	0.00033	0.00568	0.00649	2.08374
A38	2.08942	-0.00055	-0.00023	-0.00160	-0.00235	2.08707
A39	1.99833	0.00028	-0.00010	-0.00302	-0.00337	1.99496
A40	2.00641	0.00042	0.00012	0.00132	0.00160	2.00801

A41	2.02313	-0.00020	-0.00007	-0.00215	-0.00221	2.02091
A42	2.02646	0.00013	0.00004	0.00346	0.00296	2.02942
A43	2.13436	0.00021	0.00012	0.00215	0.00276	2.13711
A44	1.96924	0.00023	0.00020	-0.00693	-0.00656	1.96268
A45	2.02725	0.00007	-0.00013	-0.00086	-0.00126	2.02598
A46	2.03635	-0.00016	-0.00014	0.00005	-0.00011	2.03624
A47	2.63258	-0.00109	0.00006	-0.00611	-0.00673	2.62585
A48	2.58221	-0.00116	0.00017	-0.00821	-0.00877	2.57344
A49	1.93133	0.00002	0.00000	-0.00137	-0.00137	1.92997
A50	1.91495	0.00002	-0.00004	0.00102	0.00098	1.91593
A51	1.94317	-0.00002	0.00001	0.00038	0.00040	1.94357
A52	1.87851	0.00003	-0.00002	-0.00029	-0.00030	1.87821
A53	1.89639	-0.00003	0.00002	0.00021	0.00023	1.89663
A54	1.89799	-0.00002	0.00002	0.00003	0.00005	1.89803
A55	3.43830	-0.00145	-0.00038	-0.01595	-0.01633	3.42197
A56	2.66826	-0.00045	0.00076	-0.03129	-0.03139	2.63686
A57	2.86923	0.00054	-0.00052	-0.01757	-0.01809	2.85114
A58	3.09660	0.00047	0.00047	-0.00198	-0.00176	3.09484
D1	-0.00192	0.00028	0.00006	0.00594	0.00601	0.00408
D2	-3.13270	-0.00006	-0.00002	-0.00708	-0.00712	-3.13981
D3	3.13237	0.00026	0.00008	0.00906	0.00915	3.14152
D4	0.00160	-0.00008	0.00000	-0.00396	-0.00398	-0.00238
D5	-0.01072	0.00017	-0.00008	0.00823	0.00814	-0.00258
D6	-3.08351	-0.00009	0.00001	-0.01292	-0.01287	-3.09638
D7	3.13740	0.00019	-0.00009	0.00545	0.00533	-3.14045
D8	0.06461	-0.00007	0.00000	-0.01570	-0.01567	0.04894
D9	0.01378	-0.00064	-0.00002	-0.01796	-0.01799	-0.00421
D10	-3.13200	-0.00030	-0.00002	-0.00738	-0.00741	-3.13942
D11	-3.13764	-0.00032	0.00005	-0.00610	-0.00607	3.13947
D12	-0.00025	0.00003	0.00005	0.00449	0.00451	0.00426
D13	-0.02060	0.00074	-0.00003	0.02324	0.02323	0.00263
D14	3.10433	0.00045	-0.00013	0.01525	0.01508	3.11941
D15	3.12485	0.00043	-0.00003	0.01354	0.01351	3.13836
D16	-0.03342	0.00014	-0.00013	0.00554	0.00536	-0.02806
D17	0.07121	-0.00012	0.00028	0.01334	0.01364	0.08485
D18	-3.06368	-0.00043	0.00030	0.00101	0.00131	-3.06238
D19	-3.07508	0.00026	0.00028	0.02520	0.02549	-3.04959
D20	0.07321	-0.00004	0.00030	0.01288	0.01316	0.08637
D21	0.01940	-0.00057	0.00007	-0.01953	-0.01946	-0.00006
D22	3.09356	-0.00025	-0.00002	0.00079	0.00085	3.09441
D23	-3.10402	-0.00031	0.00018	-0.01108	-0.01097	-3.11499
D24	-0.02986	0.00001	0.00010	0.00924	0.00934	-0.02052
D25	1.30495	0.00036	0.00077	0.01780	0.01857	1.32353
D26	-2.87703	0.00002	0.00082	0.01984	0.02067	-2.85636

D27	-0.83277	0.00028	0.00081	0.02174	0.02254	-0.81022
D28	-1.75747	0.00002	0.00087	-0.00628	-0.00542	-1.76289
D29	0.34374	-0.00032	0.00092	-0.00424	-0.00332	0.34042
D30	2.38800	-0.00006	0.00091	-0.00234	-0.00145	2.38655
D31	-1.09666	0.00000	-0.00005	0.02710	0.02705	-1.06961
D32	0.94342	0.00009	-0.00010	0.03194	0.03186	0.97528
D33	3.12468	-0.00053	-0.00010	0.02756	0.02747	-3.13104
D34	3.10935	-0.00002	-0.00011	0.02383	0.02370	3.13305
D35	-1.13376	0.00008	-0.00016	0.02867	0.02851	-1.10525
D36	1.04750	-0.00055	-0.00016	0.02429	0.02413	1.07162
D37	1.02049	0.00008	-0.00006	0.02324	0.02317	1.04366
D38	3.06057	0.00017	-0.00011	0.02808	0.02798	3.08855
D39	-1.04136	-0.00045	-0.00011	0.02370	0.02359	-1.01777
D40	3.00762	-0.00013	-0.00043	-0.01755	-0.01802	2.98961
D41	-1.19193	-0.00008	-0.00039	-0.01658	-0.01695	-1.20888
D42	0.93712	-0.00031	-0.00043	-0.01762	-0.01807	0.91905
D43	3.02076	-0.00026	-0.00039	-0.01665	-0.01701	3.00375
D44	-1.16645	-0.00015	-0.00040	-0.01846	-0.01889	-1.18533
D45	0.91719	-0.00010	-0.00036	-0.01748	-0.01782	0.89937
D46	-3.13054	-0.00033	0.00004	-0.00700	-0.00696	-3.13750
D47	0.00998	-0.00010	0.00003	-0.00261	-0.00257	0.00742
D48	0.00345	0.00002	0.00002	0.00702	0.00703	0.01048
D49	-3.13921	0.00025	0.00002	0.01142	0.01142	-3.12779
D50	1.86479	0.00018	-0.00125	0.14331	0.14253	2.00732
D51	-1.10583	0.00024	0.00158	0.05261	0.05380	-1.05203
D52	-2.38425	-0.00002	-0.00105	0.13716	0.13647	-2.24778
D53	0.92831	0.00003	0.00179	0.04645	0.04774	0.97605
D54	-2.69533	-0.00089	-0.00007	-0.01722	-0.01727	-2.71260
D55	-0.00234	-0.00047	-0.00004	-0.00326	-0.00324	-0.00558
D56	-0.02264	-0.00011	-0.00003	-0.01320	-0.01326	-0.03590
D57	2.67035	0.00031	0.00000	0.00076	0.00077	2.67112
D58	0.99563	-0.00035	0.00183	-0.07909	-0.07689	0.91874
D59	-1.41097	-0.00087	0.00192	-0.07355	-0.07118	-1.48215
D60	1.45536	-0.00021	-0.00199	0.05762	0.05515	1.51051
D61	-0.96249	-0.00032	-0.00186	0.06701	0.06471	-0.89777
D62	2.56387	-0.00047	0.00001	-0.00776	-0.00768	2.55619
D63	-1.64902	-0.00041	-0.00003	-0.00832	-0.00827	-1.65730
D64	0.45292	-0.00043	-0.00002	-0.00736	-0.00731	0.44561
D65	1.36102	0.00030	0.00009	-0.00559	-0.00555	1.35547
D66	-2.85187	0.00036	0.00005	-0.00615	-0.00615	-2.85802
D67	-0.74993	0.00034	0.00006	-0.00519	-0.00518	-0.75512
D68	-1.02870	0.00002	0.00008	0.00708	0.00714	-1.02155
D69	1.04160	0.00008	0.00004	0.00653	0.00655	1.04814
D70	-3.13965	0.00006	0.00005	0.00749	0.00751	-3.13213

Item	Value	Threshold	Converged?
Maximum Force	0.004750	0.000450	NO
RMS Force	0.000593	0.000300	NO
Maximum Displacement	0.322839	0.001800	NO
RMS Displacement	0.059929	0.001200	NO

Predicted change in Energy=-1.755809D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.652909	2.071245	-0.247517
2	6	0	-3.557708	1.109306	0.065441
3	7	0	-2.857518	-0.086556	0.159675
4	6	0	-1.557915	0.152740	-0.097279
5	7	0	-1.413871	1.455226	-0.346428
6	6	0	-0.130219	2.126074	-0.616804
7	6	0	0.413000	2.871844	0.606168
8	1	0	-2.780767	3.127496	-0.410067
9	1	0	-4.618044	1.176779	0.226976
10	1	0	0.579956	1.355595	-0.918365
11	1	0	-0.273879	2.816668	-1.449014
12	1	0	-0.294817	3.652251	0.905691
13	1	0	0.494457	2.159689	1.441610
14	35	0	0.154359	-2.638838	0.322243
15	1	0	-0.781247	-0.636232	-0.065963
16	6	0	-3.347794	-1.393638	0.463030
17	6	0	-4.633231	-1.679587	0.621367
18	1	0	-2.537397	-2.116229	0.540470
19	1	0	-4.916958	-2.696902	0.853802
20	1	0	-5.430802	-0.952331	0.529318
21	7	0	1.667859	3.500840	0.212648
22	1	0	2.005008	4.125926	0.935686
23	1	0	2.376134	2.785488	0.057234
24	6	0	3.503192	-0.219769	-1.225927
25	6	0	3.315781	-0.528646	0.188016
26	8	0	2.926921	0.773802	-0.348171
27	1	0	4.497448	0.028051	-1.590963
28	1	0	2.819833	-0.636067	-1.961081
29	1	0	2.456624	-1.149552	0.435946
30	6	0	4.452382	-0.525721	1.171708
31	1	0	4.108842	-0.192631	2.155042

32	1	0	4.846647	-1.540096	1.284848
33	1	0	5.261743	0.131143	0.842874

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357178	0.000000			
3	N	2.205397	1.388968	0.000000		
4	C	2.214102	2.222761	1.346201	0.000000	
5	N	1.387256	2.210279	2.171946	1.333901	0.000000
6	C	2.550165	3.639637	3.596778	2.490435	1.473398
7	C	3.281697	4.377836	4.432581	3.431162	2.500341
8	H	1.076307	2.214235	3.265062	3.231467	2.160774
9	H	2.210649	1.074690	2.167948	3.243176	3.266964
10	H	3.378403	4.260140	3.880489	2.586799	2.076627
11	H	2.767496	3.999024	4.206160	3.251530	2.090168
12	H	3.064321	4.221261	4.593762	3.853303	2.765322
13	H	3.573078	4.406494	4.233759	3.257032	2.708333
14	Br	5.512737	5.281474	3.951199	3.301634	4.434842
15	H	3.296440	3.282210	2.159620	1.107552	2.202968
16	C	3.604602	2.543003	1.428586	2.430822	3.537132
17	C	4.329594	3.040350	2.429828	3.651225	4.596516
18	H	4.262535	3.416249	2.089749	2.552318	3.847621
19	H	5.392036	4.117802	3.396618	4.506460	5.563483
20	H	4.178777	2.823829	2.740072	4.075913	4.764347
21	N	4.574333	5.748709	5.775054	4.659554	3.740877
22	H	5.226650	6.387577	6.480074	5.435774	4.523847
23	H	5.088643	6.166046	5.970782	4.736240	4.036914
24	C	6.641055	7.300026	6.511242	5.198789	5.268456
25	C	6.524905	7.067019	6.189173	4.929360	5.156645
26	O	5.729572	6.506462	5.870082	4.534580	4.393952
27	H	7.556924	8.294475	7.561309	6.238113	6.207204
28	H	6.341668	6.915645	6.085383	4.822930	4.990477
29	H	6.078486	6.435208	5.426453	4.254035	4.730508
30	C	7.696986	8.249769	7.392680	6.180155	6.375093
31	H	7.524540	8.052170	7.247269	6.107730	6.282765
32	H	8.463644	8.896036	7.920414	6.767155	7.129313
33	H	8.221598	8.907521	8.150862	6.884191	6.908796

		6	7	8	9	10
6	C	0.000000				
7	C	1.531966	0.000000			
8	H	2.840949	3.361286	0.000000		
9	H	4.664086	5.322447	2.754398	0.000000	
10	H	1.090378	2.156637	3.833074	5.325691	0.000000

11	H	1.090932	2.167631	2.731394	4.936593	1.773515
12	H	2.162013	1.095333	2.861212	5.027813	3.060561
13	H	2.151376	1.100801	3.884901	5.345944	2.494666
14	Br	4.864893	5.524050	6.511671	6.110961	4.204253
15	H	2.890951	3.766243	4.275762	4.253685	2.558678
16	C	4.889499	5.688444	4.639447	2.876856	4.989363
17	C	6.024387	6.795602	5.253906	2.883505	6.225787
18	H	5.013075	5.795691	5.334735	3.907847	4.888726
19	H	6.952456	7.712374	6.331215	3.935437	7.055449
20	H	6.235893	6.984286	4.954808	2.298934	6.599357
21	N	2.410613	1.457794	4.507486	6.701794	2.657969
22	H	3.311922	2.053239	5.070657	7.284543	3.625329
23	H	2.677864	2.040264	5.189313	7.178808	2.494522
24	C	4.367572	4.739613	7.166446	8.367541	3.334918
25	C	4.423821	4.490470	7.133931	8.115145	3.501312
26	O	3.353641	3.410622	6.174254	7.577578	2.484322
27	H	5.173586	5.440336	7.998343	9.365718	4.190646
28	H	4.259027	4.968808	6.923639	7.962162	3.173489
29	H	4.304621	4.514089	6.814627	7.450263	3.410544
30	C	5.588473	5.308474	8.256298	9.277050	4.785755
31	H	5.570382	5.044726	8.066581	9.041640	4.929084
32	H	6.467324	6.291506	9.101461	9.903579	5.607480
33	H	5.931582	5.574745	8.673521	9.954039	5.149795

		11	12	13	14	15
11	H	0.000000				
12	H	2.498655	0.000000			
13	H	3.062299	1.771414	0.000000		
14	Br	5.751807	6.334033	4.939080	0.000000	
15	H	3.754034	4.424004	3.423065	2.244214	0.000000
16	C	5.552615	5.914187	5.324157	3.719599	2.727757
17	C	6.595964	6.879765	6.458020	4.891897	4.049543
18	H	5.780573	6.199831	5.318615	2.750690	2.375335
19	H	7.567073	7.853574	7.294889	5.099429	4.711309
20	H	6.686779	6.908124	6.754676	5.837911	4.698153
21	N	2.645668	2.086943	2.164695	6.324425	4.815715
22	H	3.548842	2.348290	2.530575	7.040117	5.607554
23	H	3.048331	2.933451	2.418435	5.867694	4.657509
24	C	4.851389	5.827625	4.672265	4.411736	4.458180
25	C	5.172683	5.570581	4.093716	3.803357	4.106302
26	O	3.953515	4.498582	3.322782	4.447771	3.977229
27	H	5.528299	6.506452	5.455669	5.443811	5.534575
28	H	4.664188	6.025704	4.980154	4.040967	4.069306
29	H	5.171037	5.554134	3.976498	2.744326	3.316507
30	C	6.354313	6.329465	4.790558	4.864140	5.379119

31	H	6.422876	5.977977	4.371060	4.998101	5.389120
32	H	7.257767	7.317027	5.714415	4.914409	5.857888
33	H	6.565662	6.578565	5.215410	5.833457	6.158943

		16	17	18	19	20
16	C	0.000000				
17	C	1.326343	0.000000			
18	H	1.088521	2.142363	0.000000		
19	H	2.076891	1.081414	2.469346	0.000000	
20	H	2.130274	1.083279	3.118746	1.847391	0.000000
21	N	7.012516	8.167473	7.024465	9.065478	8.385821
22	H	7.703342	8.824341	7.730080	9.719635	9.013607
23	H	7.098810	8.329846	6.957235	9.158619	8.668472
24	C	7.153080	8.470239	6.573084	9.019999	9.134210
25	C	6.725108	8.043585	6.074894	8.539473	8.763488
26	O	6.687891	8.007186	6.245057	8.661233	8.579106
27	H	8.233341	9.548808	7.657022	10.101153	10.199358
28	H	6.670071	7.956515	6.094961	8.486963	8.624100
29	H	5.809611	7.112057	5.087793	7.545767	7.890444
30	C	7.880244	9.175110	7.196193	9.622870	9.913223
31	H	7.739944	8.999279	7.104897	9.456725	9.706952
32	H	8.236850	9.504092	7.443799	9.841341	10.321931
33	H	8.751764	10.061726	8.122113	10.564275	10.751872

		21	22	23	24	25
21	N	0.000000				
22	H	1.013501	0.000000			
23	H	1.018595	1.645049	0.000000		
24	C	4.391000	5.079585	3.456636	0.000000	
25	C	4.353506	4.893074	3.447249	1.459371	0.000000
26	O	3.055568	3.706069	2.124759	1.445588	1.461191
27	H	4.829064	5.421143	3.849674	1.087755	2.207038
28	H	4.813123	5.633096	3.997187	1.086616	2.208195
29	H	4.722093	5.318305	3.954041	2.172930	1.088644
30	C	4.988644	5.261479	4.064107	2.596772	1.503170
31	H	4.834565	4.956095	4.033890	3.434895	2.147333
32	H	6.055192	6.348277	5.130414	3.138810	2.137667
33	H	4.966695	5.154923	3.998690	2.737806	2.156601

		26	27	28	29	30
26	O	0.000000				
27	H	2.137108	0.000000			
28	H	2.144919	1.841856	0.000000		
29	H	2.129627	3.108066	2.478170	0.000000	
30	C	2.515119	2.817987	3.534369	2.216656	0.000000
31	H	2.932065	3.772569	4.335972	2.569205	1.093579
32	H	3.421435	3.294133	3.932086	2.566198	1.094167

33	H	2.698702	2.553104	3.796538	3.110380	1.093008

	31	32	33
31	H	0.000000	
32	H	1.765576	0.000000	
33	H	1.776456	1.777831	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.370025	2.460123	-0.225476
2	6	0	-3.370680	1.571251	-0.000693
3	7	0	-2.793297	0.307988	0.004594
4	6	0	-1.471889	0.436377	-0.218237
5	7	0	-1.195896	1.733665	-0.360240
6	6	0	0.152305	2.292759	-0.561906
7	6	0	0.743217	2.881877	0.722883
8	1	0	-2.390390	3.533375	-0.303906
9	1	0	-4.422087	1.730884	0.154293
10	1	0	0.788833	1.481699	-0.916784
11	1	0	0.092806	3.057772	-1.337372
12	1	0	0.110048	3.702711	1.076552
13	1	0	0.738646	2.101408	1.499163
14	35	0	-0.050416	-2.536034	-0.006168
15	1	0	-0.777246	-0.425928	-0.242105
16	6	0	-3.415251	-0.963702	0.196517
17	6	0	-4.725304	-1.131988	0.317458
18	1	0	-2.681386	-1.767162	0.224324
19	1	0	-5.111939	-2.131201	0.464233
20	1	0	-5.445676	-0.324023	0.275603
21	7	0	2.060960	3.412046	0.394800
22	1	0	2.444328	3.941435	1.169372
23	1	0	2.698282	2.644313	0.190001
24	6	0	3.548326	-0.347371	-1.318501
25	6	0	3.305049	-0.746772	0.063910
26	8	0	3.056178	0.626151	-0.369939
27	1	0	4.568779	-0.171621	-1.651668
28	1	0	2.841233	-0.634272	-2.092092

29	1	0	2.384541	-1.296776	0.251804
30	6	0	4.417834	-0.934606	1.056859
31	1	0	4.090359	-0.647702	2.060035
32	1	0	4.708310	-1.988916	1.092286
33	1	0	5.293843	-0.337593	0.790682

Rotational constants (GHZ): 0.4261750 0.2839037 0.1794350

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1306.1534209191 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 3.70D-06 NBF= 482

NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999995 -0.001232 0.002337 0.001712 Ang= -0.36 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3205.64799771 A.U. after 11 cycles

NFock= 11 Conv=0.68D-08 -V/T= 2.0018

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1

NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000013332	-0.000087351	0.000035616
2	6	-0.000104749	0.000211127	0.000183609
3	7	0.000027673	-0.000305491	-0.000567500
4	6	-0.000154127	0.000284661	0.001009872
5	7	-0.000330612	0.000422828	0.000345765
6	6	-0.000235032	-0.000678025	-0.001046572
7	6	-0.000538311	0.000073497	-0.000344996
8	1	-0.000045112	-0.000004615	-0.000029181
9	1	0.000048435	-0.000045216	-0.000007343
10	1	0.000386010	0.000331516	0.000005208
11	1	0.000047114	0.000019673	0.000062927
12	1	0.000023167	-0.000117031	0.000249939
13	1	0.000209632	0.000192912	-0.000083227
14	35	-0.000244405	-0.000054662	-0.000025460
15	1	0.000028338	-0.000172555	-0.000075107
16	6	0.000172732	0.000183497	-0.000296493
17	6	0.000035560	-0.000132546	0.000128856
18	1	-0.000055450	0.000061573	-0.000041106
19	1	0.000010028	0.000023347	0.000012178
20	1	-0.000016502	-0.000012236	0.000030788
21	7	0.000604087	-0.000338448	0.000537680
22	1	-0.000181561	0.000111310	-0.000119860
23	1	0.000245258	0.000463839	0.000173664
24	6	0.001695773	0.001699904	-0.002713857
25	6	-0.001423742	0.000482084	0.003109767
26	8	-0.000216768	-0.002426024	-0.000662393
27	1	-0.000195962	0.000155814	-0.000329522
28	1	-0.000049698	-0.000039556	0.000337184
29	1	0.000099407	-0.000320812	0.000388126
30	6	0.000114695	-0.000002500	-0.000312935
31	1	0.000025197	0.000026021	0.000040017
32	1	-0.000028308	-0.000000090	-0.000011868
33	1	0.000033902	-0.000006446	0.000016224

Cartesian Forces: Max 0.003109767 RMS 0.000619876

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.002979551 RMS 0.000466069
Search for a local minimum.
Step number 28 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 25 26 27 28
DE= -1.82D-04 DEPred=-1.76D-04 R= 1.03D+00
TightC=F SS= 1.41D+00 RLast= 2.82D-01 DXNew= 1.1935D+00 8.4493D-01
Trust test= 1.03D+00 RLast= 2.82D-01 DXMaxT set to 8.45D-01
ITU= 1 1 0 0 -1 1 -1 1 1 1 1 1 1 1 1 0 -1 -1 1
ITU= 1 1 -1 1 0 0 -1 0
Eigenvalues --- 0.00102 0.00140 0.00251 0.00435 0.00644
Eigenvalues --- 0.00725 0.00745 0.01337 0.01512 0.01878
Eigenvalues --- 0.01946 0.02170 0.02351 0.02386 0.02466
Eigenvalues --- 0.02644 0.02843 0.03057 0.03085 0.03209
Eigenvalues --- 0.03298 0.03708 0.03725 0.03873 0.04073
Eigenvalues --- 0.04372 0.04468 0.05093 0.05442 0.05739
Eigenvalues --- 0.05830 0.05932 0.07146 0.08498 0.08533
Eigenvalues --- 0.08878 0.09655 0.10799 0.12079 0.12353
Eigenvalues --- 0.12631 0.13311 0.15022 0.15749 0.15976
Eigenvalues --- 0.16000 0.16001 0.16005 0.16020 0.16080
Eigenvalues --- 0.16300 0.17820 0.19838 0.22022 0.22228
Eigenvalues --- 0.22909 0.23416 0.24161 0.26409 0.27084
Eigenvalues --- 0.29097 0.30507 0.31699 0.32065 0.33632
Eigenvalues --- 0.33943 0.34282 0.34351 0.34522 0.34564
Eigenvalues --- 0.34707 0.34828 0.35075 0.35213 0.35373
Eigenvalues --- 0.35538 0.35573 0.35784 0.35892 0.36419
Eigenvalues --- 0.36623 0.38883 0.40201 0.41887 0.42488
Eigenvalues --- 0.44404 0.45484 0.46614 0.49661 0.54826
Eigenvalues --- 0.58172 0.60599 1.26486
En-DIIS/RFO-DIIS IScMMF= 0 using points: 28 27 26
RFO step: Lambda=-6.29188193D-05.
DidBck=F Rises=F RFO-DIIS coefs: 1.01682 0.20922 -0.22604
Iteration 1 RMS(Cart)= 0.03967156 RMS(Int)= 0.00072354
Iteration 2 RMS(Cart)= 0.00188226 RMS(Int)= 0.00029126
Iteration 3 RMS(Cart)= 0.00000211 RMS(Int)= 0.00029126
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00029126

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56469	-0.00003	-0.00005	0.00003	-0.00002	2.56467

R2	2.62153	0.00017	-0.00012	-0.00024	-0.00035	2.62118
R3	2.03392	0.00000	0.00001	0.00006	0.00008	2.03400
R4	2.62477	-0.00004	0.00002	0.00049	0.00051	2.62527
R5	2.03087	-0.00005	-0.00001	-0.00019	-0.00020	2.03067
R6	2.54395	-0.00031	-0.00009	-0.00112	-0.00121	2.54274
R7	2.69964	-0.00019	0.00000	-0.00060	-0.00060	2.69903
R8	2.52071	0.00019	0.00019	0.00010	0.00029	2.52100
R9	2.09297	0.00000	-0.00010	0.00065	0.00055	2.09352
R10	2.78432	0.00049	0.00008	0.00130	0.00138	2.78570
R11	2.89500	0.00035	-0.00038	-0.00088	-0.00125	2.89375
R12	2.06052	0.00002	0.00003	0.00039	0.00041	2.06093
R13	2.06156	-0.00004	0.00006	0.00003	0.00009	2.06165
R14	2.06988	-0.00003	-0.00001	-0.00016	-0.00017	2.06971
R15	2.08021	-0.00017	0.00001	-0.00067	-0.00066	2.07955
R16	2.75483	0.00042	0.00017	0.00144	0.00160	2.75644
R17	4.24095	-0.00006	0.00028	-0.00468	-0.00439	4.23656
R18	2.50643	0.00002	0.00000	0.00013	0.00012	2.50655
R19	2.05701	-0.00008	-0.00007	-0.00083	-0.00090	2.05611
R20	2.04358	-0.00002	-0.00001	-0.00008	-0.00009	2.04349
R21	2.04710	0.00000	-0.00002	-0.00018	-0.00020	2.04690
R22	1.91524	-0.00008	0.00005	0.00003	0.00007	1.91531
R23	1.92487	0.00040	-0.00027	-0.00112	-0.00125	1.92362
R24	4.01521	0.00034	0.00385	0.02231	0.02609	4.04130
R25	2.75781	0.00298	-0.00093	0.01430	0.01244	2.77026
R26	2.73177	-0.00035	0.00072	-0.00197	-0.00082	2.73095
R27	2.05556	-0.00003	-0.00005	-0.00026	-0.00030	2.05526
R28	2.05341	-0.00018	-0.00003	-0.00092	-0.00095	2.05246
R29	2.76125	-0.00096	0.00040	-0.00718	-0.00628	2.75497
R30	2.05724	0.00019	-0.00003	0.00069	0.00066	2.05790
R31	2.84058	-0.00007	-0.00001	-0.00008	-0.00009	2.84049
R32	2.06656	0.00003	0.00003	0.00032	0.00035	2.06692
R33	2.06768	-0.00001	0.00006	0.00020	0.00025	2.06793
R34	2.06549	0.00002	-0.00001	0.00011	0.00010	2.06558
A1	1.87250	0.00015	-0.00002	0.00016	0.00013	1.87264
A2	2.27996	-0.00012	0.00004	-0.00036	-0.00033	2.27964
A3	2.13071	-0.00004	-0.00002	0.00019	0.00017	2.13089
A4	1.86482	-0.00012	0.00001	-0.00063	-0.00062	1.86420
A5	2.27566	0.00010	-0.00015	-0.00018	-0.00033	2.27533
A6	2.14270	0.00002	0.00014	0.00082	0.00096	2.14366
A7	1.89723	0.00013	0.00007	0.00058	0.00065	1.89788
A8	2.25125	0.00032	-0.00012	0.00117	0.00105	2.25230
A9	2.13469	-0.00045	0.00005	-0.00175	-0.00170	2.13299
A10	1.88964	0.00012	-0.00012	-0.00018	-0.00032	1.88933
A11	2.14713	-0.00084	0.00107	0.00572	0.00677	2.15390

A12	2.24610	0.00073	-0.00092	-0.00531	-0.00625	2.23985
A13	1.90057	-0.00028	0.00008	0.00008	0.00015	1.90072
A14	2.20066	-0.00045	-0.00065	0.00003	-0.00065	2.20001
A15	2.18088	0.00073	0.00065	0.00023	0.00085	2.18174
A16	1.96501	-0.00115	0.00041	-0.00346	-0.00303	1.96198
A17	1.87178	0.00094	-0.00055	0.00282	0.00225	1.87403
A18	1.88965	0.00014	-0.00026	0.00058	0.00032	1.88997
A19	1.91115	0.00006	-0.00026	-0.00415	-0.00441	1.90674
A20	1.92571	0.00021	0.00016	0.00209	0.00224	1.92795
A21	1.89874	-0.00016	0.00050	0.00236	0.00286	1.90161
A22	1.91346	-0.00054	0.00049	0.00333	0.00382	1.91728
A23	1.89354	-0.00001	0.00000	0.00011	0.00012	1.89366
A24	1.87525	0.00130	-0.00069	0.00060	-0.00012	1.87513
A25	1.87677	0.00011	0.00025	-0.00050	-0.00026	1.87651
A26	1.89933	-0.00045	-0.00032	0.00111	0.00079	1.90012
A27	2.00458	-0.00044	0.00030	-0.00431	-0.00400	2.00058
A28	2.15941	0.00032	0.00006	0.00238	0.00244	2.16186
A29	1.94655	-0.00017	0.00007	-0.00060	-0.00053	1.94601
A30	2.17721	-0.00014	-0.00013	-0.00178	-0.00191	2.17530
A31	2.07459	-0.00002	0.00006	0.00025	0.00031	2.07490
A32	2.16358	0.00004	0.00000	0.00016	0.00016	2.16374
A33	2.04502	-0.00002	-0.00006	-0.00042	-0.00048	2.04454
A34	1.93894	-0.00078	-0.00065	-0.00318	-0.00365	1.93529
A35	1.91422	0.00224	-0.00067	0.00157	0.00098	1.91520
A36	1.88671	-0.00073	0.00037	0.00268	0.00298	1.88969
A37	2.08374	0.00078	-0.00332	0.00060	-0.00191	2.08183
A38	2.08707	-0.00049	0.00240	-0.00313	-0.00162	2.08546
A39	1.99496	0.00026	0.00095	0.00112	0.00184	1.99679
A40	2.00801	0.00021	-0.00118	-0.00247	-0.00360	2.00441
A41	2.02091	-0.00010	0.00070	0.00440	0.00512	2.02603
A42	2.02942	0.00021	-0.00038	-0.00311	-0.00374	2.02568
A43	2.13711	0.00006	-0.00125	-0.00609	-0.00712	2.12999
A44	1.96268	0.00042	-0.00220	-0.00361	-0.00561	1.95708
A45	2.02598	0.00006	0.00129	0.00394	0.00484	2.03082
A46	2.03624	-0.00024	0.00144	0.00733	0.00879	2.04503
A47	2.62585	-0.00088	-0.00073	-0.01900	-0.02134	2.60450
A48	2.57344	-0.00054	-0.00193	-0.00038	-0.00469	2.56875
A49	1.92997	0.00005	-0.00005	0.00071	0.00066	1.93062
A50	1.91593	-0.00006	0.00041	0.00136	0.00177	1.91771
A51	1.94357	0.00004	-0.00014	-0.00006	-0.00020	1.94337
A52	1.87821	0.00000	0.00015	0.00116	0.00131	1.87952
A53	1.89663	-0.00004	-0.00018	-0.00186	-0.00204	1.89459
A54	1.89803	0.00000	-0.00020	-0.00133	-0.00153	1.89650
A55	3.42197	0.00098	0.00374	0.01614	0.01988	3.44185

A56	2.63686	0.00127	-0.00845	-0.00224	-0.01133	2.62553
A57	2.85114	-0.00026	0.00515	0.02449	0.02965	2.88079
A58	3.09484	0.00029	-0.00499	-0.01048	-0.01567	3.07917
D1	0.00408	-0.00008	-0.00050	-0.00069	-0.00120	0.00288
D2	-3.13981	0.00007	0.00006	0.00311	0.00316	-3.13665
D3	3.14152	-0.00015	-0.00064	-0.00463	-0.00527	3.13625
D4	-0.00238	0.00000	-0.00008	-0.00083	-0.00090	-0.00328
D5	-0.00258	-0.00008	0.00095	0.00233	0.00328	0.00070
D6	-3.09638	-0.00013	-0.00035	-0.00513	-0.00545	-3.10182
D7	-3.14045	-0.00002	0.00107	0.00586	0.00692	-3.13353
D8	0.04894	-0.00008	-0.00023	-0.00160	-0.00180	0.04714
D9	-0.00421	0.00021	-0.00011	-0.00115	-0.00126	-0.00547
D10	-3.13942	0.00013	0.00011	-0.00050	-0.00038	-3.13979
D11	3.13947	0.00008	-0.00062	-0.00460	-0.00521	3.13426
D12	0.00426	-0.00001	-0.00040	-0.00394	-0.00433	-0.00007
D13	0.00263	-0.00026	0.00071	0.00262	0.00332	0.00595
D14	3.11941	0.00008	0.00167	0.01142	0.01314	3.13255
D15	3.13836	-0.00018	0.00051	0.00202	0.00252	3.14087
D16	-0.02806	0.00016	0.00147	0.01082	0.01234	-0.01572
D17	0.08485	-0.00009	-0.00275	-0.02759	-0.03035	0.05450
D18	-3.06238	-0.00003	-0.00312	-0.02754	-0.03067	-3.09305
D19	-3.04959	-0.00018	-0.00251	-0.02686	-0.02937	-3.07896
D20	0.08637	-0.00012	-0.00288	-0.02681	-0.02969	0.05668
D21	-0.00006	0.00021	-0.00102	-0.00306	-0.00408	-0.00413
D22	3.09441	0.00023	0.00019	0.00428	0.00449	3.09890
D23	-3.11499	-0.00012	-0.00210	-0.01272	-0.01478	-3.12977
D24	-0.02052	-0.00011	-0.00089	-0.00538	-0.00622	-0.02674
D25	1.32353	-0.00017	-0.00777	-0.01700	-0.02477	1.29876
D26	-2.85636	-0.00016	-0.00821	-0.02236	-0.03057	-2.88693
D27	-0.81022	0.00022	-0.00805	-0.01779	-0.02584	-0.83607
D28	-1.76289	-0.00020	-0.00922	-0.02560	-0.03482	-1.79771
D29	0.34042	-0.00019	-0.00967	-0.03096	-0.04062	0.29979
D30	2.38655	0.00019	-0.00951	-0.02639	-0.03590	2.35066
D31	-1.06961	0.00049	0.00099	-0.00423	-0.00323	-1.07284
D32	0.97528	0.00032	0.00156	-0.00290	-0.00133	0.97395
D33	-3.13104	0.00059	0.00149	-0.00771	-0.00621	-3.13725
D34	3.13305	0.00001	0.00160	-0.00277	-0.00118	3.13187
D35	-1.10525	-0.00017	0.00217	-0.00144	0.00072	-1.10452
D36	1.07162	0.00010	0.00210	-0.00626	-0.00416	1.06747
D37	1.04366	0.00004	0.00105	-0.00436	-0.00331	1.04035
D38	3.08855	-0.00014	0.00162	-0.00303	-0.00141	3.08714
D39	-1.01777	0.00013	0.00155	-0.00785	-0.00629	-1.02406
D40	2.98961	-0.00057	0.00420	-0.00274	0.00143	2.99103
D41	-1.20888	-0.00053	0.00382	-0.00039	0.00346	-1.20542

D42	0.91905	-0.00041	0.00418	-0.00763	-0.00349	0.91557
D43	3.00375	-0.00037	0.00380	-0.00529	-0.00145	3.00230
D44	-1.18533	0.00008	0.00390	-0.00492	-0.00107	-1.18640
D45	0.89937	0.00012	0.00352	-0.00258	0.00097	0.90033
D46	-3.13750	0.00005	-0.00051	-0.00322	-0.00373	-3.14123
D47	0.00742	0.00001	-0.00039	-0.00239	-0.00277	0.00465
D48	0.01048	-0.00002	-0.00009	-0.00328	-0.00338	0.00710
D49	-3.12779	-0.00006	0.00003	-0.00244	-0.00241	-3.13021
D50	2.00732	0.00013	0.01551	0.01476	0.03068	2.03800
D51	-1.05203	-0.00106	-0.01569	-0.06998	-0.08593	-1.13796
D52	-2.24778	0.00072	0.01326	0.01480	0.02831	-2.21947
D53	0.97605	-0.00046	-0.01794	-0.06994	-0.08830	0.88775
D54	-2.71260	-0.00028	0.00045	-0.00516	-0.00474	-2.71734
D55	-0.00558	-0.00024	0.00036	-0.00807	-0.00774	-0.01332
D56	-0.03590	0.00016	0.00009	0.00047	0.00042	-0.03547
D57	2.67112	0.00019	0.00000	-0.00245	-0.00258	2.66854
D58	0.91874	0.00014	-0.02043	-0.04252	-0.06226	0.85648
D59	-1.48215	-0.00026	-0.02130	-0.04804	-0.06846	-1.55062
D60	1.51051	-0.00035	0.02174	0.05100	0.07251	1.58301
D61	-0.89777	-0.00055	0.02052	0.03893	0.05937	-0.83841
D62	2.55619	-0.00026	-0.00024	-0.00468	-0.00485	2.55134
D63	-1.65730	-0.00026	0.00018	-0.00196	-0.00172	-1.65901
D64	0.44561	-0.00028	0.00012	-0.00277	-0.00259	0.44303
D65	1.35547	0.00037	-0.00103	-0.00215	-0.00321	1.35226
D66	-2.85802	0.00037	-0.00062	0.00057	-0.00007	-2.85810
D67	-0.75512	0.00036	-0.00068	-0.00023	-0.00094	-0.75606
D68	-1.02155	-0.00012	-0.00077	-0.01004	-0.01084	-1.03239
D69	1.04814	-0.00012	-0.00035	-0.00732	-0.00770	1.04044
D70	-3.13213	-0.00013	-0.00041	-0.00813	-0.00857	-3.14071

Item	Value	Threshold	Converged?
Maximum Force	0.002980	0.000450	NO
RMS Force	0.000466	0.000300	NO
Maximum Displacement	0.250908	0.001800	NO
RMS Displacement	0.038516	0.001200	NO

Predicted change in Energy=-1.029538D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.647715	2.073739	-0.239469
2	6	0	-3.558862	1.115424	0.066060

3	7	0	-2.865843	-0.085668	0.150183
4	6	0	-1.565618	0.146537	-0.106775
5	7	0	-1.412722	1.450702	-0.342315
6	6	0	-0.125450	2.115758	-0.613767
7	6	0	0.403207	2.882728	0.601622
8	1	0	-2.769532	3.131419	-0.397567
9	1	0	-4.619112	1.188505	0.224994
10	1	0	0.590264	1.340108	-0.888581
11	1	0	-0.260298	2.789748	-1.460990
12	1	0	-0.303955	3.671317	0.880196
13	1	0	0.473671	2.186032	1.450528
14	35	0	0.127291	-2.670476	0.189468
15	1	0	-0.790838	-0.645242	-0.096080
16	6	0	-3.362429	-1.392358	0.443289
17	6	0	-4.645394	-1.669953	0.633809
18	1	0	-2.558682	-2.124626	0.483520
19	1	0	-4.932424	-2.689464	0.851913
20	1	0	-5.438249	-0.933828	0.581250
21	7	0	1.667519	3.498260	0.213967
22	1	0	1.994906	4.134227	0.932039
23	1	0	2.373770	2.777565	0.079806
24	6	0	3.481566	-0.238197	-1.205007
25	6	0	3.331274	-0.539357	0.221787
26	8	0	2.896825	0.742737	-0.319387
27	1	0	4.461602	0.032518	-1.591150
28	1	0	2.791221	-0.676837	-1.919614
29	1	0	2.490615	-1.177470	0.490140
30	6	0	4.495791	-0.502714	1.171487
31	1	0	4.175739	-0.162055	2.160344
32	1	0	4.914767	-1.507196	1.285359
33	1	0	5.282208	0.165485	0.811156

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357167	0.000000			
3	N	2.205095	1.389235	0.000000		
4	C	2.214193	2.222979	1.345560	0.000000	
5	N	1.387069	2.210226	2.171301	1.334055	0.000000
6	C	2.550233	3.640213	3.597173	2.491778	1.474129
7	C	3.266501	4.371291	4.438678	3.444538	2.497862
8	H	1.076346	2.214097	3.264805	3.231639	2.160739
9	H	2.210378	1.074584	2.168655	3.243393	3.266730
10	H	3.382908	4.263457	3.880276	2.585277	2.079083

11	H	2.775707	4.001971	4.201519	3.244122	2.091067
12	H	3.049446	4.217798	4.605554	3.871690	2.766772
13	H	3.551302	4.395938	4.243097	3.277718	2.704343
14	Br	5.512914	5.285451	3.954950	3.299888	4.431540
15	H	3.295665	3.284539	2.163196	1.107841	2.200080
16	C	3.604275	2.543592	1.428267	2.428847	3.535749
17	C	4.332270	3.043225	2.431185	3.651455	4.597987
18	H	4.261092	3.416513	2.088735	2.548099	3.844243
19	H	5.394359	4.120851	3.397490	4.505260	5.563763
20	H	4.184031	2.827888	2.742711	4.078950	4.769049
21	N	4.566849	5.745854	5.779271	4.667986	3.740297
22	H	5.212675	6.380237	6.484265	5.445929	4.520753
23	H	5.080612	6.161089	5.971315	4.740875	4.034386
24	C	6.621586	7.281177	6.492258	5.179595	5.248874
25	C	6.541356	7.087773	6.214114	4.955598	5.175330
26	O	5.702621	6.477913	5.840813	4.507112	4.367372
27	H	7.519043	8.261166	7.532440	6.208361	6.170779
28	H	6.322230	6.890476	6.052761	4.790238	4.968645
29	H	6.124142	6.483315	5.477157	4.308402	4.778735
30	C	7.723897	8.289618	7.443833	6.228656	6.404526
31	H	7.570826	8.114310	7.323282	6.180472	6.332075
32	H	8.505253	8.953615	7.990448	6.831417	7.171862
33	H	8.223680	8.923120	8.178673	6.909100	6.914069

		6	7	8	9	10
6	C	0.000000				
7	C	1.531304	0.000000			
8	H	2.840682	3.335641	0.000000		
9	H	4.664367	5.313750	2.753805	0.000000	
10	H	1.090597	2.152992	3.839025	5.329224	0.000000
11	H	1.090978	2.168699	2.746610	4.940221	1.775546
12	H	2.164152	1.095242	2.828999	5.021377	3.059859
13	H	2.150627	1.100451	3.850658	5.332301	2.490103
14	Br	4.859743	5.575310	6.511388	6.117298	4.178675
15	H	2.886843	3.789341	4.274259	4.256924	2.545018
16	C	4.888996	5.699250	4.639302	2.878847	4.986384
17	C	6.026438	6.798259	5.256973	2.887664	6.228183
18	H	5.010541	5.818964	5.333552	3.910121	4.878822
19	H	6.953084	7.718869	6.334191	3.940791	7.054563
20	H	6.241304	6.977759	4.960480	2.302651	6.608642
21	N	2.410641	1.458643	4.493992	6.697523	2.652114
22	H	3.310535	2.051567	5.047112	7.274780	3.618671
23	H	2.676776	2.041193	5.177514	7.172628	2.486956
24	C	4.347555	4.741348	7.147202	8.348735	3.309200
25	C	4.438099	4.519792	7.146889	8.135979	3.504061

26	O	3.332566	3.412617	6.149757	7.548800	2.449706
27	H	5.131882	5.422408	7.957205	9.332419	4.146161
28	H	4.243913	4.972902	6.909516	7.936743	3.158372
29	H	4.348305	4.566717	6.857382	7.497757	3.442442
30	C	5.603516	5.341835	8.273679	9.318665	4.784665
31	H	5.602174	5.092378	8.101028	9.105987	4.940453
32	H	6.491246	6.331912	9.132220	9.964238	5.615558
33	H	5.922561	5.588556	8.665349	9.971273	5.126713

		11	12	13	14	15
11	H	0.000000				
12	H	2.502044	0.000000			
13	H	3.062698	1.770890	0.000000		
14	Br	5.717367	6.393858	5.029505	0.000000	
15	H	3.734114	4.452286	3.465125	2.241890	0.000000
16	C	5.544322	5.931775	5.341822	3.725071	2.731699
17	C	6.595923	6.887523	6.460687	4.896632	4.054674
18	H	5.763226	6.231702	5.358362	2.756604	2.376928
19	H	7.563072	7.866579	7.304428	5.102931	4.714899
20	H	6.696786	6.903456	6.740917	5.843344	4.705368
21	N	2.650273	2.088186	2.162475	6.358160	4.827862
22	H	3.552486	2.345578	2.525560	7.095307	5.626786
23	H	3.051641	2.934218	2.416437	5.894052	4.664899
24	C	4.820324	5.827740	4.687877	4.371694	4.432701
25	C	5.178230	5.601622	4.135631	3.848145	4.135705
26	O	3.932040	4.501176	3.329772	4.424848	3.946544
27	H	5.469515	6.485287	5.458299	5.409532	5.502973
28	H	4.641047	6.027064	4.992487	3.939461	4.019629
29	H	5.207038	5.610036	4.037766	2.811543	3.375626
30	C	6.355361	6.367492	4.846099	4.974671	5.438334
31	H	6.442486	6.033339	4.441020	5.154266	5.476477
32	H	7.265498	7.363167	5.778456	5.047190	5.933403
33	H	6.539783	6.595517	5.254849	5.916278	6.193725

		16	17	18	19	20
16	C	0.000000				
17	C	1.326408	0.000000			
18	H	1.088046	2.140954	0.000000		
19	H	2.077100	1.081369	2.467672	0.000000	
20	H	2.130331	1.083171	3.117604	1.846991	0.000000
21	N	7.019338	8.169429	7.039196	9.069407	8.382734
22	H	7.712526	8.824457	7.753037	9.724047	9.003334
23	H	7.101011	8.328025	6.965884	9.157785	8.663344
24	C	7.133669	8.454506	6.549377	9.001937	9.123471
25	C	6.751468	8.066923	6.105175	8.562051	8.785746
26	O	6.657219	7.975885	6.215222	8.628389	8.549589

27	H	8.208816	9.528181	7.631639	10.080945	10.181364
28	H	6.630437	7.925245	6.040912	8.449066	8.604914
29	H	5.857174	7.154426	5.137368	7.584096	7.933129
30	C	7.941873	9.231079	7.271140	9.683762	9.960893
31	H	7.828530	9.078351	7.212201	9.542453	9.773327
32	H	8.320712	9.583720	7.541658	9.927376	10.392760
33	H	8.791583	10.097404	8.175054	10.606182	10.779125

		21	22	23	24	25
21	N	0.000000				
22	H	1.013540	0.000000			
23	H	1.017935	1.646321	0.000000		
24	C	4.389233	5.088734	3.460170	0.000000	
25	C	4.366977	4.912507	3.455277	1.465956	0.000000
26	O	3.064077	3.725820	2.138566	1.445156	1.457868
27	H	4.803822	5.410646	3.832286	1.087595	2.211657
28	H	4.821443	5.649105	4.013083	1.086114	2.212726
29	H	4.755650	5.353048	3.977980	2.176635	1.088994
30	C	4.992370	5.273801	4.056472	2.597372	1.503121
31	H	4.845354	4.972203	4.027046	3.437042	2.147901
32	H	6.061938	6.362082	5.125349	3.141074	2.139007
33	H	4.952776	5.154791	3.977039	2.733163	2.156456

		26	27	28	29	30
26	O	0.000000				
27	H	2.137830	0.000000			
28	H	2.141744	1.844246	0.000000		
29	H	2.123096	3.111371	2.479498	0.000000	
30	C	2.516057	2.814215	3.534229	2.222669	0.000000
31	H	2.933144	3.767398	4.339118	2.580754	1.093764
32	H	3.421915	3.293993	3.933293	2.572471	1.094301
33	H	2.702109	2.542076	3.790992	3.114413	1.093060

		31	32	33
31	H	0.000000		
32	H	1.766682	0.000000	
33	H	1.775350	1.777005	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-2.352213	2.466630	-0.240193
2	6	0	-3.359600	1.590170	0.002485
3	7	0	-2.792084	0.322367	0.026440
4	6	0	-1.471300	0.435533	-0.204333
5	7	0	-1.184590	1.728424	-0.365366
6	6	0	0.167000	2.273677	-0.586636
7	6	0	0.751172	2.915995	0.674737
8	1	0	-2.364742	3.538233	-0.340347
9	1	0	-4.409479	1.761336	0.154761
10	1	0	0.805360	1.445733	-0.897130
11	1	0	0.113618	3.002935	-1.396306
12	1	0	0.122559	3.755723	0.989790
13	1	0	0.738196	2.170600	1.484187
14	35	0	-0.074621	-2.550154	-0.048697
15	1	0	-0.780208	-0.429938	-0.230089
16	6	0	-3.421848	-0.941410	0.241413
17	6	0	-4.728994	-1.097797	0.403497
18	1	0	-2.696419	-1.752300	0.248745
19	1	0	-5.120289	-2.093405	0.561648
20	1	0	-5.443010	-0.283507	0.384179
21	7	0	2.076741	3.420694	0.334466
22	1	0	2.455210	3.980285	1.090035
23	1	0	2.709035	2.640647	0.167366
24	6	0	3.528089	-0.397293	-1.272371
25	6	0	3.326295	-0.758884	0.133886
26	8	0	3.031205	0.588103	-0.339324
27	1	0	4.536202	-0.206465	-1.633141
28	1	0	2.808304	-0.724347	-2.017078
29	1	0	2.421762	-1.322365	0.357974
30	6	0	4.473799	-0.891907	1.095610
31	1	0	4.174341	-0.574933	2.098692
32	1	0	4.787975	-1.938308	1.157508
33	1	0	5.328814	-0.288049	0.780831

Rotational constants (GHZ): 0.4240164 0.2832030 0.1787006

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1304.8155087600 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 482 RedAO= T EigKep= 3.60D-06 NBF= 482
NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999993 0.003150 -0.000969 0.002021 Ang= 0.44 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3205.64808784 A.U. after 11 cycles
NFock= 11 Conv=0.86D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000062482	0.000050914	0.000064979
2	6	0.000156036	0.000165464	0.000121025
3	7	-0.000504086	-0.000784006	-0.000510272
4	6	0.000985402	0.001366148	0.000954526
5	7	-0.000188788	0.000382616	-0.000411852
6	6	-0.000612261	-0.000825302	-0.000464355
7	6	0.000371540	0.000071743	-0.000461454
8	1	-0.000038214	-0.000017258	0.000112761
9	1	-0.000013114	-0.000132591	0.000068187

10	1	-0.000115873	0.000167174	-0.000301224
11	1	0.000160558	0.000039123	0.000089878
12	1	0.000053586	-0.000009902	0.000089038
13	1	-0.000094792	-0.000040527	0.000072404
14	35	0.000144876	0.000167819	-0.000008007
15	1	-0.000514366	-0.000592146	0.000245344
16	6	-0.000087889	-0.000057107	-0.000356271
17	6	0.000062845	0.000101521	-0.000022313
18	1	0.000206810	-0.000112581	-0.000007399
19	1	0.000071019	-0.000001137	0.000079417
20	1	-0.000070563	0.000075993	0.000045620
21	7	-0.000418129	0.000386515	0.000840099
22	1	0.000233851	0.000043865	-0.000320057
23	1	0.000565621	0.000124293	0.000181346
24	6	0.000299729	0.000393618	0.000796787
25	6	-0.001199580	0.000048593	-0.001407147
26	8	0.000507511	-0.000677767	-0.000201818
27	1	-0.000232930	0.000202105	-0.000278483
28	1	0.000047212	-0.000333312	0.000195220
29	1	0.000706938	-0.000542439	0.000405131
30	6	-0.000210831	0.000389790	0.000403252
31	1	0.000101149	-0.000102169	0.000126655
32	1	-0.000232062	0.000068361	-0.000069633
33	1	-0.000078725	-0.000017410	-0.000071382

Cartesian Forces: Max 0.001407147 RMS 0.000408139

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.001432187 RMS 0.000310676
Search for a local minimum.
Step number 29 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 25 27 28 29
DE= -9.01D-05 DEPred=-1.03D-04 R= 8.75D-01
TightC=F SS= 1.41D+00 RLast= 2.22D-01 DXNew= 1.4210D+00 6.6495D-01
Trust test= 8.75D-01 RLast= 2.22D-01 DXMaxT set to 8.45D-01
ITU= 1 1 1 0 0 -1 1 -1 1 1 1 1 1 1 1 1 1 0 -1 -1
ITU= 1 1 1 -1 1 0 0 -1 0
Eigenvalues --- 0.00075 0.00145 0.00238 0.00431 0.00652

Eigenvalues --- 0.00729 0.00771 0.01336 0.01488 0.01878
Eigenvalues --- 0.01965 0.02178 0.02353 0.02386 0.02447
Eigenvalues --- 0.02731 0.02787 0.03056 0.03097 0.03222
Eigenvalues --- 0.03273 0.03692 0.03798 0.03848 0.04111
Eigenvalues --- 0.04376 0.04572 0.05293 0.05462 0.05743
Eigenvalues --- 0.05853 0.05945 0.07478 0.07837 0.08572
Eigenvalues --- 0.09108 0.09576 0.10668 0.12201 0.12462
Eigenvalues --- 0.12621 0.13744 0.15066 0.15795 0.15976
Eigenvalues --- 0.16000 0.16003 0.16005 0.16021 0.16078
Eigenvalues --- 0.16273 0.18553 0.20941 0.22074 0.22227
Eigenvalues --- 0.23072 0.23404 0.25840 0.26862 0.28896
Eigenvalues --- 0.29739 0.30407 0.31213 0.31755 0.32720
Eigenvalues --- 0.33659 0.34282 0.34359 0.34419 0.34547
Eigenvalues --- 0.34698 0.34744 0.35076 0.35202 0.35342
Eigenvalues --- 0.35556 0.35652 0.35892 0.36105 0.36423
Eigenvalues --- 0.36625 0.38924 0.40038 0.41890 0.42439
Eigenvalues --- 0.43999 0.45498 0.46463 0.49515 0.54829
Eigenvalues --- 0.58097 0.60614 1.26845
En-DIIS/RFO-DIIS IScMMF= 0 using points: 29 28 27 26
RFO step: Lambda=-3.06126635D-05.
DidBck=F Rises=F RFO-DIIS coefs: 0.93154 0.30500 -0.27208 0.03554
Iteration 1 RMS(Cart)= 0.03481188 RMS(Int)= 0.00063065
Iteration 2 RMS(Cart)= 0.00145363 RMS(Int)= 0.00028188
Iteration 3 RMS(Cart)= 0.00000149 RMS(Int)= 0.00028188
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00028188

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56467	0.00032	0.00002	0.00015	0.00017	2.56484
R2	2.62118	0.00012	-0.00012	-0.00037	-0.00048	2.62070
R3	2.03400	-0.00003	-0.00003	0.00002	-0.00001	2.03399
R4	2.62527	0.00013	0.00025	0.00017	0.00041	2.62569
R5	2.03067	0.00001	0.00001	-0.00014	-0.00013	2.03054
R6	2.54274	-0.00002	-0.00020	-0.00091	-0.00111	2.54163
R7	2.69903	-0.00011	-0.00034	0.00002	-0.00033	2.69871
R8	2.52100	-0.00042	-0.00013	0.00042	0.00029	2.52129
R9	2.09352	0.00005	0.00012	-0.00143	-0.00132	2.09220
R10	2.78570	-0.00032	0.00058	0.00067	0.00125	2.78695
R11	2.89375	0.00037	-0.00028	0.00021	-0.00006	2.89368
R12	2.06093	-0.00012	0.00006	0.00002	0.00008	2.06101
R13	2.06165	-0.00007	-0.00009	-0.00025	-0.00033	2.06132
R14	2.06971	-0.00002	-0.00002	-0.00035	-0.00037	2.06934
R15	2.07955	0.00007	-0.00030	-0.00089	-0.00119	2.07836
R16	2.75644	-0.00007	0.00102	0.00140	0.00242	2.75885
R17	4.23656	-0.00009	0.00094	0.01063	0.01157	4.24812

R18	2.50655	-0.00009	0.00011	-0.00004	0.00006	2.50661
R19	2.05611	0.00023	-0.00020	0.00000	-0.00020	2.05591
R20	2.04349	0.00000	0.00000	-0.00001	-0.00001	2.04348
R21	2.04690	0.00010	0.00002	0.00002	0.00004	2.04694
R22	1.91531	-0.00012	0.00007	-0.00027	-0.00020	1.91512
R23	1.92362	0.00041	0.00060	0.00058	0.00137	1.92499
R24	4.04130	0.00050	0.00152	0.03131	0.03273	4.07404
R25	2.77026	-0.00029	0.00057	-0.00168	-0.00193	2.76832
R26	2.73095	-0.00031	-0.00019	0.00188	0.00201	2.73296
R27	2.05526	-0.00006	0.00010	-0.00039	-0.00029	2.05497
R28	2.05246	-0.00003	0.00016	-0.00025	-0.00009	2.05237
R29	2.75497	-0.00035	0.00099	0.00083	0.00232	2.75729
R30	2.05790	-0.00013	0.00010	0.00049	0.00059	2.05849
R31	2.84049	-0.00007	-0.00048	-0.00008	-0.00056	2.83993
R32	2.06692	0.00005	-0.00015	0.00034	0.00020	2.06711
R33	2.06793	-0.00016	-0.00007	0.00001	-0.00006	2.06787
R34	2.06558	-0.00004	0.00013	0.00001	0.00014	2.06573
A1	1.87264	-0.00020	0.00030	0.00011	0.00041	1.87304
A2	2.27964	0.00004	-0.00033	-0.00024	-0.00057	2.27907
A3	2.13089	0.00016	0.00004	0.00011	0.00015	2.13103
A4	1.86420	0.00011	-0.00042	-0.00025	-0.00069	1.86351
A5	2.27533	0.00009	0.00076	0.00038	0.00115	2.27648
A6	2.14366	-0.00020	-0.00033	-0.00014	-0.00047	2.14319
A7	1.89788	-0.00029	0.00024	0.00023	0.00044	1.89832
A8	2.25230	0.00038	-0.00053	0.00040	-0.00013	2.25217
A9	2.13299	-0.00009	0.00029	-0.00060	-0.00030	2.13269
A10	1.88933	0.00036	0.00000	0.00009	0.00008	1.88940
A11	2.15390	-0.00039	0.00176	0.00182	0.00359	2.15748
A12	2.23985	0.00004	-0.00181	-0.00178	-0.00359	2.23626
A13	1.90072	0.00002	-0.00006	-0.00014	-0.00023	1.90049
A14	2.20001	0.00141	-0.00069	-0.00060	-0.00133	2.19868
A15	2.18174	-0.00143	0.00099	0.00084	0.00180	2.18353
A16	1.96198	-0.00041	0.00136	-0.00081	0.00059	1.96257
A17	1.87403	-0.00013	0.00010	0.00105	0.00114	1.87517
A18	1.88997	0.00046	-0.00086	-0.00071	-0.00159	1.88838
A19	1.90674	0.00020	0.00007	-0.00168	-0.00162	1.90511
A20	1.92795	0.00004	-0.00107	0.00125	0.00016	1.92811
A21	1.90161	-0.00016	0.00042	0.00097	0.00139	1.90300
A22	1.91728	-0.00023	0.00004	0.00191	0.00196	1.91925
A23	1.89366	-0.00017	0.00078	0.00083	0.00162	1.89528
A24	1.87513	0.00074	-0.00089	0.00050	-0.00044	1.87470
A25	1.87651	0.00005	0.00039	0.00002	0.00039	1.87690
A26	1.90012	0.00000	0.00022	0.00061	0.00084	1.90096
A27	2.00058	-0.00041	-0.00051	-0.00367	-0.00417	1.99642

A28	2.16186	-0.00008	0.00021	0.00060	0.00080	2.16266
A29	1.94601	-0.00002	0.00049	-0.00028	0.00020	1.94621
A30	2.17530	0.00010	-0.00069	-0.00032	-0.00102	2.17428
A31	2.07490	-0.00009	0.00014	-0.00016	-0.00002	2.07488
A32	2.16374	0.00005	-0.00021	0.00036	0.00015	2.16389
A33	2.04454	0.00004	0.00007	-0.00020	-0.00013	2.04441
A34	1.93529	0.00059	0.00028	0.00129	0.00175	1.93704
A35	1.91520	-0.00070	0.00065	0.00038	0.00110	1.91629
A36	1.88969	-0.00006	-0.00034	0.00039	-0.00002	1.88967
A37	2.08183	0.00043	0.00221	-0.00041	0.00253	2.08436
A38	2.08546	-0.00038	-0.00083	-0.00196	-0.00360	2.08185
A39	1.99679	-0.00061	-0.00108	0.00101	-0.00044	1.99635
A40	2.00441	0.00067	0.00082	-0.00289	-0.00188	2.00253
A41	2.02603	-0.00005	-0.00099	0.00250	0.00153	2.02757
A42	2.02568	0.00019	0.00102	-0.00482	-0.00444	2.02124
A43	2.12999	0.00040	0.00134	-0.00164	0.00030	2.13030
A44	1.95708	0.00103	-0.00084	-0.00244	-0.00301	1.95406
A45	2.03082	-0.00069	-0.00084	-0.00006	-0.00133	2.02949
A46	2.04503	-0.00057	-0.00086	0.00553	0.00472	2.04975
A47	2.60450	0.00007	-0.00004	-0.01242	-0.01411	2.59040
A48	2.56875	0.00000	-0.00147	-0.01071	-0.01403	2.55472
A49	1.93062	0.00028	-0.00036	0.00118	0.00082	1.93144
A50	1.91771	-0.00029	0.00005	0.00068	0.00073	1.91843
A51	1.94337	-0.00011	0.00013	-0.00050	-0.00037	1.94300
A52	1.87952	-0.00004	-0.00019	0.00024	0.00005	1.87958
A53	1.89459	0.00000	0.00022	-0.00084	-0.00062	1.89397
A54	1.89650	0.00017	0.00015	-0.00078	-0.00064	1.89587
A55	3.44185	-0.00080	-0.00586	0.01598	0.01013	3.45198
A56	2.62553	0.00006	-0.00540	-0.02276	-0.02901	2.59652
A57	2.88079	0.00022	-0.00717	0.00804	0.00088	2.88167
A58	3.07917	0.00063	0.00144	0.00433	0.00549	3.08465
D1	0.00288	0.00001	0.00160	-0.00269	-0.00109	0.00179
D2	-3.13665	0.00009	-0.00193	0.00100	-0.00093	-3.13758
D3	3.13625	-0.00006	0.00265	-0.00508	-0.00242	3.13383
D4	-0.00328	0.00001	-0.00088	-0.00139	-0.00226	-0.00554
D5	0.00070	-0.00026	0.00157	-0.00161	-0.00004	0.00066
D6	-3.10182	-0.00011	-0.00265	-0.00442	-0.00704	-3.10887
D7	-3.13353	-0.00019	0.00063	0.00053	0.00115	-3.13237
D8	0.04714	-0.00004	-0.00359	-0.00228	-0.00585	0.04129
D9	-0.00547	0.00023	-0.00420	0.00606	0.00186	-0.00361
D10	-3.13979	0.00010	-0.00176	0.00166	-0.00010	-3.13990
D11	3.13426	0.00016	-0.00100	0.00271	0.00171	3.13597
D12	-0.00007	0.00003	0.00144	-0.00169	-0.00025	-0.00032
D13	0.00595	-0.00039	0.00522	-0.00712	-0.00190	0.00405

D14	3.13255	-0.00012	0.00245	0.00180	0.00426	3.13681
D15	3.14087	-0.00027	0.00298	-0.00307	-0.00010	3.14078
D16	-0.01572	0.00000	0.00021	0.00584	0.00606	-0.00966
D17	0.05450	-0.00007	0.00577	-0.00338	0.00239	0.05690
D18	-3.09305	0.00003	0.00290	-0.00289	0.00001	-3.09304
D19	-3.07896	-0.00022	0.00850	-0.00831	0.00020	-3.07876
D20	0.05668	-0.00012	0.00563	-0.00782	-0.00219	0.05449
D21	-0.00413	0.00040	-0.00421	0.00542	0.00121	-0.00292
D22	3.09890	0.00034	-0.00013	0.00814	0.00805	3.10694
D23	-3.12977	0.00012	-0.00128	-0.00411	-0.00540	-3.13516
D24	-0.02674	0.00005	0.00280	-0.00139	0.00144	-0.02529
D25	1.29876	0.00012	0.00736	0.01946	0.02681	1.32557
D26	-2.88693	0.00003	0.00833	0.01758	0.02591	-2.86102
D27	-0.83607	0.00001	0.00843	0.01890	0.02733	-0.80874
D28	-1.79771	0.00024	0.00254	0.01625	0.01878	-1.77893
D29	0.29979	0.00015	0.00351	0.01437	0.01787	0.31767
D30	2.35066	0.00014	0.00361	0.01570	0.01929	2.36995
D31	-1.07284	-0.00025	0.00654	-0.00654	-0.00001	-1.07285
D32	0.97395	-0.00041	0.00747	-0.00496	0.00251	0.97646
D33	-3.13725	-0.00055	0.00676	-0.00861	-0.00184	-3.13909
D34	3.13187	0.00004	0.00550	-0.00622	-0.00073	3.13114
D35	-1.10452	-0.00012	0.00643	-0.00464	0.00180	-1.10273
D36	1.06747	-0.00026	0.00572	-0.00829	-0.00256	1.06490
D37	1.04035	0.00009	0.00560	-0.00712	-0.00152	1.03883
D38	3.08714	-0.00007	0.00653	-0.00554	0.00100	3.08814
D39	-1.02406	-0.00021	0.00583	-0.00919	-0.00336	-1.02741
D40	2.99103	-0.00001	-0.00507	-0.02500	-0.03011	2.96092
D41	-1.20542	-0.00017	-0.00489	-0.02346	-0.02833	-1.23375
D42	0.91557	-0.00016	-0.00474	-0.02789	-0.03266	0.88291
D43	3.00230	-0.00031	-0.00457	-0.02635	-0.03088	2.97142
D44	-1.18640	0.00005	-0.00506	-0.02591	-0.03101	-1.21741
D45	0.90033	-0.00011	-0.00488	-0.02437	-0.02923	0.87111
D46	-3.14123	0.00013	-0.00133	0.00042	-0.00091	3.14105
D47	0.00465	0.00001	-0.00036	-0.00027	-0.00063	0.00402
D48	0.00710	0.00002	0.00193	-0.00014	0.00178	0.00889
D49	-3.13021	-0.00010	0.00289	-0.00082	0.00206	-3.12814
D50	2.03800	-0.00003	0.02955	0.08045	0.11050	2.14850
D51	-1.13796	0.00030	0.02122	-0.04638	-0.02555	-1.16351
D52	-2.21947	-0.00013	0.02862	0.07348	0.10245	-2.11702
D53	0.88775	0.00021	0.02028	-0.05335	-0.03360	0.85415
D54	-2.71734	0.00021	-0.00388	0.00141	-0.00241	-2.71975
D55	-0.01332	0.00010	-0.00030	0.00042	0.00017	-0.01316
D56	-0.03547	0.00018	-0.00322	0.00237	-0.00090	-0.03637
D57	2.66854	0.00007	0.00036	0.00138	0.00168	2.67022

D58	0.85648	-0.00049	-0.01092	-0.07881	-0.08915	0.76734
D59	-1.55062	-0.00047	-0.00899	-0.08063	-0.08888	-1.63950
D60	1.58301	-0.00001	0.00481	0.08039	0.08458	1.66759
D61	-0.83841	0.00048	0.00819	0.07445	0.08213	-0.75627
D62	2.55134	-0.00003	-0.00147	-0.00320	-0.00455	2.54679
D63	-1.65901	-0.00009	-0.00189	-0.00175	-0.00352	-1.66253
D64	0.44303	-0.00015	-0.00159	-0.00261	-0.00407	0.43895
D65	1.35226	0.00018	-0.00095	-0.00387	-0.00492	1.34733
D66	-2.85810	0.00012	-0.00137	-0.00242	-0.00390	-2.86199
D67	-0.75606	0.00006	-0.00107	-0.00328	-0.00445	-0.76051
D68	-1.03239	0.00004	0.00257	-0.00666	-0.00411	-1.03650
D69	1.04044	-0.00002	0.00215	-0.00521	-0.00308	1.03736
D70	-3.14071	-0.00008	0.00245	-0.00606	-0.00363	3.13885

Item	Value	Threshold	Converged?
Maximum Force	0.001432	0.000450	NO
RMS Force	0.000311	0.000300	NO
Maximum Displacement	0.163845	0.001800	NO
RMS Displacement	0.034906	0.001200	NO

Predicted change in Energy=-7.364320D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.651492	2.079089	-0.220457
2	6	0	-3.556483	1.115412	0.086889
3	7	0	-2.857529	-0.083413	0.156626
4	6	0	-1.560735	0.155787	-0.108059
5	7	0	-1.414996	1.462070	-0.337191
6	6	0	-0.134473	2.135244	-0.623722
7	6	0	0.423019	2.874749	0.595755
8	1	0	-2.779422	3.136966	-0.372259
9	1	0	-4.615513	1.182344	0.255867
10	1	0	0.576275	1.367849	-0.932651
11	1	0	-0.291692	2.828341	-1.451217
12	1	0	-0.276194	3.656346	0.910925
13	1	0	0.517474	2.159997	1.426303
14	35	0	0.137351	-2.666685	0.137737
15	1	0	-0.781214	-0.630393	-0.113865
16	6	0	-3.345978	-1.393919	0.445499
17	6	0	-4.626073	-1.679602	0.643466
18	1	0	-2.539117	-2.123168	0.473542

19	1	0	-4.906123	-2.702076	0.856702
20	1	0	-5.423296	-0.947495	0.601481
21	7	0	1.679502	3.498653	0.191573
22	1	0	2.011298	4.140206	0.902469
23	1	0	2.390403	2.782840	0.050516
24	6	0	3.500130	-0.255961	-1.208786
25	6	0	3.311687	-0.554870	0.212894
26	8	0	2.870319	0.718738	-0.345741
27	1	0	4.485129	0.032531	-1.568068
28	1	0	2.838017	-0.711025	-1.939585
29	1	0	2.472786	-1.206814	0.453302
30	6	0	4.444772	-0.492381	1.198132
31	1	0	4.089036	-0.150290	2.174336
32	1	0	4.877519	-1.488455	1.332257
33	1	0	5.230724	0.186755	0.857546

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357257	0.000000			
3	N	2.204781	1.389454	0.000000		
4	C	2.213927	2.223037	1.344971	0.000000	
5	N	1.386816	2.210426	2.171007	1.334210	0.000000
6	C	2.549737	3.640767	3.598113	2.493669	1.474790
7	C	3.279008	4.380714	4.439093	3.438516	2.498870
8	H	1.076343	2.213893	3.264454	3.231475	2.160593
9	H	2.210977	1.074513	2.168525	3.243136	3.266998
10	H	3.381059	4.264138	3.883773	2.591498	2.080532
11	H	2.764924	3.994842	4.200832	3.249168	2.090350
12	H	3.067540	4.230329	4.606306	3.865525	2.769388
13	H	3.572213	4.413878	4.246835	3.269568	2.707665
14	Br	5.516187	5.286895	3.955118	3.303069	4.436436
15	H	3.294024	3.284853	2.164125	1.107143	2.197716
16	C	3.603831	2.543552	1.428095	2.427984	3.535246
17	C	4.332792	3.043994	2.431580	3.650991	4.598130
18	H	4.260661	3.416568	2.088642	2.547376	3.843809
19	H	5.394735	4.121571	3.397681	4.504415	5.563583
20	H	4.185534	2.829378	2.743665	4.079222	4.770071
21	N	4.576291	5.753811	5.780750	4.665155	3.742083
22	H	5.220228	6.388642	6.488507	5.445749	4.522020
23	H	5.097979	6.176334	5.980590	4.747425	4.046704
24	C	6.653699	7.304467	6.504918	5.195527	5.279184
25	C	6.533378	7.069475	6.187460	4.934425	5.168383
26	O	5.688290	6.453550	5.805520	4.472991	4.349315

27	H	7.545582	8.281247	7.543384	6.220876	6.194362
28	H	6.393343	6.952129	6.101413	4.843023	5.037671
29	H	6.124486	6.471404	5.455483	4.294310	4.781492
30	C	7.679961	8.236501	7.387529	6.179998	6.365059
31	H	7.492654	8.025796	7.233974	6.101059	6.261137
32	H	8.474922	8.914228	7.949039	6.799203	7.147616
33	H	8.177551	8.869686	8.123061	6.859831	6.871640

		6	7	8	9	10
6	C	0.000000				
7	C	1.531270	0.000000			
8	H	2.839443	3.355807	0.000000		
9	H	4.664914	5.326027	2.754328	0.000000	
10	H	1.090640	2.151804	3.834647	5.329320	0.000000
11	H	1.090802	2.168655	2.729140	4.931417	1.776320
12	H	2.165404	1.095045	2.860501	5.037805	3.059851
13	H	2.151336	1.099818	3.880569	5.354744	2.489100
14	Br	4.869521	5.567664	6.515369	6.117083	4.197124
15	H	2.885650	3.773560	4.272306	4.257296	2.550717
16	C	4.889989	5.696441	4.638818	2.878335	4.991065
17	C	6.027710	6.799832	5.257484	2.888092	6.231815
18	H	5.012024	5.811055	5.333117	3.909631	4.885719
19	H	6.954133	7.718084	6.334636	3.941341	7.058524
20	H	6.243081	6.984911	4.961961	2.303948	6.611296
21	N	2.411244	1.459921	4.508961	6.707954	2.649777
22	H	3.309602	2.053798	5.057907	7.285717	3.621177
23	H	2.692392	2.043608	5.199157	7.189341	2.501975
24	C	4.389818	4.746191	7.186412	8.371237	3.355882
25	C	4.451142	4.500363	7.146585	8.115434	3.534346
26	O	3.333547	3.394713	6.145576	7.524264	2.455289
27	H	5.162743	5.409351	7.990068	9.352567	4.179231
28	H	4.320699	5.011780	6.987072	7.997498	3.232818
29	H	4.373458	4.569572	6.865541	7.482716	3.485184
30	C	5.585074	5.279670	8.235731	9.261821	4.792281
31	H	5.557951	5.008238	8.029129	9.012525	4.929260
32	H	6.486688	6.278738	9.106517	9.920154	5.638172
33	H	5.897127	5.514333	8.624304	9.914717	5.124811

		11	12	13	14	15
11	H	0.000000				
12	H	2.503107	0.000000			
13	H	3.062932	1.770475	0.000000		
14	Br	5.736215	6.383538	5.010165	0.000000	
15	H	3.740452	4.436369	3.441654	2.248011	0.000000
16	C	5.545600	5.928353	5.340276	3.721321	2.733839
17	C	6.595157	6.889508	6.466176	4.890839	4.056764

18	H	5.768281	6.222130	5.347523	2.751664	2.379842
19	H	7.563397	7.865666	7.306134	5.094585	4.716858
20	H	6.693569	6.912580	6.754967	5.838791	4.707569
21	N	2.652110	2.089756	2.160293	6.355511	4.816372
22	H	3.544657	2.338122	2.535181	7.101427	5.620469
23	H	3.074233	2.934971	2.405948	5.897556	4.662224
24	C	4.893834	5.836090	4.655834	4.351206	4.434970
25	C	5.215335	5.576242	4.080501	3.813374	4.106618
26	O	3.958638	4.484338	3.279214	4.377666	3.899694
27	H	5.536084	6.476700	5.406908	5.394322	5.503503
28	H	4.749810	6.074343	4.995686	3.928545	4.054452
29	H	5.249000	5.605053	4.013152	2.772194	3.352977
30	C	6.362416	6.291418	4.744559	4.940234	5.389927
31	H	6.419318	5.928061	4.318915	5.108404	5.402378
32	H	7.287194	7.294331	5.685952	5.028349	5.903287
33	H	6.542587	6.508998	5.141196	5.882406	6.144491

		16	17	18	19	20
16	C	0.000000				
17	C	1.326442	0.000000			
18	H	1.087941	2.140330	0.000000		
19	H	2.077117	1.081365	2.466711	0.000000	
20	H	2.130464	1.083193	3.117221	1.846932	0.000000
21	N	7.018347	8.171830	7.034282	9.069834	8.389637
22	H	7.715942	8.831305	7.753716	9.729832	9.013794
23	H	7.106855	8.336421	6.967642	9.163707	8.675993
24	C	7.134480	8.455340	6.541345	8.995266	9.131420
25	C	6.714358	8.028602	6.062953	8.518062	8.752433
26	O	6.612997	7.932620	6.165197	8.580262	8.512204
27	H	8.210691	9.530807	7.625958	10.077361	10.190402
28	H	6.663089	7.957571	6.060602	8.470845	8.646515
29	H	5.821776	7.117126	5.095025	7.539684	7.901728
30	C	7.878769	9.165008	7.208273	9.614497	9.896559
31	H	7.734010	8.979726	7.121611	9.442491	9.674392
32	H	8.271709	9.530438	7.493113	9.870090	10.340864
33	H	8.730872	10.034220	8.115025	10.540446	10.717287

		21	22	23	24	25
21	N	0.000000				
22	H	1.013435	0.000000			
23	H	1.018659	1.646811	0.000000		
24	C	4.401457	5.099049	3.471548	0.000000	
25	C	4.369844	4.920393	3.466329	1.464934	0.000000
26	O	3.071592	3.741976	2.155888	1.446218	1.459095
27	H	4.793942	5.394107	3.817315	1.087444	2.212201
28	H	4.858537	5.682884	4.045732	1.086068	2.209505

29	H	4.779039	5.385661	4.010780	2.173038	1.089304
30	C	4.958652	5.241190	4.032930	2.596439	1.502824
31	H	4.801248	4.933861	3.999901	3.435621	2.148304
32	H	6.033218	6.331016	5.106130	3.142156	2.139249
33	H	4.901364	5.098676	3.931714	2.731425	2.155989

		26	27	28	29	30
26	O	0.000000				
27	H	2.138358	0.000000			
28	H	2.141402	1.844960	0.000000		
29	H	2.122323	3.109894	2.470852	0.000000	
30	C	2.515801	2.815852	3.531958	2.225739	0.000000
31	H	2.931087	3.767745	4.336336	2.586593	1.093869
32	H	3.422899	3.298371	3.933054	2.575777	1.094269
33	H	2.702299	2.542302	3.788799	3.116356	1.093135

		31	32	33
31	H	0.000000		
32	H	1.766774	0.000000	
33	H	1.775102	1.776635	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.361145	2.465254	-0.233390
2	6	0	-3.362136	1.583073	0.015446
3	7	0	-2.786275	0.318746	0.036472
4	6	0	-1.467725	0.439883	-0.199537
5	7	0	-1.189724	1.734451	-0.363623
6	6	0	0.155862	2.289574	-0.600777
7	6	0	0.761970	2.912336	0.660013
8	1	0	-2.381322	3.536528	-0.335750
9	1	0	-4.412210	1.747034	0.173688
10	1	0	0.792741	1.470541	-0.937029
11	1	0	0.082488	3.032677	-1.395927
12	1	0	0.137858	3.744046	1.003330
13	1	0	0.770704	2.153807	1.456354
14	35	0	-0.061154	-2.545830	-0.067845
15	1	0	-0.769635	-0.418787	-0.233055

16	6	0	-3.406732	-0.948726	0.255574
17	6	0	-4.712076	-1.114615	0.422927
18	1	0	-2.676419	-1.755105	0.258958
19	1	0	-5.095414	-2.112995	0.583053
20	1	0	-5.432271	-0.305705	0.405881
21	7	0	2.080854	3.426360	0.302671
22	1	0	2.461731	3.997908	1.047867
23	1	0	2.720008	2.650758	0.136566
24	6	0	3.546455	-0.421324	-1.253017
25	6	0	3.304309	-0.765943	0.150064
26	8	0	3.000766	0.569886	-0.352310
27	1	0	4.561321	-0.215780	-1.585181
28	1	0	2.855687	-0.773737	-2.013403
29	1	0	2.401030	-1.341728	0.347906
30	6	0	4.420423	-0.862421	1.151793
31	1	0	4.082980	-0.532520	2.138630
32	1	0	4.750293	-1.901753	1.243430
33	1	0	5.275475	-0.249674	0.854519

Rotational constants (GHZ): 0.4236257 0.2850398 0.1795482

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1306.1799186928 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 3.63D-06 NBF= 482

NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999999 0.000729 0.000553 -0.000805 Ang= 0.14 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3205.64817135 A.U. after 11 cycles
NFock= 11 Conv=0.46D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000296597	0.000107076	0.000133431
2	6	0.000467709	0.000012229	0.000026936
3	7	-0.000854045	-0.000926360	-0.000018080
4	6	0.001707586	0.001903173	0.000372853
5	7	-0.000164094	0.000554783	-0.000695488
6	6	-0.000638464	-0.001077711	-0.000105224
7	6	0.001369736	0.000434169	-0.000418707
8	1	0.000008130	0.000016671	0.000154959
9	1	-0.000052486	-0.000085319	0.000035579
10	1	-0.000205911	0.000108608	-0.000324963
11	1	0.000225945	0.000014692	0.000018093
12	1	0.000014801	0.000041178	-0.000102955
13	1	-0.000367045	-0.000257225	0.000194391
14	35	-0.000058928	0.000041121	-0.000021321
15	1	-0.000733258	-0.000942560	0.000422973
16	6	-0.000242485	-0.000297362	-0.000417387
17	6	0.000045863	0.000249932	-0.000019721
18	1	0.000328775	-0.000138465	0.000010398
19	1	0.000089060	-0.000006255	0.000075052
20	1	-0.000063387	0.000086537	0.000061762
21	7	-0.000350853	-0.000014482	0.000659710
22	1	0.000133013	-0.000055996	-0.000178821
23	1	-0.000144032	0.000373880	0.000197860
24	6	-0.000177363	0.000917057	0.000515297
25	6	-0.001495926	0.000343258	-0.001338636

26	8	0.000838556	-0.001105646	-0.000355929
27	1	-0.000126264	0.000129301	-0.000277089
28	1	0.000163101	-0.000222748	-0.000017899
29	1	0.001002380	-0.000398664	0.000926214
30	6	-0.000141746	0.000376186	0.000529087
31	1	0.000054686	-0.000189194	0.000086875
32	1	-0.000250321	0.000019246	-0.000062960
33	1	-0.000086137	-0.000011109	-0.000066291

Cartesian Forces: Max 0.001903173 RMS 0.000520441

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.001510965 RMS 0.000319538
Search for a local minimum.
Step number 30 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 25 28 29 30
DE= -8.35D-05 DEPred=-7.36D-05 R= 1.13D+00
TightC=F SS= 1.41D+00 RLast= 2.57D-01 DXNew= 1.4210D+00 7.7183D-01
Trust test= 1.13D+00 RLast= 2.57D-01 DXMaxT set to 8.45D-01
ITU= 1 1 1 1 0 0 -1 1 -1 1 1 1 1 1 1 1 1 0 -1
ITU= -1 1 1 1 -1 1 0 0 -1 0

Eigenvalues ---	0.00051	0.00174	0.00234	0.00429	0.00653
Eigenvalues ---	0.00729	0.00767	0.01309	0.01516	0.01886
Eigenvalues ---	0.01961	0.02176	0.02355	0.02390	0.02473
Eigenvalues ---	0.02690	0.02871	0.03052	0.03096	0.03246
Eigenvalues ---	0.03340	0.03661	0.03795	0.03868	0.04065
Eigenvalues ---	0.04374	0.04551	0.05263	0.05460	0.05741
Eigenvalues ---	0.05796	0.05922	0.06908	0.07594	0.08653
Eigenvalues ---	0.08988	0.09560	0.10479	0.12209	0.12566
Eigenvalues ---	0.12735	0.13741	0.14888	0.15883	0.15991
Eigenvalues ---	0.16001	0.16004	0.16011	0.16024	0.16088
Eigenvalues ---	0.16264	0.20047	0.21167	0.22148	0.22454
Eigenvalues ---	0.23132	0.23472	0.25356	0.26336	0.27827
Eigenvalues ---	0.28933	0.29447	0.30824	0.31748	0.32446
Eigenvalues ---	0.33783	0.34281	0.34351	0.34372	0.34547
Eigenvalues ---	0.34688	0.34727	0.35079	0.35223	0.35364
Eigenvalues ---	0.35546	0.35633	0.35892	0.36236	0.36425
Eigenvalues ---	0.36670	0.39268	0.40585	0.41848	0.42446

Eigenvalues --- 0.44982 0.45490 0.46265 0.49474 0.55082

Eigenvalues --- 0.58071 0.60619 1.29170

En-DIIS/RFO-DIIS IScMMF= 0 using points: 30 29 28 27 26

RFO step: Lambda=-3.33224649D-05.

DidBck=F Rises=F RFO-DIIS coefs: 1.47887 -0.23407 -0.34979 -0.04551 0.15051

Iteration 1 RMS(Cart)= 0.04116671 RMS(Int)= 0.00110425

Iteration 2 RMS(Cart)= 0.00193604 RMS(Int)= 0.00043125

Iteration 3 RMS(Cart)= 0.00000355 RMS(Int)= 0.00043124

Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00043124

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56484	0.00014	0.00010	-0.00008	0.00001	2.56486
R2	2.62070	0.00025	-0.00018	0.00024	0.00006	2.62076
R3	2.03399	-0.00001	0.00001	-0.00001	0.00001	2.03400
R4	2.62569	-0.00010	0.00020	-0.00015	0.00005	2.62573
R5	2.03054	0.00005	-0.00011	0.00008	-0.00003	2.03050
R6	2.54163	0.00038	-0.00065	0.00072	0.00008	2.54170
R7	2.69871	-0.00001	-0.00015	0.00008	-0.00007	2.69864
R8	2.52129	-0.00006	0.00012	0.00027	0.00039	2.52168
R9	2.09220	0.00008	-0.00048	-0.00020	-0.00068	2.09152
R10	2.78695	-0.00039	0.00061	-0.00071	-0.00010	2.78684
R11	2.89368	0.00056	0.00008	0.00099	0.00108	2.89476
R12	2.06101	-0.00012	0.00009	-0.00020	-0.00011	2.06090
R13	2.06132	-0.00004	-0.00015	0.00001	-0.00014	2.06117
R14	2.06934	-0.00001	-0.00020	-0.00003	-0.00022	2.06911
R15	2.07836	0.00028	-0.00060	0.00053	-0.00008	2.07828
R16	2.75885	-0.00059	0.00098	-0.00084	0.00014	2.75899
R17	4.24812	-0.00006	0.00401	0.00676	0.01077	4.25889
R18	2.50661	-0.00012	0.00002	-0.00014	-0.00012	2.50649
R19	2.05591	0.00034	-0.00017	0.00061	0.00045	2.05636
R20	2.04348	0.00000	-0.00002	0.00000	-0.00001	2.04347
R21	2.04694	0.00010	-0.00002	0.00014	0.00012	2.04706
R22	1.91512	-0.00012	-0.00014	-0.00026	-0.00040	1.91471
R23	1.92499	-0.00042	0.00035	-0.00091	-0.00038	1.92461
R24	4.07404	0.00008	0.01796	0.02336	0.04124	4.11527
R25	2.76832	0.00036	0.00224	-0.00133	-0.00038	2.76795
R26	2.73296	-0.00075	0.00033	0.00055	0.00144	2.73439
R27	2.05497	0.00001	-0.00021	-0.00009	-0.00030	2.05467
R28	2.05237	0.00001	-0.00029	-0.00010	-0.00039	2.05198
R29	2.75729	-0.00074	-0.00094	-0.00062	-0.00081	2.75648
R30	2.05849	-0.00033	0.00041	-0.00050	-0.00009	2.05839
R31	2.83993	0.00001	-0.00009	0.00033	0.00024	2.84016
R32	2.06711	0.00000	0.00020	0.00015	0.00036	2.06747

R33	2.06787	-0.00013	0.00001	-0.00006	-0.00005	2.06782
R34	2.06573	-0.00005	0.00005	-0.00009	-0.00004	2.06568
A1	1.87304	-0.00007	0.00013	-0.00015	-0.00003	1.87302
A2	2.27907	0.00001	-0.00024	-0.00003	-0.00028	2.27879
A3	2.13103	0.00005	0.00011	0.00018	0.00029	2.13132
A4	1.86351	0.00025	-0.00031	0.00067	0.00036	1.86387
A5	2.27648	-0.00003	0.00029	-0.00023	0.00006	2.27654
A6	2.14319	-0.00022	0.00001	-0.00043	-0.00042	2.14277
A7	1.89832	-0.00029	0.00021	-0.00064	-0.00041	1.89791
A8	2.25217	0.00029	0.00046	0.00015	0.00060	2.25277
A9	2.13269	0.00001	-0.00067	0.00048	-0.00020	2.13249
A10	1.88940	0.00025	0.00006	0.00029	0.00034	1.88974
A11	2.15748	-0.00151	0.00173	-0.00413	-0.00244	2.15505
A12	2.23626	0.00126	-0.00170	0.00386	0.00213	2.23839
A13	1.90049	-0.00014	-0.00011	-0.00017	-0.00026	1.90023
A14	2.19868	0.00064	-0.00004	0.00100	0.00097	2.19964
A15	2.18353	-0.00051	0.00019	-0.00080	-0.00061	2.18293
A16	1.96257	-0.00058	-0.00121	-0.00082	-0.00198	1.96059
A17	1.87517	0.00003	0.00140	-0.00035	0.00103	1.87620
A18	1.88838	0.00035	-0.00017	-0.00003	-0.00022	1.88816
A19	1.90511	0.00045	-0.00157	0.00052	-0.00106	1.90405
A20	1.92811	-0.00004	0.00087	0.00034	0.00120	1.92931
A21	1.90300	-0.00022	0.00076	0.00034	0.00111	1.90411
A22	1.91925	-0.00038	0.00140	-0.00027	0.00114	1.92038
A23	1.89528	-0.00041	0.00050	-0.00164	-0.00111	1.89417
A24	1.87470	0.00100	0.00061	0.00256	0.00311	1.87780
A25	1.87690	0.00013	-0.00020	-0.00068	-0.00089	1.87601
A26	1.90096	-0.00038	0.00072	-0.00215	-0.00143	1.89954
A27	1.99642	0.00001	-0.00288	0.00212	-0.00074	1.99568
A28	2.16266	-0.00027	0.00079	-0.00077	0.00002	2.16268
A29	1.94621	0.00002	-0.00026	0.00003	-0.00023	1.94598
A30	2.17428	0.00026	-0.00054	0.00076	0.00022	2.17450
A31	2.07488	-0.00011	-0.00004	-0.00054	-0.00058	2.07430
A32	2.16389	0.00005	0.00019	0.00042	0.00061	2.16450
A33	2.04441	0.00006	-0.00015	0.00012	-0.00003	2.04438
A34	1.93704	0.00022	0.00040	0.00124	0.00183	1.93887
A35	1.91629	0.00005	0.00097	0.00011	0.00115	1.91745
A36	1.88967	-0.00020	0.00050	0.00042	0.00084	1.89051
A37	2.08436	0.00040	0.00235	0.00243	0.00605	2.09041
A38	2.08185	-0.00019	-0.00350	-0.00436	-0.00923	2.07262
A39	1.99635	-0.00049	-0.00008	-0.00094	-0.00145	1.99490
A40	2.00253	0.00073	-0.00114	0.00065	-0.00032	2.00221
A41	2.02757	-0.00018	0.00173	0.00158	0.00335	2.03092
A42	2.02124	0.00052	-0.00306	-0.00200	-0.00568	2.01557

A43	2.13030	0.00052	-0.00103	0.00341	0.00294	2.13324
A44	1.95406	0.00118	-0.00074	0.00238	0.00204	1.95610
A45	2.02949	-0.00045	-0.00019	-0.00239	-0.00324	2.02625
A46	2.04975	-0.00100	0.00347	-0.00122	0.00230	2.05205
A47	2.59040	-0.00016	-0.01087	-0.01880	-0.03191	2.55849
A48	2.55472	-0.00019	-0.00576	-0.01592	-0.02524	2.52949
A49	1.93144	0.00021	0.00071	0.00116	0.00187	1.93331
A50	1.91843	-0.00033	0.00041	-0.00090	-0.00048	1.91795
A51	1.94300	-0.00008	-0.00017	-0.00003	-0.00020	1.94280
A52	1.87958	-0.00003	0.00027	-0.00049	-0.00022	1.87936
A53	1.89397	0.00004	-0.00070	0.00032	-0.00038	1.89360
A54	1.89587	0.00019	-0.00055	-0.00008	-0.00063	1.89524
A55	3.45198	0.00016	0.00875	0.00691	0.01567	3.46765
A56	2.59652	0.00035	-0.00809	-0.02867	-0.03749	2.55903
A57	2.88167	0.00000	0.00594	0.01307	0.01901	2.90068
A58	3.08465	0.00034	0.00228	-0.00062	0.00138	3.08604
D1	0.00179	0.00001	-0.00105	0.00110	0.00005	0.00184
D2	-3.13758	0.00007	0.00096	0.00103	0.00199	-3.13559
D3	3.13383	0.00000	-0.00288	0.00120	-0.00169	3.13214
D4	-0.00554	0.00006	-0.00088	0.00113	0.00025	-0.00529
D5	0.00066	-0.00019	-0.00061	0.00010	-0.00052	0.00014
D6	-3.10887	-0.00004	-0.00327	-0.00051	-0.00381	-3.11268
D7	-3.13237	-0.00018	0.00103	0.00001	0.00105	-3.13132
D8	0.04129	-0.00003	-0.00162	-0.00060	-0.00224	0.03905
D9	-0.00361	0.00017	0.00234	-0.00193	0.00042	-0.00319
D10	-3.13990	0.00009	0.00048	0.00036	0.00085	-3.13905
D11	3.13597	0.00012	0.00052	-0.00186	-0.00133	3.13463
D12	-0.00032	0.00004	-0.00134	0.00043	-0.00091	-0.00122
D13	0.00405	-0.00029	-0.00275	0.00200	-0.00075	0.00331
D14	3.13681	-0.00008	0.00273	0.00450	0.00723	-3.13915
D15	3.14078	-0.00022	-0.00104	-0.00010	-0.00114	3.13964
D16	-0.00966	0.00000	0.00444	0.00240	0.00684	-0.00282
D17	0.05690	-0.00013	-0.00573	-0.01928	-0.02501	0.03188
D18	-3.09304	-0.00001	-0.00555	-0.01787	-0.02342	-3.11646
D19	-3.07876	-0.00022	-0.00781	-0.01672	-0.02454	-3.10330
D20	0.05449	-0.00009	-0.00763	-0.01531	-0.02294	0.03155
D21	-0.00292	0.00030	0.00209	-0.00131	0.00078	-0.00214
D22	3.10694	0.00017	0.00475	-0.00066	0.00407	3.11101
D23	-3.13516	0.00009	-0.00377	-0.00389	-0.00766	3.14037
D24	-0.02529	-0.00004	-0.00111	-0.00325	-0.00437	-0.02966
D25	1.32557	-0.00022	0.01021	-0.01212	-0.00191	1.32366
D26	-2.86102	0.00001	0.00845	-0.01219	-0.00374	-2.86475
D27	-0.80874	-0.00004	0.01001	-0.01200	-0.00199	-0.81073
D28	-1.77893	-0.00006	0.00712	-0.01284	-0.00573	-1.78466

D29	0.31767	0.00017	0.00536	-0.01292	-0.00756	0.31011
D30	2.36995	0.00012	0.00692	-0.01272	-0.00581	2.36414
D31	-1.07285	0.00004	-0.00399	-0.00073	-0.00471	-1.07757
D32	0.97646	-0.00026	-0.00315	-0.00266	-0.00580	0.97066
D33	-3.13909	0.00012	-0.00597	0.00051	-0.00545	3.13864
D34	3.13114	0.00006	-0.00393	-0.00012	-0.00406	3.12709
D35	-1.10273	-0.00024	-0.00308	-0.00206	-0.00514	-1.10787
D36	1.06490	0.00014	-0.00591	0.00112	-0.00479	1.06011
D37	1.03883	0.00007	-0.00441	-0.00109	-0.00550	1.03333
D38	3.08814	-0.00023	-0.00357	-0.00302	-0.00658	3.08156
D39	-1.02741	0.00015	-0.00640	0.00015	-0.00624	-1.03365
D40	2.96092	-0.00013	-0.01518	0.00055	-0.01467	2.94625
D41	-1.23375	-0.00021	-0.01368	0.00194	-0.01171	-1.24546
D42	0.88291	-0.00004	-0.01758	0.00061	-0.01700	0.86591
D43	2.97142	-0.00012	-0.01608	0.00200	-0.01404	2.95738
D44	-1.21741	0.00007	-0.01593	0.00164	-0.01434	-1.23175
D45	0.87111	-0.00001	-0.01443	0.00303	-0.01138	0.85973
D46	3.14105	0.00015	-0.00036	-0.00062	-0.00097	3.14008
D47	0.00402	0.00001	-0.00048	-0.00148	-0.00196	0.00206
D48	0.00889	0.00000	-0.00057	-0.00221	-0.00277	0.00611
D49	-3.12814	-0.00013	-0.00069	-0.00307	-0.00376	-3.13190
D50	2.14850	-0.00004	0.03673	0.08333	0.12053	2.26903
D51	-1.16351	-0.00015	-0.02787	-0.06107	-0.08931	-1.25282
D52	-2.11702	0.00008	0.03436	0.07430	0.10899	-2.00804
D53	0.85415	-0.00003	-0.03024	-0.07010	-0.10085	0.75330
D54	-2.71975	0.00020	-0.00099	0.00185	0.00085	-2.71890
D55	-0.01316	0.00003	-0.00175	0.00195	0.00020	-0.01296
D56	-0.03637	0.00021	0.00086	0.00142	0.00210	-0.03427
D57	2.67022	0.00004	0.00010	0.00152	0.00145	2.67167
D58	0.76734	-0.00027	-0.03712	-0.09159	-0.12764	0.63970
D59	-1.63950	-0.00025	-0.03847	-0.09380	-0.13095	-1.77045
D60	1.66759	-0.00032	0.03860	0.08888	0.12692	1.79451
D61	-0.75627	0.00040	0.03413	0.09078	0.12454	-0.63174
D62	2.54679	-0.00008	-0.00249	0.00070	-0.00164	2.54515
D63	-1.66253	-0.00019	-0.00145	0.00025	-0.00105	-1.66359
D64	0.43895	-0.00022	-0.00198	-0.00047	-0.00230	0.43665
D65	1.34733	0.00027	-0.00194	0.00010	-0.00194	1.34540
D66	-2.86199	0.00016	-0.00090	-0.00035	-0.00135	-2.86334
D67	-0.76051	0.00013	-0.00142	-0.00107	-0.00259	-0.76310
D68	-1.03650	0.00011	-0.00478	0.00065	-0.00417	-1.04067
D69	1.03736	0.00000	-0.00374	0.00020	-0.00358	1.03378
D70	3.13885	-0.00003	-0.00427	-0.00052	-0.00483	3.13402

Item	Value	Threshold	Converged?
Maximum Force	0.001511	0.000450	NO

RMS	Force	0.000320	0.000300	NO
Maximum	Displacement	0.255559	0.001800	NO
RMS	Displacement	0.042182	0.001200	NO

Predicted change in Energy=-6.612525D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.642885	2.085253	-0.195214
2	6	0	-3.543926	1.117226	0.110102
3	7	0	-2.844700	-0.082704	0.153658
4	6	0	-1.551316	0.160467	-0.123977
5	7	0	-1.408106	1.469969	-0.336964
6	6	0	-0.131461	2.145407	-0.634963
7	6	0	0.440909	2.872971	0.585522
8	1	0	-2.773171	3.144960	-0.331469
9	1	0	-4.600917	1.181396	0.292295
10	1	0	0.575986	1.381274	-0.958980
11	1	0	-0.300026	2.845902	-1.453850
12	1	0	-0.251504	3.654548	0.915017
13	1	0	0.539524	2.150337	1.408679
14	35	0	0.123753	-2.688464	0.002500
15	1	0	-0.775313	-0.628013	-0.156966
16	6	0	-3.329354	-1.397458	0.429137
17	6	0	-4.603046	-1.682190	0.665596
18	1	0	-2.525165	-2.130367	0.413187
19	1	0	-4.880153	-2.708466	0.863853
20	1	0	-5.397734	-0.946058	0.670727
21	7	0	1.696674	3.496698	0.178569
22	1	0	2.029874	4.140883	0.886117
23	1	0	2.407911	2.781774	0.036149
24	6	0	3.489254	-0.283952	-1.200381
25	6	0	3.290110	-0.573388	0.221595
26	8	0	2.815017	0.678779	-0.356400
27	1	0	4.465722	0.037681	-1.554286
28	1	0	2.850656	-0.775799	-1.927960
29	1	0	2.471893	-1.254819	0.451049
30	6	0	4.401861	-0.457915	1.226347
31	1	0	4.017820	-0.117284	2.192497
32	1	0	4.867791	-1.435996	1.380086
33	1	0	5.169136	0.244716	0.890944

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357265	0.000000			
3	N	2.205103	1.389477	0.000000		
4	C	2.213910	2.222763	1.345011	0.000000	
5	N	1.386848	2.210435	2.171476	1.334417	0.000000
6	C	2.550343	3.641043	3.598343	2.493408	1.474734
7	C	3.277169	4.380362	4.440468	3.439481	2.497649
8	H	1.076346	2.213764	3.264703	3.231592	2.160793
9	H	2.210998	1.074496	2.168287	3.242783	3.266999
10	H	3.382316	4.264544	3.883593	2.590949	2.081200
11	H	2.766178	3.994640	4.199545	3.247438	2.090087
12	H	3.068225	4.233902	4.612091	3.870093	2.770842
13	H	3.564328	4.407741	4.244352	3.268062	2.702486
14	Br	5.521028	5.286466	3.952789	3.307304	4.444592
15	H	3.294101	3.283657	2.162455	1.106784	2.198717
16	C	3.604209	2.543906	1.428060	2.427856	3.535568
17	C	4.333227	3.044182	2.431505	3.651283	4.598792
18	H	4.260922	3.417103	2.088631	2.546536	3.843562
19	H	5.395065	4.121840	3.397362	4.504191	5.563847
20	H	4.186633	2.829850	2.744216	4.080549	4.771767
21	N	4.578610	5.755907	5.782458	4.665985	3.743402
22	H	5.218196	6.388423	6.491276	5.448755	4.522103
23	H	5.103843	6.180659	5.984060	4.751039	4.052410
24	C	6.650309	7.290149	6.480192	5.173345	5.273126
25	C	6.514793	7.040927	6.154777	4.908907	5.153690
26	O	5.638514	6.391089	5.733447	4.403128	4.296641
27	H	7.521431	8.251671	7.508251	6.185920	6.167267
28	H	6.431720	6.973372	6.103326	4.848537	5.070680
29	H	6.142856	6.475563	5.452380	4.303475	4.806227
30	C	7.623450	8.176956	7.335128	6.135641	6.317943
31	H	7.410622	7.939797	7.159067	6.038085	6.193401
32	H	8.443401	8.881936	7.925783	6.783497	7.125993
33	H	8.099073	8.791384	8.054338	6.797178	6.802140

		6	7	8	9	10
6	C	0.000000				
7	C	1.531842	0.000000			
8	H	2.840748	3.353381	0.000000		
9	H	4.665315	5.326107	2.754146	0.000000	
10	H	1.090581	2.151486	3.836824	5.329725	0.000000
11	H	1.090726	2.169967	2.732329	4.931254	1.776915
12	H	2.166646	1.094927	2.858708	5.041989	3.060127

13	H	2.150980	1.099778	3.871865	5.348766	2.489698
14	Br	4.882397	5.600899	6.521698	6.114107	4.206154
15	H	2.887020	3.779864	4.272847	4.255707	2.550779
16	C	4.889859	5.698763	4.639119	2.878556	4.989981
17	C	6.028021	6.796867	5.257753	2.887817	6.232692
18	H	5.011056	5.818994	5.333395	3.910388	4.881763
19	H	6.953892	7.716451	6.334885	3.941533	7.058198
20	H	6.244647	6.977249	4.962777	2.303083	6.614965
21	N	2.414518	1.459997	4.512580	6.710679	2.650467
22	H	3.311643	2.054938	5.054070	7.285505	3.624033
23	H	2.702548	2.044315	5.206790	7.193781	2.511500
24	C	4.396709	4.737933	7.192385	8.356206	3.364280
25	C	4.453390	4.486399	7.134099	8.084093	3.546960
26	O	3.303079	3.367207	6.108234	7.461200	2.422780
27	H	5.140210	5.368125	7.971954	9.323191	4.158086
28	H	4.370161	5.043609	7.039074	8.017860	3.281159
29	H	4.417964	4.602350	6.890652	7.482311	3.540004
30	C	5.549124	5.214845	8.178545	9.198359	4.774473
31	H	5.507343	4.931357	7.945451	8.920760	4.901398
32	H	6.471429	6.228628	9.071873	9.883848	5.641616
33	H	5.834153	5.418222	8.543181	9.833091	5.080453

		11	12	13	14	15
11	H	0.000000				
12	H	2.503556	0.000000			
13	H	3.063124	1.769768	0.000000		
14	Br	5.738445	6.419292	5.056105	0.000000	
15	H	3.738434	4.445655	3.449531	2.253710	0.000000
16	C	5.543335	5.935655	5.339903	3.711154	2.731060
17	C	6.596337	6.890494	6.456506	4.878003	4.054559
18	H	5.761972	6.235912	5.357961	2.738047	2.375737
19	H	7.563089	7.868605	7.299157	5.077539	4.713817
20	H	6.699210	6.907165	6.736710	5.828321	4.706698
21	N	2.659913	2.088701	2.159827	6.384459	4.820430
22	H	3.546950	2.332819	2.540962	7.145213	5.630228
23	H	3.091461	2.933706	2.402794	5.928071	4.668710
24	C	4.921267	5.829233	4.629671	4.307575	4.403819
25	C	5.233329	5.558714	4.048897	3.814101	4.083375
26	O	3.950229	4.458167	3.234015	4.325510	3.825957
27	H	5.532499	6.436724	5.353271	5.357999	5.464805
28	H	4.823721	6.110146	5.003675	3.849801	4.038058
29	H	5.303591	5.633297	4.030656	2.787525	3.362575
30	C	6.340852	6.217965	4.664105	4.977486	5.361494
31	H	6.381231	5.838304	4.225520	5.154688	5.362363
32	H	7.285065	7.234439	5.621076	5.096304	5.904234

33	H	6.494301	6.403973	5.033164	5.903285	6.098872
		16	17	18	19	20
16	C	0.000000				
17	C	1.326378	0.000000			
18	H	1.088178	2.140599	0.000000		
19	H	2.076704	1.081358	2.466428	0.000000	
20	H	2.130803	1.083257	3.117782	1.846962	0.000000
21	N	7.019722	8.169734	7.038667	9.067984	8.385161
22	H	7.720323	8.829069	7.765348	9.729469	9.005150
23	H	7.108912	8.335269	6.971838	9.162080	8.673380
24	C	7.098495	8.421536	6.495082	8.954680	9.105931
25	C	6.673790	7.983013	6.023148	8.469017	8.707424
26	O	6.533079	7.851517	6.082854	8.495769	8.434712
27	H	8.170484	9.493598	7.579175	10.036638	10.159045
28	H	6.643410	7.943913	6.017913	8.443627	8.649746
29	H	5.803042	7.091082	5.073323	7.505736	7.878745
30	C	7.828792	9.105035	7.172309	9.557833	9.827465
31	H	7.663501	8.893801	7.073125	9.362341	9.573678
32	H	8.252211	9.500940	7.488180	9.844190	10.301662
33	H	8.668006	9.962896	8.066693	10.474265	10.636032
		21	22	23	24	25
21	N	0.000000				
22	H	1.013223	0.000000			
23	H	1.018458	1.646977	0.000000		
24	C	4.405469	5.105137	3.478072	0.000000	
25	C	4.371096	4.924848	3.474158	1.464734	0.000000
26	O	3.078563	3.761178	2.177709	1.446979	1.458668
27	H	4.757648	5.359589	3.780757	1.087284	2.215676
28	H	4.901364	5.724201	4.087796	1.085860	2.203333
29	H	4.822045	5.431230	4.058364	2.169061	1.089255
30	C	4.904573	5.185656	3.985975	2.598485	1.502948
31	H	4.743889	4.877555	3.955525	3.437845	2.149895
32	H	5.985908	6.276891	5.064263	3.144262	2.138989
33	H	4.810494	5.003509	3.845997	2.734069	2.155936
		26	27	28	29	30
26	O	0.000000				
27	H	2.137935	0.000000			
28	H	2.141698	1.846570	0.000000		
29	H	2.123325	3.109225	2.456136	0.000000	
30	C	2.513013	2.825175	3.529440	2.227313	0.000000
31	H	2.928707	3.776641	4.332907	2.591625	1.094058
32	H	3.420751	3.308160	3.930377	2.576095	1.094243
33	H	2.699287	2.552803	3.789858	3.117248	1.093113
		31	32	33		

31 H 0.000000

32 H 1.766767 0.000000

33 H 1.774997 1.776193 0.000000

Stoichiometry C10H18BrN3O

Framework group C1[X(C10H18BrN3O)]

Deg. of freedom 93

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.332223	2.484678	-0.235196
2	6	0	-3.335448	1.610544	0.032380
3	7	0	-2.767247	0.342802	0.057381
4	6	0	-1.450681	0.454259	-0.194187
5	7	0	-1.166687	1.745809	-0.372840
6	6	0	0.179081	2.289233	-0.634450
7	6	0	0.802813	2.924396	0.612172
8	1	0	-2.347823	3.555036	-0.347488
9	1	0	-4.382922	1.781831	0.199719
10	1	0	0.807909	1.462211	-0.966081
11	1	0	0.099885	3.022013	-1.438467
12	1	0	0.190670	3.767047	0.949937
13	1	0	0.810052	2.176896	1.418834
14	35	0	-0.087197	-2.557774	-0.111541
15	1	0	-0.761476	-0.410811	-0.234447
16	6	0	-3.392409	-0.919326	0.293091
17	6	0	-4.693029	-1.073247	0.502790
18	1	0	-2.669639	-1.732514	0.271659
19	1	0	-5.080090	-2.068752	0.671575
20	1	0	-5.405818	-0.257612	0.513634
21	7	0	2.124337	3.421089	0.240066
22	1	0	2.510705	4.010261	0.968227
23	1	0	2.758849	2.638468	0.091218
24	6	0	3.533666	-0.495458	-1.203058
25	6	0	3.279672	-0.794438	0.208163
26	8	0	2.949417	0.513692	-0.346309
27	1	0	4.544752	-0.270799	-1.533846
28	1	0	2.860033	-0.900475	-1.952239
29	1	0	2.390313	-1.390678	0.408200
30	6	0	4.379179	-0.819852	1.232513

```
      31        1        0        4.015820   -0.462580    2.200650
      32        1        0        4.736779   -1.844904    1.369470
      33        1        0        5.222019   -0.194750    0.926302
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.4205321           0.2879179           0.1804496
 Standard basis: 6-311++G(d,p) (5D, 7F)
 There are     499 symmetry adapted cartesian basis functions of A      symmetry.
 There are     482 symmetry adapted basis functions of A      symmetry.
   482 basis functions,      760 primitive gaussians,      499 cartesian basis functions
    71 alpha electrons              71 beta electrons
         nuclear repulsion energy           1307.5355431886 Hartrees.
 NAtoms=       33 NActive=       33 NUniq=       33 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      482 RedAO= T EigKep=    3.60D-06    NBF=      482
 NBsUse=      482 1.00D-06 EigRej= -1.00D+00 NBFU=      482
 Initial                guess                from                the                checkpoint                file:
"/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"
 B after Tr=          0.000000        0.000000        0.000000
             Rot=        0.999987        0.003032      -0.000058        0.004111 Ang=      0.59 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn=                5 AccDes=
0.00D+00
 Harris functional with IExCor=    402 and IRadAn=             5 diagonalized for initial guess.
 HarFok:    IExCor=    402 AccDes= 0.00D+00 IRadAn=                5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=    3500011 ScaDFX=    1.000000    1.000000    1.000000    1.000000
 FoFCou: FMM=F IPFlag=                  0 FMFlag=           100000 FMFlg1=                  0
             NFxFlg=                  0 DoJE=T BraDBF=F KetDBF=T FulRan=T
             wScrn=      0.000000  ICntrl=             500  IOpCl=      0  I1Cent=        200000004  NGrid=
0
             NMat0=         1 NMatS0=             1 NMatT0=         0 NMatD0=         1 NMtDS0=         0
NMtDT0=         0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3205.64826304          A.U. after      11 cycles
                  NFock= 11    Conv=0.60D-08         -V/T= 2.0018
 Calling FoFJK, ICntrl=             2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
```

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000263866	0.000043598	0.000098035
2	6	0.000368712	-0.000081698	0.000067928
3	7	-0.000741978	-0.000614462	0.000010396
4	6	0.001580922	0.001750950	0.000234856
5	7	-0.000111083	0.000107522	-0.000739047
6	6	-0.000435467	-0.000646566	0.000209968
7	6	0.001466830	0.000508148	-0.000236477
8	1	0.000038102	0.000009374	0.000156975
9	1	-0.000065978	-0.000050972	0.000020655
10	1	-0.000336465	-0.000018492	-0.000273146
11	1	0.000243926	0.000089163	-0.000011067
12	1	-0.000131475	0.000037045	-0.000201176
13	1	-0.000321445	-0.000281966	0.000179601
14	35	0.000028784	0.000118289	-0.000035456
15	1	-0.000508782	-0.000816476	0.000381528
16	6	-0.000222293	-0.000272037	-0.000352742
17	6	-0.000043863	0.000221756	-0.000010269
18	1	0.000262232	-0.000123612	-0.000001404
19	1	0.000060474	-0.000016274	0.000068656
20	1	-0.000024361	0.000069546	0.000048083
21	7	-0.000402696	-0.000181051	0.000253424
22	1	0.000080568	-0.000060805	-0.000025857
23	1	-0.000291350	0.000201344	0.000189592
24	6	-0.000410240	0.000955235	0.000661930
25	6	-0.000812406	0.000721777	-0.001133872
26	8	0.000435950	-0.001460504	-0.000548708
27	1	0.000033433	-0.000149163	-0.000087936
28	1	0.000123554	0.000156631	-0.000442939
29	1	0.000685243	0.000047118	0.001209154
30	6	-0.000006658	-0.000018992	0.000441553
31	1	-0.000052990	-0.000221627	-0.000058975
32	1	-0.000137911	-0.000014261	0.000016445
33	1	-0.000087421	-0.000008535	-0.000089708

Cartesian Forces: Max 0.001750950 RMS 0.000471862

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.001041616 RMS 0.000289476
Search for a local minimum.
Step number 31 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 29 30 31
DE= -9.17D-05 DEPred=-6.61D-05 R= 1.39D+00
TightC=F SS= 1.41D+00 RLast= 3.46D-01 DXNew= 1.4210D+00 1.0374D+00
Trust test= 1.39D+00 RLast= 3.46D-01 DXMaxT set to 1.04D+00
ITU= 1 1 1 1 1 0 0 -1 1 -1 1 1 1 1 1 1 1 1 0
ITU= -1 -1 1 1 1 -1 1 0 0 -1 0

Eigenvalues ---	0.00057	0.00173	0.00223	0.00407	0.00658
Eigenvalues ---	0.00728	0.00773	0.01272	0.01520	0.01887
Eigenvalues ---	0.01977	0.02175	0.02357	0.02388	0.02480
Eigenvalues ---	0.02636	0.02862	0.03045	0.03086	0.03232
Eigenvalues ---	0.03331	0.03601	0.03767	0.03852	0.03985
Eigenvalues ---	0.04379	0.04506	0.05216	0.05459	0.05717
Eigenvalues ---	0.05731	0.05900	0.06089	0.07548	0.08663
Eigenvalues ---	0.09029	0.09554	0.10647	0.12212	0.12553
Eigenvalues ---	0.12746	0.13824	0.15026	0.15864	0.15993
Eigenvalues ---	0.16001	0.16004	0.16010	0.16023	0.16106
Eigenvalues ---	0.16323	0.20372	0.21549	0.22115	0.22381
Eigenvalues ---	0.23011	0.23424	0.23897	0.26035	0.27332
Eigenvalues ---	0.29077	0.29513	0.31367	0.31747	0.32403
Eigenvalues ---	0.33790	0.34283	0.34342	0.34412	0.34546
Eigenvalues ---	0.34688	0.34737	0.35079	0.35219	0.35446
Eigenvalues ---	0.35594	0.35620	0.35890	0.36038	0.36421
Eigenvalues ---	0.36658	0.39338	0.40496	0.41899	0.42446
Eigenvalues ---	0.45005	0.45485	0.46363	0.49542	0.55135
Eigenvalues ---	0.58065	0.60612	1.30414		

En-DIIS/RFO-DIIS IScMMF= 0 using points: 31 30 29 28 27
RFO step: Lambda=-2.61146919D-05.
DidBck=F Rises=F RFO-DIIS coefs: 1.33982 -0.32456 -0.07314 -0.10094 0.15882
Iteration 1 RMS(Cart)= 0.02017681 RMS(Int)= 0.00020486
Iteration 2 RMS(Cart)= 0.00035472 RMS(Int)= 0.00004352
Iteration 3 RMS(Cart)= 0.00000011 RMS(Int)= 0.00004352

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56486	0.00013	0.00000	-0.00007	-0.00007	2.56479
R2	2.62076	0.00016	0.00014	0.00022	0.00035	2.62112
R3	2.03400	-0.00002	0.00001	-0.00005	-0.00004	2.03396
R4	2.62573	-0.00010	-0.00020	-0.00012	-0.00031	2.62542

R5	2.03050	0.00007	0.00000	0.00008	0.00008	2.03059
R6	2.54170	0.00049	0.00028	0.00056	0.00084	2.54254
R7	2.69864	0.00006	0.00026	-0.00008	0.00018	2.69882
R8	2.52168	-0.00036	0.00017	-0.00036	-0.00018	2.52150
R9	2.09152	0.00016	-0.00037	0.00047	0.00009	2.09161
R10	2.78684	-0.00047	-0.00055	-0.00031	-0.00087	2.78598
R11	2.89476	0.00026	0.00072	0.00078	0.00150	2.89626
R12	2.06090	-0.00012	-0.00012	-0.00023	-0.00035	2.06055
R13	2.06117	0.00003	-0.00001	-0.00001	-0.00003	2.06115
R14	2.06911	0.00005	-0.00005	0.00012	0.00008	2.06919
R15	2.07828	0.00029	0.00023	0.00023	0.00046	2.07874
R16	2.75899	-0.00083	-0.00077	-0.00093	-0.00170	2.75729
R17	4.25889	-0.00010	0.00364	0.00010	0.00374	4.26263
R18	2.50649	-0.00003	-0.00012	0.00010	-0.00002	2.50647
R19	2.05636	0.00028	0.00038	0.00038	0.00076	2.05712
R20	2.04347	0.00001	0.00000	0.00004	0.00004	2.04351
R21	2.04706	0.00006	0.00005	0.00007	0.00012	2.04718
R22	1.91471	-0.00003	-0.00020	-0.00012	-0.00031	1.91440
R23	1.92461	-0.00048	-0.00035	-0.00035	-0.00074	1.92387
R24	4.11527	-0.00008	0.01041	0.00813	0.01855	4.13383
R25	2.76795	0.00044	-0.00172	0.00345	0.00168	2.76963
R26	2.73439	-0.00096	0.00066	-0.00266	-0.00198	2.73241
R27	2.05467	0.00002	-0.00014	0.00009	-0.00005	2.05462
R28	2.05198	0.00015	-0.00014	0.00015	0.00001	2.05199
R29	2.75648	-0.00075	-0.00029	-0.00306	-0.00332	2.75316
R30	2.05839	-0.00029	-0.00015	-0.00036	-0.00051	2.05788
R31	2.84016	-0.00003	0.00040	0.00014	0.00054	2.84070
R32	2.06747	-0.00010	0.00018	-0.00022	-0.00003	2.06744
R33	2.06782	-0.00005	0.00000	-0.00007	-0.00007	2.06775
R34	2.06568	-0.00004	-0.00011	0.00003	-0.00008	2.06561
A1	1.87302	-0.00009	-0.00021	0.00019	-0.00003	1.87299
A2	2.27879	0.00005	0.00014	-0.00019	-0.00004	2.27875
A3	2.13132	0.00004	0.00006	0.00000	0.00006	2.13138
A4	1.86387	0.00017	0.00046	-0.00008	0.00038	1.86425
A5	2.27654	-0.00003	-0.00042	0.00036	-0.00006	2.27648
A6	2.14277	-0.00015	-0.00005	-0.00029	-0.00033	2.14243
A7	1.89791	-0.00026	-0.00037	-0.00004	-0.00040	1.89751
A8	2.25277	0.00008	0.00046	-0.00021	0.00025	2.25302
A9	2.13249	0.00018	-0.00009	0.00025	0.00015	2.13265
A10	1.88974	0.00016	0.00016	0.00005	0.00020	1.88995
A11	2.15505	-0.00086	-0.00275	-0.00323	-0.00600	2.14904
A12	2.23839	0.00069	0.00262	0.00318	0.00578	2.24418
A13	1.90023	0.00002	-0.00008	-0.00011	-0.00017	1.90006
A14	2.19964	0.00085	0.00091	0.00127	0.00221	2.20185

A15	2.18293	-0.00087	-0.00099	-0.00120	-0.00217	2.18076
A16	1.96059	-0.00013	-0.00130	-0.00052	-0.00182	1.95876
A17	1.87620	-0.00035	0.00012	-0.00024	-0.00012	1.87609
A18	1.88816	0.00038	0.00047	0.00067	0.00115	1.88931
A19	1.90405	0.00039	0.00006	0.00140	0.00146	1.90551
A20	1.92931	-0.00018	0.00087	-0.00056	0.00032	1.92963
A21	1.90411	-0.00013	-0.00023	-0.00077	-0.00100	1.90311
A22	1.92038	-0.00022	-0.00006	-0.00154	-0.00160	1.91878
A23	1.89417	-0.00024	-0.00088	-0.00087	-0.00175	1.89241
A24	1.87780	0.00025	0.00172	0.00138	0.00312	1.88092
A25	1.87601	0.00006	-0.00055	-0.00020	-0.00075	1.87526
A26	1.89954	0.00004	-0.00066	0.00104	0.00037	1.89991
A27	1.99568	0.00010	0.00041	0.00007	0.00048	1.99615
A28	2.16268	-0.00031	-0.00038	-0.00044	-0.00081	2.16187
A29	1.94598	0.00007	-0.00035	0.00002	-0.00033	1.94565
A30	2.17450	0.00024	0.00073	0.00043	0.00116	2.17566
A31	2.07430	-0.00006	-0.00033	-0.00022	-0.00055	2.07375
A32	2.16450	0.00001	0.00034	0.00004	0.00038	2.16488
A33	2.04438	0.00005	0.00000	0.00018	0.00017	2.04455
A34	1.93887	0.00055	0.00091	0.00109	0.00197	1.94084
A35	1.91745	-0.00084	-0.00005	0.00009	0.00003	1.91747
A36	1.89051	0.00011	0.00016	0.00094	0.00112	1.89163
A37	2.09041	-0.00021	0.00118	-0.00056	0.00045	2.09087
A38	2.07262	0.00053	-0.00273	0.00274	0.00017	2.07279
A39	1.99490	0.00013	-0.00007	0.00040	0.00035	1.99525
A40	2.00221	0.00011	-0.00018	-0.00035	-0.00056	2.00165
A41	2.03092	-0.00028	0.00122	-0.00113	0.00009	2.03101
A42	2.01557	0.00089	-0.00225	0.00707	0.00486	2.02042
A43	2.13324	0.00016	0.00098	-0.00104	-0.00010	2.13314
A44	1.95610	0.00047	0.00201	0.00180	0.00376	1.95986
A45	2.02625	0.00037	-0.00120	0.00068	-0.00048	2.02578
A46	2.05205	-0.00104	0.00036	-0.00513	-0.00477	2.04728
A47	2.55849	-0.00027	-0.00875	-0.00374	-0.01280	2.54569
A48	2.52949	-0.00049	-0.00713	-0.00913	-0.01631	2.51318
A49	1.93331	-0.00006	0.00083	-0.00049	0.00034	1.93365
A50	1.91795	-0.00010	-0.00041	-0.00060	-0.00101	1.91694
A51	1.94280	-0.00010	-0.00013	0.00027	0.00014	1.94294
A52	1.87936	-0.00001	-0.00010	-0.00064	-0.00074	1.87862
A53	1.89360	0.00015	-0.00006	0.00093	0.00087	1.89447
A54	1.89524	0.00013	-0.00014	0.00053	0.00039	1.89563
A55	3.46765	-0.00026	0.00692	0.00535	0.01228	3.47993
A56	2.55903	-0.00075	-0.00754	-0.00592	-0.01328	2.54575
A57	2.90068	0.00016	0.00763	0.00954	0.01718	2.91786
A58	3.08604	0.00004	0.00174	-0.00629	-0.00448	3.08155

D1	0.00184	0.00002	-0.00088	0.00111	0.00023	0.00207
D2	-3.13559	0.00006	0.00161	0.00152	0.00313	-3.13245
D3	3.13214	0.00002	-0.00176	0.00101	-0.00075	3.13138
D4	-0.00529	0.00006	0.00073	0.00142	0.00215	-0.00314
D5	0.00014	-0.00017	-0.00166	-0.00251	-0.00417	-0.00403
D6	-3.11268	-0.00001	0.00096	-0.00092	0.00001	-3.11266
D7	-3.13132	-0.00017	-0.00087	-0.00242	-0.00329	-3.13461
D8	0.03905	-0.00001	0.00174	-0.00083	0.00089	0.03994
D9	-0.00319	0.00014	0.00310	0.00066	0.00375	0.00056
D10	-3.13905	0.00007	0.00149	0.00084	0.00231	-3.13674
D11	3.13463	0.00010	0.00084	0.00028	0.00112	3.13576
D12	-0.00122	0.00004	-0.00078	0.00046	-0.00032	-0.00155
D13	0.00331	-0.00025	-0.00416	-0.00223	-0.00639	-0.00309
D14	-3.13915	-0.00010	-0.00063	0.00091	0.00021	-3.13894
D15	3.13964	-0.00019	-0.00268	-0.00240	-0.00507	3.13457
D16	-0.00282	-0.00004	0.00085	0.00074	0.00154	-0.00128
D17	0.03188	-0.00011	-0.00887	-0.01014	-0.01901	0.01288
D18	-3.11646	0.00000	-0.00639	-0.00907	-0.01546	-3.13192
D19	-3.10330	-0.00018	-0.01068	-0.00993	-0.02062	-3.12392
D20	0.03155	-0.00007	-0.00820	-0.00887	-0.01707	0.01447
D21	-0.00214	0.00026	0.00361	0.00293	0.00653	0.00439
D22	3.11101	0.00013	0.00111	0.00140	0.00251	3.11352
D23	3.14037	0.00010	-0.00009	-0.00040	-0.00053	3.13983
D24	-0.02966	-0.00002	-0.00259	-0.00192	-0.00456	-0.03422
D25	1.32366	-0.00014	-0.00176	0.01273	0.01097	1.33463
D26	-2.86475	0.00003	-0.00239	0.01399	0.01160	-2.85315
D27	-0.81073	-0.00010	-0.00234	0.01330	0.01096	-0.79976
D28	-1.78466	0.00003	0.00121	0.01454	0.01575	-1.76891
D29	0.31011	0.00020	0.00058	0.01580	0.01638	0.32649
D30	2.36414	0.00007	0.00063	0.01511	0.01574	2.37988
D31	-1.07757	-0.00019	-0.00571	-0.00292	-0.00863	-1.08619
D32	0.97066	-0.00038	-0.00691	-0.00453	-0.01145	0.95922
D33	3.13864	-0.00026	-0.00588	-0.00412	-0.01001	3.12864
D34	3.12709	0.00007	-0.00509	-0.00322	-0.00831	3.11878
D35	-1.10787	-0.00012	-0.00629	-0.00484	-0.01113	-1.11900
D36	1.06011	0.00000	-0.00526	-0.00443	-0.00969	1.05042
D37	1.03333	0.00008	-0.00538	-0.00281	-0.00818	1.02514
D38	3.08156	-0.00011	-0.00658	-0.00442	-0.01101	3.07055
D39	-1.03365	0.00001	-0.00555	-0.00401	-0.00957	-1.04321
D40	2.94625	0.00004	-0.00267	-0.00872	-0.01138	2.93487
D41	-1.24546	-0.00002	-0.00192	-0.00679	-0.00871	-1.25417
D42	0.86591	0.00013	-0.00320	-0.00825	-0.01145	0.85446
D43	2.95738	0.00008	-0.00246	-0.00631	-0.00877	2.94861
D44	-1.23175	-0.00004	-0.00228	-0.00880	-0.01108	-1.24282

D45	0.85973	-0.00009	-0.00154	-0.00686	-0.00840	0.85133
D46	3.14008	0.00013	0.00098	0.00004	0.00102	3.14109
D47	0.00206	0.00001	-0.00011	-0.00058	-0.00069	0.00138
D48	0.00611	0.00001	-0.00184	-0.00115	-0.00299	0.00312
D49	-3.13190	-0.00011	-0.00292	-0.00177	-0.00469	-3.13659
D50	2.26903	0.00024	0.01823	0.02868	0.04680	2.31583
D51	-1.25282	0.00001	-0.03431	-0.00446	-0.03867	-1.29149
D52	-2.00804	-0.00004	0.01529	0.02960	0.04480	-1.96324
D53	0.75330	-0.00027	-0.03725	-0.00354	-0.04068	0.71262
D54	-2.71890	0.00016	0.00327	-0.00174	0.00154	-2.71735
D55	-0.01296	-0.00006	0.00103	-0.00064	0.00041	-0.01254
D56	-0.03427	0.00019	0.00278	0.00049	0.00328	-0.03099
D57	2.67167	-0.00002	0.00054	0.00159	0.00215	2.67382
D58	0.63970	-0.00004	-0.02892	-0.01951	-0.04859	0.59111
D59	-1.77045	0.00012	-0.03059	-0.01775	-0.04848	-1.81892
D60	1.79451	-0.00054	0.03147	0.00808	0.03956	1.83407
D61	-0.63174	0.00015	0.02986	0.01343	0.04330	-0.58843
D62	2.54515	-0.00006	0.00087	0.00035	0.00123	2.54639
D63	-1.66359	-0.00017	0.00100	-0.00112	-0.00010	-1.66369
D64	0.43665	-0.00014	0.00047	-0.00067	-0.00020	0.43646
D65	1.34540	0.00013	0.00033	0.00177	0.00210	1.34749
D66	-2.86334	0.00002	0.00046	0.00030	0.00076	-2.86258
D67	-0.76310	0.00005	-0.00007	0.00075	0.00067	-0.76243
D68	-1.04067	0.00018	-0.00199	0.00436	0.00237	-1.03830
D69	1.03378	0.00007	-0.00186	0.00289	0.00103	1.03481
D70	3.13402	0.00010	-0.00239	0.00333	0.00094	3.13496

Item	Value	Threshold	Converged?
Maximum Force	0.001042	0.000450	NO
RMS Force	0.000289	0.000300	YES
Maximum Displacement	0.086235	0.001800	NO
RMS Displacement	0.020312	0.001200	NO

Predicted change in Energy=-3.852278D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.643585	2.089164	-0.194447
2	6	0	-3.538293	1.115838	0.112482
3	7	0	-2.833192	-0.080642	0.150718
4	6	0	-1.540941	0.170621	-0.127146
5	7	0	-1.406121	1.480465	-0.342888

6	6	0	-0.133082	2.160039	-0.644620
7	6	0	0.447960	2.873607	0.581014
8	1	0	-2.780088	3.148350	-0.328487
9	1	0	-4.595312	1.173843	0.296832
10	1	0	0.571513	1.400333	-0.984264
11	1	0	-0.308328	2.870009	-1.453870
12	1	0	-0.239967	3.655697	0.918717
13	1	0	0.541880	2.142108	1.397183
14	35	0	0.119356	-2.689725	-0.043133
15	1	0	-0.765346	-0.618218	-0.162678
16	6	0	-3.310531	-1.398852	0.422919
17	6	0	-4.579183	-1.686838	0.681435
18	1	0	-2.504636	-2.129801	0.387516
19	1	0	-4.851019	-2.715228	0.876117
20	1	0	-5.374285	-0.951588	0.709781
21	7	0	1.706578	3.493481	0.180263
22	1	0	2.039895	4.136836	0.888272
23	1	0	2.415483	2.776671	0.038500
24	6	0	3.479762	-0.297316	-1.198268
25	6	0	3.273018	-0.584048	0.224087
26	8	0	2.788890	0.658793	-0.362048
27	1	0	4.454851	0.034578	-1.546370
28	1	0	2.851615	-0.798039	-1.928893
29	1	0	2.463403	-1.274811	0.454860
30	6	0	4.375752	-0.451157	1.237020
31	1	0	3.980352	-0.112857	2.199380
32	1	0	4.851647	-1.423314	1.397400
33	1	0	5.137070	0.259371	0.904827

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357229	0.000000			
3	N	2.205254	1.389314	0.000000		
4	C	2.213856	2.222672	1.345457	0.000000	
5	N	1.387036	2.210537	2.171920	1.334321	0.000000
6	C	2.551530	3.641294	3.597750	2.491512	1.474276
7	C	3.282429	4.381721	4.436068	3.429773	2.496408
8	H	1.076325	2.213692	3.264788	3.231546	2.160980
9	H	2.210974	1.074541	2.167982	3.242744	3.267139
10	H	3.381591	4.263132	3.882459	2.590233	2.080582
11	H	2.765735	3.995403	4.201902	3.250573	2.090517
12	H	3.077424	4.240266	4.612469	3.864210	2.771858
13	H	3.561359	4.399034	4.229114	3.247843	2.694499

14	Br	5.522184	5.280618	3.944925	3.308357	4.450552
15	H	3.295255	3.282057	2.159443	1.106832	2.201712
16	C	3.604471	2.543996	1.428154	2.428429	3.536058
17	C	4.332655	3.043379	2.431052	3.651694	4.598845
18	H	4.261180	3.417348	2.088798	2.546670	3.843729
19	H	5.394538	4.121098	3.396891	4.504584	5.563913
20	H	4.185752	2.828760	2.743766	4.080971	4.771721
21	N	4.586549	5.759032	5.777953	4.656423	3.743636
22	H	5.224963	6.390968	6.486763	5.439147	4.521846
23	H	5.110881	6.181528	5.977075	4.740488	4.053426
24	C	6.648182	7.277923	6.459110	5.154971	5.269158
25	C	6.505953	7.021113	6.127365	4.885396	5.145679
26	O	5.620128	6.361392	5.693637	4.363591	4.274766
27	H	7.512445	8.234760	7.483913	6.162973	6.155481
28	H	6.445268	6.975749	6.095612	4.845529	5.082845
29	H	6.149736	6.469373	5.438057	4.296834	4.816759
30	C	7.600883	8.145684	7.299741	6.103673	6.297407
31	H	7.379420	7.899041	7.114945	5.998146	6.165702
32	H	8.429116	8.859425	7.900237	6.762400	7.114787
33	H	8.068156	8.753472	8.013075	6.757860	6.772090

		6	7	8	9	10
6	C	0.000000				
7	C	1.532634	0.000000			
8	H	2.843122	3.364962	0.000000		
9	H	4.665877	5.329591	2.754041	0.000000	
10	H	1.090397	2.153113	3.836514	5.328094	0.000000
11	H	1.090712	2.170884	2.730121	4.931548	1.776119
12	H	2.166205	1.094967	2.874914	5.051274	3.060475
13	H	2.150548	1.100020	3.876329	5.342195	2.494474
14	Br	4.893436	5.607869	6.524670	6.104984	4.221225
15	H	2.889764	3.770680	4.274776	4.253383	2.556706
16	C	4.888919	5.692552	4.639291	2.878423	4.988574
17	C	6.026998	6.788218	5.256969	2.886464	6.231761
18	H	5.009222	5.812861	5.333612	3.910654	4.879172
19	H	6.952682	7.707226	6.334143	3.940282	7.057103
20	H	6.243944	6.967584	4.961587	2.301039	6.614669
21	N	2.417199	1.459097	4.528589	6.716258	2.650616
22	H	3.313505	2.055338	5.068516	7.290755	3.626429
23	H	2.709626	2.043249	5.221761	7.196322	2.518051
24	C	4.404289	4.734176	7.198254	8.343048	3.374273
25	C	4.459393	4.479255	7.132757	8.062635	3.563146
26	O	3.297197	3.357785	6.100208	7.431409	2.419461
27	H	5.136134	5.351731	7.970142	9.305954	4.154704
28	H	4.394087	5.055510	7.060551	8.018659	3.305152

29	H	4.443961	4.613816	6.904505	7.473041	3.578648
30	C	5.539720	5.187673	8.161698	9.165401	4.778531
31	H	5.493153	4.900598	7.920172	8.877910	4.903622
32	H	6.469760	6.206648	9.062129	9.859083	5.653747
33	H	5.812730	5.378367	8.517550	9.794139	5.070973

		11	12	13	14	15
11	H	0.000000				
12	H	2.500230	0.000000			
13	H	3.062874	1.769510	0.000000		
14	Br	5.751845	6.427959	5.059609	0.000000	
15	H	3.747501	4.439796	3.429490	2.255689	0.000000
16	C	5.546055	5.934867	5.322467	3.694277	2.725854
17	C	6.600347	6.886783	6.434160	4.858709	4.049670
18	H	5.763035	6.235615	5.343210	2.717408	2.369119
19	H	7.567016	7.864623	7.276577	5.054730	4.708425
20	H	6.704469	6.901591	6.711519	5.811032	4.702621
21	N	2.668137	2.088221	2.159543	6.387582	4.809790
22	H	3.550301	2.330278	2.545973	7.152476	5.620001
23	H	3.107255	2.932386	2.399808	5.929616	4.656546
24	C	4.944381	5.826176	4.617175	4.283723	4.381366
25	C	5.250913	5.549686	4.033261	3.801429	4.056987
26	O	3.959080	4.449244	3.216236	4.294262	3.781944
27	H	5.544015	6.421097	5.330810	5.336484	5.439780
28	H	4.864717	6.123932	5.004211	3.820969	4.029177
29	H	5.339033	5.642100	4.031819	2.782900	3.352207
30	C	6.341265	6.186472	4.631334	4.976634	5.330850
31	H	6.374676	5.801137	4.189448	5.155230	5.325069
32	H	7.292990	7.207637	5.593419	5.106223	5.884950
33	H	6.483151	6.359855	4.990279	5.896884	6.062033

		16	17	18	19	20
16	C	0.000000				
17	C	1.326365	0.000000			
18	H	1.088581	2.141577	0.000000		
19	H	2.076375	1.081379	2.467178	0.000000	
20	H	2.131060	1.083321	3.118803	1.847133	0.000000
21	N	7.011789	8.160740	7.028412	9.057281	8.377210
22	H	7.712811	8.818739	7.757207	9.717799	8.994109
23	H	7.097183	8.322358	6.957216	9.146836	8.662045
24	C	7.067511	8.391105	6.456448	8.919152	9.080907
25	C	6.636758	7.942441	5.983088	8.424194	8.668728
26	O	6.484830	7.802522	6.029886	8.443061	8.389254
27	H	8.138426	9.462566	7.540485	10.001454	10.132851
28	H	6.622994	7.925941	5.985714	8.418685	8.640117
29	H	5.775355	7.058266	5.041523	7.466795	7.848492

30	C	7.787158	9.056845	7.132969	9.507343	9.777098
31	H	7.613578	8.834433	7.028939	9.301423	9.509553
32	H	8.220180	9.461639	7.458813	9.802168	10.259875
33	H	8.622291	9.911771	8.023180	10.421659	10.582677

		21	22	23	24	25
21	N	0.000000				
22	H	1.013056	0.000000			
23	H	1.018067	1.647188	0.000000		
24	C	4.406208	5.107697	3.480184	0.000000	
25	C	4.368283	4.924274	3.473361	1.465623	0.000000
26	O	3.082362	3.771084	2.187527	1.445930	1.456910
27	H	4.743235	5.346776	3.766949	1.087257	2.216742
28	H	4.916991	5.740062	4.103584	1.085866	2.204245
29	H	4.835783	5.445469	4.073102	2.172858	1.088984
30	C	4.878667	5.160187	3.962067	2.599441	1.503235
31	H	4.717260	4.852243	3.932885	3.439277	2.150377
32	H	5.962194	6.251434	5.041962	3.144429	2.138481
33	H	4.769982	4.962610	3.807145	2.734882	2.156259

		26	27	28	29	30
26	O	0.000000				
27	H	2.137216	0.000000			
28	H	2.140397	1.846602	0.000000		
29	H	2.124172	3.112119	2.461768	0.000000	
30	C	2.511402	2.826563	3.530769	2.224244	0.000000
31	H	2.928470	3.778562	4.334301	2.587397	1.094040
32	H	3.418449	3.308878	3.931326	2.571798	1.094206
33	H	2.697862	2.554275	3.790962	3.115233	1.093072

		31	32	33
31	H	0.000000		
32	H	1.766247	0.000000	
33	H	1.775504	1.776379	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.329171	2.489711	-0.240641
2	6	0	-3.327553	1.612548	0.034837

3	7	0	-2.754333	0.347327	0.063619
4	6	0	-1.437941	0.463830	-0.188950
5	7	0	-1.160909	1.755066	-0.379669
6	6	0	0.182307	2.299809	-0.648960
7	6	0	0.813839	2.928248	0.598116
8	1	0	-2.349971	3.559370	-0.358417
9	1	0	-4.375558	1.779920	0.203095
10	1	0	0.808179	1.474766	-0.990360
11	1	0	0.097972	3.036928	-1.448457
12	1	0	0.206950	3.773800	0.938234
13	1	0	0.814910	2.178279	1.402844
14	35	0	-0.092643	-2.558037	-0.127943
15	1	0	-0.750016	-0.402477	-0.225686
16	6	0	-3.373789	-0.916627	0.305112
17	6	0	-4.670275	-1.071851	0.538081
18	1	0	-2.649593	-1.728610	0.270001
19	1	0	-5.053250	-2.068348	0.710432
20	1	0	-5.383157	-0.256632	0.566386
21	7	0	2.138149	3.416717	0.228564
22	1	0	2.525200	4.009802	0.952943
23	1	0	2.769323	2.630779	0.085804
24	6	0	3.523004	-0.519427	-1.186928
25	6	0	3.261561	-0.804638	0.226704
26	8	0	2.922754	0.491678	-0.345453
27	1	0	4.533902	-0.287889	-1.513430
28	1	0	2.858395	-0.938955	-1.936191
29	1	0	2.379153	-1.408756	0.432335
30	6	0	4.353874	-0.805750	1.259451
31	1	0	3.979494	-0.442299	2.221047
32	1	0	4.720865	-1.825443	1.410548
33	1	0	5.192179	-0.175257	0.951993

Rotational constants (GHZ): 0.4194888 0.2900321 0.1812828

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1309.0142633472 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.
NBasis= 482 RedAO= T EigKep= 3.60D-06 NBF= 482
NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999999 0.000664 -0.000048 0.000880 Ang= 0.13 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3205.64831655 A.U. after 11 cycles
NFock= 11 Conv=0.35D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000129670	0.000050722	-0.000114004
2	6	0.000181234	-0.000165575	-0.000092460
3	7	-0.000341803	-0.000172088	0.000383186
4	6	0.000658519	0.000818039	-0.000216366
5	7	0.000005152	-0.000133694	-0.000300693
6	6	-0.000085941	-0.000099449	0.000402173
7	6	0.000950606	0.000243597	-0.000014898
8	1	0.000049297	0.000018433	0.000092670
9	1	-0.000042374	-0.000007594	-0.000012578
10	1	-0.000230832	-0.000106518	-0.000087584
11	1	0.000093274	0.000076033	-0.000008376
12	1	-0.000098495	0.000033487	-0.000193780

13	1	-0.000214046	-0.000167713	0.000121018
14	35	0.000051314	0.000021917	-0.000033799
15	1	-0.000165397	-0.000365070	0.000071370
16	6	-0.000164577	-0.000135661	-0.000057424
17	6	-0.000047720	0.000126447	0.000006788
18	1	0.000078739	-0.000084355	-0.000046530
19	1	0.000014780	-0.000010551	0.000017713
20	1	-0.000000210	0.000033026	0.000020030
21	7	-0.000354017	-0.000111910	-0.000095199
22	1	0.000035732	-0.000070397	0.000084019
23	1	-0.000108477	0.000035651	0.000089105
24	6	-0.000541293	0.000380868	0.000871244
25	6	-0.000012823	0.000546891	-0.000872068
26	8	-0.000061629	-0.000536319	-0.000374999
27	1	0.000111024	-0.000184227	-0.000020802
28	1	0.000115853	0.000091919	-0.000374352
29	1	0.000285049	0.000134994	0.000581589
30	6	0.000101699	-0.000126695	0.000238455
31	1	-0.000086043	-0.000121850	-0.000077856
32	1	-0.000019949	-0.000016838	0.000029839
33	1	-0.000026978	0.000004479	-0.000015430

Cartesian Forces: Max 0.000950606 RMS 0.000264331

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000516091 RMS 0.000150445
Search for a local minimum.
Step number 32 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 30 31 32
DE= -5.35D-05 DEPred=-3.85D-05 R= 1.39D+00
TightC=F SS= 1.41D+00 RLast= 1.46D-01 DXNew= 1.7446D+00 4.3819D-01
Trust test= 1.39D+00 RLast= 1.46D-01 DXMaxT set to 1.04D+00
ITU= 1 1 1 1 1 1 0 0 -1 1 -1 1 1 1 1 1 1 1 1
ITU= 0 -1 -1 1 1 1 -1 1 0 0 -1 0
Eigenvalues --- 0.00051 0.00175 0.00229 0.00440 0.00656
Eigenvalues --- 0.00727 0.00762 0.01222 0.01516 0.01889
Eigenvalues --- 0.01953 0.02176 0.02360 0.02381 0.02480
Eigenvalues --- 0.02648 0.02854 0.03037 0.03073 0.03208

Eigenvalues --- 0.03320 0.03698 0.03755 0.03903 0.04083
Eigenvalues --- 0.04391 0.04466 0.05126 0.05461 0.05592
Eigenvalues --- 0.05730 0.05871 0.05947 0.07572 0.08643
Eigenvalues --- 0.08994 0.09561 0.10898 0.12103 0.12317
Eigenvalues --- 0.12742 0.13949 0.14193 0.15814 0.15972
Eigenvalues --- 0.16001 0.16002 0.16005 0.16020 0.16098
Eigenvalues --- 0.16153 0.18545 0.21454 0.21874 0.22185
Eigenvalues --- 0.22985 0.23454 0.24602 0.26351 0.27615
Eigenvalues --- 0.28655 0.29515 0.31016 0.31827 0.32313
Eigenvalues --- 0.33677 0.34282 0.34338 0.34407 0.34546
Eigenvalues --- 0.34674 0.34741 0.35080 0.35195 0.35394
Eigenvalues --- 0.35579 0.35673 0.35736 0.35894 0.36418
Eigenvalues --- 0.36630 0.39290 0.39858 0.41893 0.42455
Eigenvalues --- 0.44497 0.45492 0.46483 0.49542 0.54860
Eigenvalues --- 0.58050 0.60618 1.29387
En-DIIS/RFO-DIIS IScMMF= 0 using points: 32 31 30 29 28
RFO step: Lambda=-8.80450647D-06.
DidBck=F Rises=F RFO-DIIS coefs: 1.27324 -0.08583 -0.59649 0.35333 0.05574
Iteration 1 RMS(Cart)= 0.01469056 RMS(Int)= 0.00035523
Iteration 2 RMS(Cart)= 0.00016817 RMS(Int)= 0.00034321
Iteration 3 RMS(Cart)= 0.00000019 RMS(Int)= 0.00034321

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56479	0.00003	-0.00008	0.00007	-0.00001	2.56478
R2	2.62112	0.00002	0.00032	-0.00008	0.00025	2.62136
R3	2.03396	0.00000	-0.00001	-0.00001	-0.00002	2.03394
R4	2.62542	-0.00012	-0.00027	-0.00013	-0.00040	2.62503
R5	2.03059	0.00004	0.00008	0.00003	0.00011	2.03070
R6	2.54254	0.00047	0.00077	0.00037	0.00114	2.54368
R7	2.69882	0.00010	0.00020	0.00003	0.00023	2.69905
R8	2.52150	-0.00014	-0.00011	-0.00022	-0.00033	2.52117
R9	2.09161	0.00017	0.00041	0.00030	0.00071	2.09232
R10	2.78598	-0.00018	-0.00084	0.00012	-0.00072	2.78526
R11	2.89626	0.00006	0.00071	-0.00013	0.00057	2.89683
R12	2.06055	-0.00005	-0.00017	-0.00010	-0.00027	2.06028
R13	2.06115	0.00004	0.00010	0.00013	0.00023	2.06138
R14	2.06919	0.00003	0.00014	0.00007	0.00021	2.06939
R15	2.07874	0.00018	0.00064	0.00016	0.00079	2.07953
R16	2.75729	-0.00048	-0.00152	-0.00024	-0.00176	2.75554
R17	4.26263	0.00000	-0.00145	-0.00110	-0.00255	4.26009
R18	2.50647	0.00001	-0.00006	0.00006	-0.00001	2.50646
R19	2.05712	0.00012	0.00042	-0.00002	0.00040	2.05752
R20	2.04351	0.00001	0.00002	0.00002	0.00003	2.04354

R21	2.04718	0.00002	0.00005	-0.00001	0.00004	2.04722
R22	1.91440	0.00002	-0.00008	0.00006	-0.00003	1.91437
R23	1.92387	-0.00028	-0.00076	0.00033	-0.00062	1.92325
R24	4.13383	-0.00022	-0.00205	0.00406	0.00210	4.13593
R25	2.76963	-0.00018	0.00048	-0.00263	-0.00117	2.76846
R26	2.73241	-0.00052	-0.00105	0.00000	-0.00145	2.73096
R27	2.05462	0.00005	0.00006	0.00008	0.00014	2.05476
R28	2.05199	0.00014	0.00002	0.00022	0.00024	2.05223
R29	2.75316	-0.00025	-0.00166	0.00020	-0.00204	2.75112
R30	2.05788	-0.00018	-0.00043	-0.00013	-0.00057	2.05731
R31	2.84070	0.00007	0.00043	0.00043	0.00085	2.84156
R32	2.06744	-0.00008	-0.00004	-0.00006	-0.00010	2.06734
R33	2.06775	0.00001	-0.00002	0.00004	0.00002	2.06777
R34	2.06561	-0.00001	-0.00009	0.00003	-0.00006	2.06554
A1	1.87299	-0.00002	-0.00019	0.00005	-0.00014	1.87285
A2	2.27875	0.00004	0.00019	0.00008	0.00027	2.27902
A3	2.13138	-0.00002	0.00000	-0.00012	-0.00011	2.13126
A4	1.86425	0.00012	0.00049	0.00004	0.00053	1.86478
A5	2.27648	-0.00005	-0.00046	0.00001	-0.00045	2.27603
A6	2.14243	-0.00007	-0.00003	-0.00005	-0.00008	2.14235
A7	1.89751	-0.00015	-0.00040	-0.00015	-0.00055	1.89696
A8	2.25302	-0.00021	0.00018	-0.00049	-0.00031	2.25271
A9	2.13265	0.00035	0.00022	0.00063	0.00085	2.13350
A10	1.88995	0.00000	0.00011	0.00007	0.00018	1.89013
A11	2.14904	-0.00022	-0.00394	0.00032	-0.00360	2.14544
A12	2.24418	0.00022	0.00380	-0.00040	0.00341	2.24759
A13	1.90006	0.00004	-0.00001	-0.00001	-0.00002	1.90004
A14	2.20185	0.00008	0.00137	-0.00008	0.00130	2.20315
A15	2.18076	-0.00013	-0.00149	0.00009	-0.00139	2.17937
A16	1.95876	0.00020	-0.00094	0.00101	0.00003	1.95879
A17	1.87609	-0.00028	-0.00043	-0.00149	-0.00191	1.87418
A18	1.88931	0.00006	0.00090	0.00019	0.00111	1.89043
A19	1.90551	0.00021	0.00111	0.00052	0.00164	1.90715
A20	1.92963	-0.00020	0.00012	-0.00066	-0.00052	1.92911
A21	1.90311	0.00000	-0.00080	0.00039	-0.00042	1.90269
A22	1.91878	-0.00013	-0.00124	-0.00132	-0.00257	1.91621
A23	1.89241	-0.00009	-0.00136	0.00025	-0.00115	1.89127
A24	1.88092	-0.00002	0.00162	-0.00009	0.00159	1.88251
A25	1.87526	0.00003	-0.00052	0.00023	-0.00028	1.87498
A26	1.89991	-0.00001	-0.00055	-0.00022	-0.00078	1.89914
A27	1.99615	0.00021	0.00192	0.00105	0.00295	1.99910
A28	2.16187	-0.00024	-0.00068	-0.00018	-0.00087	2.16100
A29	1.94565	0.00012	-0.00019	0.00039	0.00020	1.94585
A30	2.17566	0.00012	0.00088	-0.00020	0.00067	2.17633

A31	2.07375	-0.00001	-0.00027	0.00008	-0.00019	2.07356
A32	2.16488	-0.00001	0.00015	-0.00010	0.00005	2.16493
A33	2.04455	0.00002	0.00012	0.00002	0.00014	2.04469
A34	1.94084	0.00016	0.00037	0.00057	0.00074	1.94158
A35	1.91747	-0.00021	-0.00028	0.00072	0.00036	1.91783
A36	1.89163	0.00000	0.00030	-0.00081	-0.00041	1.89121
A37	2.09087	-0.00030	0.00033	-0.00191	-0.00257	2.08830
A38	2.07279	0.00046	-0.00012	0.00185	0.00280	2.07558
A39	1.99525	0.00016	-0.00010	0.00076	0.00111	1.99636
A40	2.00165	-0.00003	0.00075	-0.00015	0.00035	2.00200
A41	2.03101	-0.00019	-0.00026	-0.00046	-0.00075	2.03026
A42	2.02042	0.00041	0.00229	0.00010	0.00318	2.02360
A43	2.13314	0.00008	0.00080	0.00048	0.00052	2.13366
A44	1.95986	0.00005	0.00295	-0.00048	0.00214	1.96200
A45	2.02578	0.00035	-0.00046	0.00085	0.00092	2.02670
A46	2.04728	-0.00050	-0.00329	-0.00076	-0.00410	2.04318
A47	2.54569	0.00003	-0.00252	-0.00472	-0.00525	2.54044
A48	2.51318	-0.00029	-0.00319	-0.00817	-0.00895	2.50423
A49	1.93365	-0.00016	0.00007	-0.00086	-0.00079	1.93286
A50	1.91694	0.00002	-0.00076	0.00032	-0.00045	1.91649
A51	1.94294	0.00000	0.00016	0.00045	0.00062	1.94355
A52	1.87862	0.00002	-0.00034	-0.00008	-0.00041	1.87821
A53	1.89447	0.00010	0.00053	0.00017	0.00070	1.89517
A54	1.89563	0.00002	0.00033	0.00000	0.00033	1.89596
A55	3.47993	-0.00018	0.00104	-0.00390	-0.00286	3.47707
A56	2.54575	-0.00042	0.00184	-0.00948	-0.00698	2.53877
A57	2.91786	0.00015	0.00624	0.00707	0.01332	2.93117
A58	3.08155	-0.00002	-0.00234	0.00253	0.00045	3.08200
D1	0.00207	0.00001	0.00059	-0.00030	0.00029	0.00236
D2	-3.13245	-0.00001	0.00144	0.00015	0.00158	-3.13087
D3	3.13138	0.00007	0.00076	0.00097	0.00174	3.13312
D4	-0.00314	0.00005	0.00161	0.00142	0.00303	-0.00012
D5	-0.00403	0.00002	-0.00140	0.00092	-0.00048	-0.00451
D6	-3.11266	0.00007	0.00247	0.00071	0.00319	-3.10947
D7	-3.13461	-0.00004	-0.00156	-0.00022	-0.00178	-3.13639
D8	0.03994	0.00001	0.00232	-0.00043	0.00189	0.04184
D9	0.00056	-0.00003	0.00042	-0.00041	-0.00001	0.00055
D10	-3.13674	0.00001	0.00085	0.00043	0.00127	-3.13547
D11	3.13576	-0.00001	-0.00035	-0.00082	-0.00118	3.13458
D12	-0.00155	0.00003	0.00009	0.00002	0.00010	-0.00144
D13	-0.00309	0.00004	-0.00130	0.00099	-0.00030	-0.00338
D14	-3.13894	0.00003	-0.00106	0.00264	0.00154	-3.13740
D15	3.13457	0.00001	-0.00170	0.00022	-0.00147	3.13310
D16	-0.00128	-0.00001	-0.00146	0.00186	0.00036	-0.00091

D17	0.01288	-0.00010	-0.00917	-0.00947	-0.01863	-0.00576
D18	-3.13192	-0.00008	-0.00691	-0.00887	-0.01577	3.13549
D19	-3.12392	-0.00005	-0.00868	-0.00852	-0.01720	-3.14112
D20	0.01447	-0.00003	-0.00641	-0.00792	-0.01434	0.00013
D21	0.00439	-0.00004	0.00166	-0.00118	0.00048	0.00487
D22	3.11352	-0.00008	-0.00209	-0.00098	-0.00307	3.11045
D23	3.13983	-0.00003	0.00145	-0.00294	-0.00153	3.13831
D24	-0.03422	-0.00007	-0.00231	-0.00274	-0.00508	-0.03930
D25	1.33463	-0.00015	-0.00695	-0.00183	-0.00878	1.32585
D26	-2.85315	0.00005	-0.00643	-0.00156	-0.00798	-2.86114
D27	-0.79976	-0.00006	-0.00712	-0.00180	-0.00891	-0.80867
D28	-1.76891	-0.00010	-0.00251	-0.00207	-0.00458	-1.77349
D29	0.32649	0.00010	-0.00199	-0.00179	-0.00378	0.32271
D30	2.37988	-0.00001	-0.00268	-0.00203	-0.00471	2.37517
D31	-1.08619	-0.00006	-0.00306	0.00087	-0.00219	-1.08838
D32	0.95922	-0.00015	-0.00517	0.00055	-0.00463	0.95459
D33	3.12864	0.00004	-0.00266	0.00192	-0.00074	3.12789
D34	3.11878	0.00003	-0.00267	0.00175	-0.00091	3.11787
D35	-1.11900	-0.00006	-0.00478	0.00143	-0.00335	-1.12235
D36	1.05042	0.00012	-0.00227	0.00280	0.00054	1.05096
D37	1.02514	0.00002	-0.00246	0.00135	-0.00111	1.02403
D38	3.07055	-0.00007	-0.00457	0.00103	-0.00355	3.06700
D39	-1.04321	0.00011	-0.00206	0.00240	0.00033	-1.04288
D40	2.93487	-0.00001	0.00638	-0.00112	0.00530	2.94017
D41	-1.25417	-0.00005	0.00682	-0.00129	0.00549	-1.24867
D42	0.85446	0.00016	0.00724	0.00063	0.00790	0.86236
D43	2.94861	0.00012	0.00768	0.00046	0.00810	2.95670
D44	-1.24282	-0.00001	0.00703	-0.00020	0.00688	-1.23594
D45	0.85133	-0.00005	0.00747	-0.00037	0.00707	0.85840
D46	3.14109	0.00003	0.00067	0.00026	0.00094	-3.14115
D47	0.00138	-0.00001	-0.00014	-0.00068	-0.00082	0.00055
D48	0.00312	0.00001	-0.00188	-0.00042	-0.00230	0.00083
D49	-3.13659	-0.00003	-0.00270	-0.00136	-0.00406	-3.14065
D50	2.31583	0.00013	-0.01154	0.01491	0.00290	2.31874
D51	-1.29149	-0.00010	-0.01206	-0.02393	-0.03566	-1.32715
D52	-1.96324	0.00002	-0.01082	0.01166	0.00054	-1.96269
D53	0.71262	-0.00020	-0.01135	-0.02718	-0.03802	0.67460
D54	-2.71735	0.00016	0.00183	0.00167	0.00346	-2.71389
D55	-0.01254	0.00002	0.00051	0.00101	0.00147	-0.01107
D56	-0.03099	0.00004	0.00163	0.00030	0.00202	-0.02897
D57	2.67382	-0.00010	0.00031	-0.00035	0.00003	2.67385
D58	0.59111	-0.00001	0.00274	-0.02243	-0.02047	0.57065
D59	-1.81892	0.00015	0.00239	-0.02241	-0.02100	-1.83993
D60	1.83407	-0.00031	-0.00404	0.02002	0.01674	1.85082

D61	-0.58843	0.00004	-0.00173	0.02084	0.01971	-0.56872
D62	2.54639	0.00003	0.00216	0.00187	0.00389	2.55027
D63	-1.66369	-0.00003	0.00131	0.00144	0.00260	-1.66109
D64	0.43646	0.00001	0.00133	0.00194	0.00312	0.43958
D65	1.34749	0.00000	0.00240	0.00071	0.00322	1.35072
D66	-2.86258	-0.00007	0.00155	0.00028	0.00194	-2.86064
D67	-0.76243	-0.00002	0.00157	0.00078	0.00245	-0.75998
D68	-1.03830	0.00011	0.00215	0.00141	0.00360	-1.03470
D69	1.03481	0.00004	0.00130	0.00098	0.00231	1.03712
D70	3.13496	0.00009	0.00131	0.00148	0.00283	3.13779

Item	Value	Threshold	Converged?
Maximum Force	0.000516	0.000450	NO
RMS Force	0.000150	0.000300	YES
Maximum Displacement	0.072957	0.001800	NO
RMS Displacement	0.014643	0.001200	NO

Predicted change in Energy=-1.609249D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.639671	2.089376	-0.195922
2	6	0	-3.535025	1.116091	0.109219
3	7	0	-2.831770	-0.081345	0.143703
4	6	0	-1.538971	0.169570	-0.134845
5	7	0	-1.402972	1.479610	-0.347544
6	6	0	-0.128255	2.157113	-0.644956
7	6	0	0.448200	2.872816	0.581976
8	1	0	-2.774744	3.149272	-0.325633
9	1	0	-4.592042	1.174950	0.293643
10	1	0	0.575279	1.394761	-0.980380
11	1	0	-0.298013	2.865874	-1.456595
12	1	0	-0.241221	3.657194	0.911588
13	1	0	0.532871	2.142867	1.401106
14	35	0	0.120112	-2.693547	-0.081740
15	1	0	-0.766913	-0.623095	-0.173770
16	6	0	-3.311518	-1.399697	0.411584
17	6	0	-4.577404	-1.682426	0.688767
18	1	0	-2.509701	-2.134370	0.358501
19	1	0	-4.851940	-2.710887	0.879330
20	1	0	-5.367265	-0.942615	0.738034
21	7	0	1.709173	3.490153	0.188154

22	1	0	2.042054	4.130668	0.898917
23	1	0	2.416697	2.772369	0.046756
24	6	0	3.460853	-0.305439	-1.191111
25	6	0	3.271175	-0.584054	0.234595
26	8	0	2.771973	0.650296	-0.354145
27	1	0	4.431442	0.029101	-1.549346
28	1	0	2.829641	-0.813627	-1.914087
29	1	0	2.470834	-1.279514	0.481622
30	6	0	4.383533	-0.437507	1.235723
31	1	0	3.994387	-0.099370	2.200625
32	1	0	4.868760	-1.405213	1.395140
33	1	0	5.135556	0.277995	0.893305

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357223	0.000000			
3	N	2.205511	1.389104	0.000000		
4	C	2.213803	2.222543	1.346059	0.000000	
5	N	1.387165	2.210526	2.172410	1.334144	0.000000
6	C	2.552142	3.641234	3.597453	2.490112	1.473895
7	C	3.279307	4.379003	4.435916	3.430776	2.496371
8	H	1.076313	2.213808	3.265029	3.231433	2.161020
9	H	2.210792	1.074598	2.167791	3.242782	3.267125
10	H	3.381385	4.261394	3.879488	2.585744	2.078739
11	H	2.770489	3.998970	4.203211	3.249162	2.091090
12	H	3.072002	4.236761	4.612728	3.865579	2.770731
13	H	3.552236	4.389876	4.224806	3.247395	2.691686
14	Br	5.523205	5.282975	3.948168	3.309504	4.450357
15	H	3.296242	3.281355	2.158220	1.107206	2.203664
16	C	3.604729	2.543731	1.428275	2.429631	3.536839
17	C	4.331740	3.042060	2.430595	3.652438	4.598851
18	H	4.261961	3.417444	2.089205	2.548303	3.845023
19	H	5.393776	4.119841	3.396576	4.505702	5.564249
20	H	4.183899	2.826797	2.742946	4.081018	4.770878
21	N	4.584990	5.757084	5.777346	4.656290	3.743622
22	H	5.223418	6.388670	6.485796	5.438998	4.522165
23	H	5.108056	6.178200	5.974904	4.738655	4.051737
24	C	6.628872	7.256302	6.436540	5.132210	5.249267
25	C	6.501590	7.016450	6.124288	4.882821	5.142494
26	O	5.601953	6.341127	5.673190	4.343205	4.256521
27	H	7.488466	8.209566	7.458744	6.137294	6.130962
28	H	6.425954	6.951729	6.068138	4.818417	5.062411
29	H	6.158389	6.476723	5.446779	4.307948	4.827697

30	C	7.600009	8.147775	7.306158	6.109260	6.298072
31	H	7.385443	7.908436	7.129352	6.012054	6.173963
32	H	8.433278	8.867591	7.913083	6.773464	7.119956
33	H	8.057398	8.746208	8.010574	6.754121	6.762834

		6	7	8	9	10
6	C	0.000000				
7	C	1.532937	0.000000			
8	H	2.844336	3.359695	0.000000		
9	H	4.665941	5.326342	2.753910	0.000000	
10	H	1.090253	2.154473	3.837923	5.326599	0.000000
11	H	1.090834	2.170865	2.737441	4.935711	1.775836
12	H	2.164678	1.095077	2.864863	5.047082	3.060199
13	H	2.150269	1.100440	3.864556	5.331798	2.496584
14	Br	4.889560	5.615386	6.525198	6.108238	4.210580
15	H	2.891272	3.777439	4.276119	4.252417	2.554181
16	C	4.888797	5.693758	4.639475	2.877926	4.985353
17	C	6.026259	6.783681	5.255844	2.884603	6.229387
18	H	5.009495	5.819883	5.334338	3.910492	4.874882
19	H	6.952271	7.704391	6.333098	3.938312	7.054755
20	H	6.242452	6.957119	4.959444	2.298377	6.612874
21	N	2.418101	1.458168	4.526112	6.713911	2.653650
22	H	3.314921	2.054996	5.065985	7.287925	3.628825
23	H	2.708097	2.042433	5.218409	7.192713	2.518657
24	C	4.386816	4.724535	7.180999	8.321368	3.355835
25	C	4.454631	4.476585	7.127742	8.057776	3.558051
26	O	3.281218	3.349006	6.083729	7.411046	2.402471
27	H	5.112455	5.338115	7.947456	9.280778	4.130223
28	H	4.380084	5.048906	7.045344	7.994366	3.291038
29	H	4.453634	4.619845	6.912445	7.479568	3.589196
30	C	5.534008	5.183867	8.157435	9.167795	4.771909
31	H	5.494108	4.901974	7.921918	8.887476	4.903215
32	H	6.467018	6.205169	9.062425	9.867994	5.649507
33	H	5.796985	5.366687	8.503110	9.787251	5.055095

		11	12	13	14	15
11	H	0.000000				
12	H	2.497540	0.000000			
13	H	3.062607	1.769755	0.000000		
14	Br	5.742144	6.438103	5.075440	0.000000	
15	H	3.746787	4.446934	3.438054	2.254341	0.000000
16	C	5.546747	5.937076	5.320548	3.700473	2.724107
17	C	6.603242	6.882127	6.423021	4.866488	4.047961
18	H	5.760954	6.244527	5.351544	2.724410	2.367399
19	H	7.569350	7.862075	7.268243	5.064115	4.706946
20	H	6.709568	6.889462	6.691148	5.817998	4.700715

21	N	2.669030	2.086935	2.161045	6.390313	4.814644
22	H	3.553034	2.331883	2.545816	7.157196	5.624874
23	H	3.104587	2.931787	2.404025	5.930181	4.659740
24	C	4.925118	5.816284	4.613770	4.253741	4.360034
25	C	5.244162	5.548282	4.036726	3.805157	4.058872
26	O	3.943222	4.441042	3.212826	4.276430	3.765339
27	H	5.515762	6.407264	5.326540	5.306057	5.416684
28	H	4.850798	6.115788	5.000650	3.772683	4.000026
29	H	5.348593	5.649000	4.039040	2.800492	3.368001
30	C	6.330701	6.185466	4.638241	5.000218	5.343052
31	H	6.371234	5.806355	4.201065	5.191238	5.346215
32	H	7.284925	7.209278	5.602575	5.137182	5.902034
33	H	6.460868	6.350515	4.992025	5.910622	6.065456

		16	17	18	19	20
16	C	0.000000				
17	C	1.326361	0.000000			
18	H	1.088794	2.142130	0.000000		
19	H	2.076273	1.081395	2.467735	0.000000	
20	H	2.131101	1.083342	3.119295	1.847244	0.000000
21	N	7.011981	8.156423	7.033006	9.054216	8.368260
22	H	7.712532	8.812119	7.762810	9.712590	8.981207
23	H	7.095891	8.317140	6.960077	9.142886	8.652690
24	C	7.044930	8.369206	6.433802	8.898058	9.058878
25	C	6.635393	7.938065	5.986431	8.421645	8.660523
26	O	6.465112	7.780913	6.013179	8.422771	8.365251
27	H	8.114193	9.439162	7.516645	9.979338	10.108957
28	H	6.592879	7.898985	5.951268	8.391035	8.616244
29	H	5.784024	7.062783	5.054866	7.471949	7.849525
30	C	7.798642	9.063518	7.153009	9.517838	9.776548
31	H	7.633332	8.846885	7.059590	9.317904	9.512663
32	H	8.239197	9.476593	7.486520	9.821551	10.267522
33	H	8.625529	9.910937	8.034642	10.425147	10.574651

		21	22	23	24	25
21	N	0.000000				
22	H	1.013041	0.000000			
23	H	1.017741	1.646667	0.000000		
24	C	4.401962	5.104924	3.477856	0.000000	
25	C	4.363619	4.917384	3.468572	1.465006	0.000000
26	O	3.080328	3.770402	2.188638	1.445164	1.455829
27	H	4.733765	5.340975	3.759289	1.087332	2.214639
28	H	4.919083	5.742763	4.107894	1.085991	2.205558
29	H	4.839005	5.443166	4.075512	2.174166	1.088684
30	C	4.865811	5.144335	3.947833	2.599674	1.503687
31	H	4.707112	4.837278	3.921114	3.439622	2.150170

32	H	5.950161	6.235582	5.028215	3.143311	2.138562
33	H	4.749241	4.940938	3.785596	2.736753	2.157069

		26	27	28	29	30
26	O	0.000000				
27	H	2.137341	0.000000			
28	H	2.140050	1.846346	0.000000		
29	H	2.124467	3.111477	2.466823	0.000000	
30	C	2.511597	2.824293	3.532329	2.221725	0.000000
31	H	2.929700	3.777540	4.335625	2.582426	1.093987
32	H	3.417840	3.304316	3.931789	2.569118	1.094218
33	H	2.698381	2.554265	3.793459	3.113850	1.093038

		31	32	33
31	H	0.000000		
32	H	1.765945	0.000000	
33	H	1.775882	1.776572	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.324344	2.489916	-0.247429
2	6	0	-3.323236	1.615329	0.034290
3	7	0	-2.752355	0.349393	0.067596
4	6	0	-1.435813	0.463100	-0.188651
5	7	0	-1.157431	1.752837	-0.386196
6	6	0	0.186938	2.292766	-0.657334
7	6	0	0.816414	2.932645	0.585328
8	1	0	-2.343480	3.559212	-0.368631
9	1	0	-4.370804	1.785211	0.203116
10	1	0	0.810512	1.462437	-0.989540
11	1	0	0.106957	3.022288	-1.464377
12	1	0	0.209314	3.783413	0.912157
13	1	0	0.809423	2.191081	1.398349
14	35	0	-0.092635	-2.561167	-0.138702
15	1	0	-0.752168	-0.407135	-0.223662
16	6	0	-3.374263	-0.912353	0.314978
17	6	0	-4.667421	-1.060555	0.569955
18	1	0	-2.654619	-1.727992	0.266844

19	1	0	-5.053141	-2.055354	0.746053
20	1	0	-5.374571	-0.241053	0.614508
21	7	0	2.142270	3.415018	0.216987
22	1	0	2.529965	4.010422	0.939094
23	1	0	2.771410	2.626971	0.079280
24	6	0	3.501341	-0.534408	-1.173063
25	6	0	3.259876	-0.802948	0.246734
26	8	0	2.904806	0.482480	-0.337250
27	1	0	4.507768	-0.302486	-1.513076
28	1	0	2.831366	-0.966284	-1.910623
29	1	0	2.386018	-1.410976	0.474566
30	6	0	4.365096	-0.784316	1.266153
31	1	0	3.998598	-0.414541	2.228313
32	1	0	4.741692	-1.799593	1.423326
33	1	0	5.194607	-0.150413	0.942407

Rotational constants (GHZ): 0.4192324 0.2905085 0.1814994

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1309.4800706457 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 3.59D-06 NBF= 482

NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999999 0.001086 -0.000438 0.000252 Ang= 0.14 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3205.64833838 A.U. after 10 cycles

NFock= 10 Conv=0.84D-08 -V/T= 2.0018

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000030972	0.000023189	-0.000060804
2	6	-0.000053688	-0.000048359	-0.000068124
3	7	0.000065681	0.000109187	0.000138981
4	6	-0.000003943	0.000034970	-0.000035895
5	7	-0.000046243	-0.000205096	-0.000011853
6	6	0.000098821	0.000076329	0.000095235
7	6	0.000103810	0.000018906	0.000074586
8	1	0.000020345	0.000004467	0.000026828
9	1	-0.000010353	0.000007394	-0.000028436
10	1	-0.000045753	-0.000046144	-0.000008698
11	1	-0.000004451	0.000042230	0.000029853
12	1	-0.000036323	0.000020233	-0.000028353
13	1	0.000020071	0.000017245	0.000000348
14	35	-0.000011934	0.000096266	-0.000030696
15	1	0.000125110	-0.000041417	-0.000044493
16	6	0.000041754	0.000012383	0.000012540
17	6	-0.000018545	-0.000023749	0.000039848
18	1	-0.000053588	0.000022618	-0.000023790
19	1	-0.000017112	-0.000000722	-0.000023612
20	1	0.000022501	0.000003080	0.000000893
21	7	-0.000107530	-0.000013523	-0.000177450
22	1	-0.000044776	-0.000020638	0.000102205
23	1	0.000044122	-0.000172305	0.000041158
24	6	-0.000181780	0.000010945	0.000244035
25	6	0.000162383	0.000083634	-0.000080482
26	8	-0.000102623	0.000017230	-0.000159498
27	1	0.000059572	-0.000007580	-0.000074453
28	1	0.000069195	-0.000019950	-0.000097844

29	1	-0.000042741	0.000134438	0.000127023
30	6	0.000012989	-0.000107754	0.000071747
31	1	-0.000038368	-0.000025427	-0.000040473
32	1	0.000022767	-0.000003346	0.000002024
33	1	-0.000018397	0.000001266	-0.000012350

Cartesian Forces: Max 0.000244035 RMS 0.000073214

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000300065 RMS 0.000073288
Search for a local minimum.
Step number 33 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 30 31 32 33
DE= -2.18D-05 DEPred=-1.61D-05 R= 1.36D+00
TightC=F SS= 1.41D+00 RLast= 8.15D-02 DXNew= 1.7446D+00 2.4453D-01
Trust test= 1.36D+00 RLast= 8.15D-02 DXMaxT set to 1.04D+00
ITU= 1 1 1 1 1 1 1 0 0 -1 1 -1 1 1 1 1 1 1 1 1
ITU= 1 0 -1 -1 1 1 1 -1 1 0 0 -1 0

Eigenvalues ---	0.00059	0.00161	0.00226	0.00435	0.00643
Eigenvalues ---	0.00720	0.00733	0.01180	0.01513	0.01888
Eigenvalues ---	0.01983	0.02176	0.02363	0.02377	0.02463
Eigenvalues ---	0.02684	0.02855	0.03011	0.03082	0.03192
Eigenvalues ---	0.03448	0.03666	0.03743	0.03876	0.04089
Eigenvalues ---	0.04400	0.04419	0.05265	0.05436	0.05462
Eigenvalues ---	0.05740	0.05848	0.05957	0.07605	0.08641
Eigenvalues ---	0.08889	0.09535	0.10383	0.11505	0.12316
Eigenvalues ---	0.12836	0.13162	0.14362	0.15861	0.15940
Eigenvalues ---	0.16001	0.16003	0.16005	0.16020	0.16058
Eigenvalues ---	0.16149	0.18790	0.21298	0.21938	0.22182
Eigenvalues ---	0.23003	0.23502	0.25325	0.26022	0.27635
Eigenvalues ---	0.28114	0.29441	0.30395	0.31802	0.32310
Eigenvalues ---	0.33655	0.34282	0.34336	0.34371	0.34546
Eigenvalues ---	0.34665	0.34733	0.35083	0.35128	0.35311
Eigenvalues ---	0.35562	0.35644	0.35881	0.35895	0.36417
Eigenvalues ---	0.36622	0.39161	0.39604	0.41867	0.42467
Eigenvalues ---	0.44633	0.45498	0.46378	0.49487	0.54737
Eigenvalues ---	0.58051	0.60622	1.29107		

En-DIIS/RFO-DIIS IScMMF= 0 using points: 33 32 31 30 29
RFO step: Lambda=-1.73085268D-06.
DidBck=F Rises=F RFO-DIIS coefs: 1.16039 -0.07202 -0.12518 0.02955 0.00726
Iteration 1 RMS(Cart)= 0.01305436 RMS(Int)= 0.00006355
Iteration 2 RMS(Cart)= 0.00008839 RMS(Int)= 0.00003094
Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00003094

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56478	0.00001	-0.00001	0.00001	0.00000	2.56478
R2	2.62136	0.00000	0.00007	0.00000	0.00007	2.62144
R3	2.03394	0.00000	-0.00001	0.00000	-0.00001	2.03393
R4	2.62503	0.00002	-0.00010	-0.00002	-0.00012	2.62491
R5	2.03070	0.00001	0.00003	0.00001	0.00003	2.03073
R6	2.54368	0.00002	0.00026	0.00001	0.00027	2.54395
R7	2.69905	0.00000	0.00006	0.00004	0.00010	2.69915
R8	2.52117	-0.00020	-0.00009	-0.00016	-0.00025	2.52092
R9	2.09232	0.00005	0.00016	0.00013	0.00029	2.09261
R10	2.78526	-0.00004	-0.00020	0.00000	-0.00020	2.78506
R11	2.89683	-0.00007	0.00018	-0.00010	0.00008	2.89691
R12	2.06028	0.00001	-0.00007	0.00001	-0.00006	2.06022
R13	2.06138	0.00001	0.00004	0.00000	0.00004	2.06142
R14	2.06939	0.00003	0.00005	0.00005	0.00010	2.06950
R15	2.07953	-0.00001	0.00018	-0.00001	0.00017	2.07970
R16	2.75554	-0.00017	-0.00045	-0.00039	-0.00085	2.75469
R17	4.26009	-0.00009	-0.00056	-0.00182	-0.00238	4.25771
R18	2.50646	0.00002	0.00000	0.00002	0.00002	2.50648
R19	2.05752	-0.00005	0.00012	-0.00008	0.00004	2.05756
R20	2.04354	0.00000	0.00001	0.00000	0.00001	2.04355
R21	2.04722	-0.00002	0.00001	-0.00003	-0.00002	2.04720
R22	1.91437	0.00004	-0.00002	0.00007	0.00006	1.91443
R23	1.92325	0.00005	-0.00016	0.00020	0.00003	1.92328
R24	4.13593	-0.00010	0.00022	0.00030	0.00053	4.13645
R25	2.76846	-0.00001	-0.00001	-0.00082	-0.00074	2.76772
R26	2.73096	-0.00006	-0.00047	0.00037	-0.00014	2.73082
R27	2.05476	0.00008	0.00003	0.00021	0.00024	2.05500
R28	2.05223	0.00003	0.00005	-0.00003	0.00003	2.05225
R29	2.75112	-0.00001	-0.00061	-0.00020	-0.00086	2.75026
R30	2.05731	-0.00003	-0.00014	-0.00016	-0.00029	2.05702
R31	2.84156	-0.00001	0.00018	0.00012	0.00030	2.84186
R32	2.06734	-0.00003	-0.00003	0.00002	-0.00002	2.06732
R33	2.06777	0.00001	0.00000	0.00003	0.00003	2.06780
R34	2.06554	-0.00001	-0.00002	-0.00003	-0.00005	2.06550
A1	1.87285	-0.00005	-0.00003	-0.00014	-0.00017	1.87268

A2	2.27902	0.00004	0.00005	0.00018	0.00023	2.27925
A3	2.13126	0.00001	-0.00002	-0.00003	-0.00006	2.13121
A4	1.86478	-0.00003	0.00011	-0.00002	0.00009	1.86487
A5	2.27603	0.00001	-0.00009	-0.00014	-0.00022	2.27580
A6	2.14235	0.00003	-0.00002	0.00015	0.00013	2.14248
A7	1.89696	0.00002	-0.00011	0.00012	0.00001	1.89697
A8	2.25271	-0.00005	-0.00005	-0.00015	-0.00020	2.25252
A9	2.13350	0.00003	0.00016	0.00002	0.00018	2.13368
A10	1.89013	-0.00003	0.00003	-0.00019	-0.00016	1.88997
A11	2.14544	0.00022	-0.00104	0.00055	-0.00049	2.14495
A12	2.24759	-0.00019	0.00101	-0.00038	0.00063	2.24821
A13	1.90004	0.00010	-0.00001	0.00024	0.00023	1.90027
A14	2.20315	0.00014	0.00038	0.00006	0.00044	2.20359
A15	2.17937	-0.00024	-0.00041	-0.00032	-0.00073	2.17864
A16	1.95879	0.00012	-0.00009	0.00045	0.00036	1.95915
A17	1.87418	-0.00014	-0.00036	-0.00070	-0.00106	1.87312
A18	1.89043	0.00003	0.00030	-0.00001	0.00029	1.89071
A19	1.90715	0.00002	0.00044	0.00014	0.00058	1.90773
A20	1.92911	-0.00007	-0.00010	-0.00013	-0.00023	1.92888
A21	1.90269	0.00003	-0.00021	0.00024	0.00003	1.90272
A22	1.91621	0.00003	-0.00061	0.00004	-0.00058	1.91563
A23	1.89127	0.00009	-0.00031	0.00030	-0.00001	1.89126
A24	1.88251	-0.00023	0.00042	-0.00064	-0.00022	1.88229
A25	1.87498	-0.00002	-0.00008	0.00022	0.00014	1.87512
A26	1.89914	0.00013	-0.00004	0.00007	0.00002	1.89916
A27	1.99910	0.00000	0.00057	0.00002	0.00059	1.99970
A28	2.16100	0.00000	-0.00022	-0.00001	-0.00023	2.16077
A29	1.94585	0.00002	0.00001	0.00000	0.00001	1.94586
A30	2.17633	-0.00001	0.00021	0.00001	0.00022	2.17655
A31	2.07356	0.00003	-0.00006	0.00010	0.00005	2.07361
A32	2.16493	-0.00003	0.00002	-0.00009	-0.00007	2.16486
A33	2.04469	0.00000	0.00004	-0.00002	0.00002	2.04472
A34	1.94158	0.00009	0.00021	-0.00072	-0.00053	1.94105
A35	1.91783	-0.00030	0.00001	-0.00063	-0.00063	1.91720
A36	1.89121	0.00008	0.00000	-0.00032	-0.00031	1.89091
A37	2.08830	-0.00008	-0.00061	-0.00004	-0.00075	2.08755
A38	2.07558	0.00015	0.00083	-0.00035	0.00058	2.07616
A39	1.99636	0.00008	0.00027	0.00001	0.00031	1.99667
A40	2.00200	-0.00003	0.00003	0.00053	0.00054	2.00255
A41	2.03026	-0.00008	-0.00025	0.00003	-0.00022	2.03004
A42	2.02360	0.00005	0.00118	-0.00042	0.00082	2.02442
A43	2.13366	0.00004	-0.00004	0.00015	0.00006	2.13372
A44	1.96200	-0.00009	0.00062	-0.00083	-0.00023	1.96177
A45	2.02670	0.00015	0.00023	0.00039	0.00067	2.02737

A46	2.04318	-0.00009	-0.00120	0.00027	-0.00094	2.04225
A47	2.54044	0.00007	-0.00070	-0.00082	-0.00135	2.53909
A48	2.50423	-0.00015	-0.00185	-0.00240	-0.00401	2.50022
A49	1.93286	-0.00007	-0.00017	-0.00010	-0.00027	1.93259
A50	1.91649	0.00004	-0.00015	0.00017	0.00003	1.91652
A51	1.94355	-0.00002	0.00012	-0.00015	-0.00003	1.94352
A52	1.87821	0.00002	-0.00012	0.00023	0.00011	1.87832
A53	1.89517	0.00004	0.00021	-0.00005	0.00016	1.89533
A54	1.89596	0.00000	0.00012	-0.00010	0.00002	1.89597
A55	3.47707	-0.00008	-0.00002	0.00576	0.00574	3.48280
A56	2.53877	-0.00023	-0.00070	-0.00223	-0.00289	2.53588
A57	2.93117	0.00010	0.00295	0.00731	0.01026	2.94143
A58	3.08200	0.00009	-0.00042	0.00540	0.00501	3.08701
D1	0.00236	0.00002	0.00007	0.00053	0.00060	0.00296
D2	-3.13087	0.00000	0.00046	0.00111	0.00157	-3.12930
D3	3.13312	0.00004	0.00029	0.00028	0.00057	3.13369
D4	-0.00012	0.00002	0.00068	0.00086	0.00154	0.00143
D5	-0.00451	0.00002	-0.00043	0.00000	-0.00042	-0.00494
D6	-3.10947	0.00003	0.00070	0.00055	0.00125	-3.10822
D7	-3.13639	0.00000	-0.00062	0.00022	-0.00040	-3.13679
D8	0.04184	0.00001	0.00051	0.00076	0.00127	0.04311
D9	0.00055	-0.00005	0.00030	-0.00088	-0.00058	-0.00002
D10	-3.13547	-0.00001	0.00038	0.00038	0.00076	-3.13471
D11	3.13458	-0.00003	-0.00005	-0.00140	-0.00146	3.13313
D12	-0.00144	0.00000	0.00002	-0.00014	-0.00012	-0.00156
D13	-0.00338	0.00006	-0.00057	0.00089	0.00032	-0.00306
D14	-3.13740	0.00005	-0.00003	0.00257	0.00253	-3.13486
D15	3.13310	0.00003	-0.00064	-0.00027	-0.00091	3.13219
D16	-0.00091	0.00002	-0.00010	0.00141	0.00130	0.00039
D17	-0.00576	-0.00004	-0.00376	-0.00658	-0.01034	-0.01610
D18	3.13549	-0.00005	-0.00303	-0.00670	-0.00973	3.12576
D19	-3.14112	0.00000	-0.00368	-0.00517	-0.00885	3.13322
D20	0.00013	-0.00001	-0.00295	-0.00528	-0.00823	-0.00810
D21	0.00487	-0.00005	0.00062	-0.00056	0.00006	0.00493
D22	3.11045	-0.00005	-0.00048	-0.00108	-0.00155	3.10889
D23	3.13831	-0.00003	0.00003	-0.00236	-0.00233	3.13598
D24	-0.03930	-0.00003	-0.00107	-0.00288	-0.00395	-0.04325
D25	1.32585	0.00000	-0.00056	-0.00054	-0.00110	1.32475
D26	-2.86114	0.00001	-0.00031	-0.00055	-0.00086	-2.86200
D27	-0.80867	-0.00001	-0.00059	-0.00066	-0.00124	-0.80992
D28	-1.77349	0.00000	0.00073	0.00008	0.00081	-1.77268
D29	0.32271	0.00001	0.00099	0.00006	0.00105	0.32376
D30	2.37517	-0.00001	0.00071	-0.00005	0.00067	2.37584
D31	-1.08838	-0.00009	-0.00094	-0.00285	-0.00379	-1.09218

D32	0.95459	-0.00005	-0.00156	-0.00239	-0.00395	0.95064
D33	3.12789	-0.00014	-0.00079	-0.00258	-0.00337	3.12452
D34	3.11787	-0.00001	-0.00073	-0.00235	-0.00307	3.11479
D35	-1.12235	0.00003	-0.00134	-0.00189	-0.00323	-1.12558
D36	1.05096	-0.00005	-0.00057	-0.00208	-0.00265	1.04831
D37	1.02403	-0.00002	-0.00069	-0.00265	-0.00334	1.02069
D38	3.06700	0.00003	-0.00131	-0.00219	-0.00350	3.06350
D39	-1.04288	-0.00006	-0.00054	-0.00238	-0.00292	-1.04580
D40	2.94017	0.00003	0.00060	-0.00007	0.00054	2.94071
D41	-1.24867	-0.00001	0.00075	-0.00134	-0.00060	-1.24927
D42	0.86236	0.00005	0.00112	0.00021	0.00134	0.86370
D43	2.95670	0.00001	0.00126	-0.00106	0.00020	2.95690
D44	-1.23594	-0.00001	0.00088	-0.00014	0.00075	-1.23519
D45	0.85840	-0.00006	0.00102	-0.00141	-0.00039	0.85801
D46	-3.14115	-0.00003	0.00028	-0.00105	-0.00077	3.14127
D47	0.00055	-0.00001	-0.00012	-0.00077	-0.00088	-0.00033
D48	0.00083	-0.00001	-0.00054	-0.00092	-0.00146	-0.00063
D49	-3.14065	0.00000	-0.00094	-0.00064	-0.00158	3.14096
D50	2.31874	0.00008	-0.00064	-0.00182	-0.00250	2.31624
D51	-1.32715	0.00010	-0.00566	-0.01200	-0.01764	-1.34479
D52	-1.96269	-0.00010	-0.00071	-0.00581	-0.00654	-1.96923
D53	0.67460	-0.00009	-0.00574	-0.01599	-0.02168	0.65292
D54	-2.71389	0.00000	0.00068	-0.00062	0.00005	-2.71384
D55	-0.01107	-0.00001	0.00026	-0.00058	-0.00031	-0.01139
D56	-0.02897	-0.00005	0.00054	-0.00148	-0.00093	-0.02989
D57	2.67385	-0.00006	0.00013	-0.00144	-0.00130	2.67256
D58	0.57065	-0.00008	-0.00223	-0.00643	-0.00873	0.56191
D59	-1.83993	-0.00001	-0.00219	-0.00712	-0.00940	-1.84933
D60	1.85082	-0.00011	0.00090	0.00464	0.00559	1.85641
D61	-0.56872	-0.00004	0.00181	0.00475	0.00660	-0.56212
D62	2.55027	0.00001	0.00083	0.00085	0.00166	2.55194
D63	-1.66109	0.00001	0.00047	0.00119	0.00165	-1.65944
D64	0.43958	0.00002	0.00060	0.00108	0.00166	0.44124
D65	1.35072	-0.00004	0.00081	0.00017	0.00099	1.35170
D66	-2.86064	-0.00004	0.00046	0.00051	0.00097	-2.85967
D67	-0.75998	-0.00003	0.00058	0.00040	0.00099	-0.75899
D68	-1.03470	0.00004	0.00097	0.00073	0.00171	-1.03300
D69	1.03712	0.00004	0.00062	0.00107	0.00169	1.03881
D70	3.13779	0.00005	0.00074	0.00096	0.00171	3.13949

Item	Value	Threshold	Converged?
Maximum Force	0.000300	0.000450	YES
RMS Force	0.000073	0.000300	YES
Maximum Displacement	0.086072	0.001800	NO
RMS Displacement	0.013033	0.001200	NO

Predicted change in Energy=-3.969900D-06
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.639462	2.091002	-0.193641
2	6	0	-3.533029	1.115743	0.110448
3	7	0	-2.828443	-0.080974	0.139797
4	6	0	-1.536510	0.172103	-0.141488
5	7	0	-1.402596	1.482816	-0.350503
6	6	0	-0.128751	2.161969	-0.647367
7	6	0	0.449563	2.873856	0.580965
8	1	0	-2.775720	3.151217	-0.319417
9	1	0	-4.589868	1.172934	0.296510
10	1	0	0.573775	1.400408	-0.986573
11	1	0	-0.299718	2.873476	-1.456375
12	1	0	-0.238244	3.659293	0.911603
13	1	0	0.532159	2.142106	1.398817
14	35	0	0.116390	-2.693334	-0.127288
15	1	0	-0.764432	-0.620417	-0.186792
16	6	0	-3.306623	-1.400709	0.403920
17	6	0	-4.569760	-1.683799	0.693059
18	1	0	-2.506087	-2.135731	0.337590
19	1	0	-4.843692	-2.713283	0.878927
20	1	0	-5.357877	-0.943245	0.756782
21	7	0	1.711439	3.488831	0.188008
22	1	0	2.045900	4.126710	0.900440
23	1	0	2.416971	2.769255	0.045654
24	6	0	3.444973	-0.317694	-1.181539
25	6	0	3.267143	-0.585023	0.247448
26	8	0	2.761294	0.643490	-0.346677
27	1	0	4.412714	0.014878	-1.549557
28	1	0	2.809344	-0.832623	-1.895843
29	1	0	2.469856	-1.279071	0.507304
30	6	0	4.387581	-0.429855	1.238458
31	1	0	4.005541	-0.085930	2.204142
32	1	0	4.875831	-1.395645	1.400356
33	1	0	5.135453	0.284614	0.885046

Distance matrix (angstroms):

	1	2	3	4	5

1	C	0.000000				
2	C	1.357225	0.000000			
3	N	2.205533	1.389042	0.000000		
4	C	2.213910	2.222614	1.346201	0.000000	
5	N	1.387204	2.210421	2.172296	1.334013	0.000000
6	C	2.552367	3.641151	3.597048	2.489431	1.473791
7	C	3.279474	4.378742	4.435197	3.430145	2.496621
8	H	1.076310	2.213923	3.265076	3.231474	2.161018
9	H	2.210696	1.074616	2.167825	3.242915	3.267010
10	H	3.380910	4.260319	3.877923	2.583836	2.077840
11	H	2.771492	3.999857	4.203688	3.249000	2.091227
12	H	3.073589	4.238762	4.614587	3.867169	2.772307
13	H	3.549326	4.386236	4.221476	3.245434	2.690365
14	Br	5.521684	5.280516	3.945605	3.308022	4.449423
15	H	3.296601	3.281422	2.158193	1.107359	2.204006
16	C	3.604751	2.543604	1.428327	2.429919	3.536833
17	C	4.331445	3.041659	2.430501	3.652594	4.598630
18	H	4.262073	3.417351	2.089273	2.548664	3.845133
19	H	5.393532	4.119447	3.396556	4.506013	5.564161
20	H	4.183269	2.826173	2.742667	4.080898	4.770335
21	N	4.585839	5.756909	5.775497	4.653862	3.743168
22	H	5.224341	6.388619	6.484011	5.436745	4.521854
23	H	5.107328	6.175823	5.970513	4.733945	4.049810
24	C	6.618014	7.239923	6.415428	5.112415	5.237498
25	C	6.499512	7.010971	6.117338	4.878483	5.141981
26	O	5.593468	6.328545	5.657443	4.328445	4.247642
27	H	7.475425	8.191602	7.436226	6.115607	6.116404
28	H	6.413623	6.931596	6.040980	4.793087	5.048739
29	H	6.160669	6.475125	5.444489	4.310198	4.833191
30	C	7.601642	8.148457	7.307515	6.112403	6.301529
31	H	7.392189	7.915655	7.138968	6.023528	6.183455
32	H	8.436655	8.870166	7.916640	6.778881	7.125285
33	H	8.054558	8.742617	8.007039	6.751409	6.760795

		6	7	8	9	10
6	C	0.000000				
7	C	1.532980	0.000000			
8	H	2.844752	3.360069	0.000000		
9	H	4.665904	5.326341	2.753925	0.000000	
10	H	1.090219	2.154914	3.837909	5.325528	0.000000
11	H	1.090856	2.170755	2.738686	4.936581	1.775846
12	H	2.164337	1.095131	2.865717	5.049450	3.060230
13	H	2.150364	1.100528	3.861696	5.328182	2.498387
14	Br	4.889227	5.621942	6.523802	6.105448	4.207885
15	H	2.891002	3.777986	4.276458	4.252487	2.552290

16	C	4.888430	5.693170	4.639516	2.877828	4.983695
17	C	6.025715	6.780736	5.255576	2.884195	6.228118
18	H	5.009201	5.821602	5.334434	3.910383	4.872703
19	H	6.951858	7.702172	6.332843	3.937806	7.053474
20	H	6.241614	6.951800	4.958867	2.297804	6.611845
21	N	2.417584	1.457718	4.528362	6.714285	2.652439
22	H	3.314366	2.054264	5.068299	7.288548	3.627767
23	H	2.707355	2.041615	5.219503	7.190755	2.517262
24	C	4.382416	4.718569	7.174512	8.304533	3.351667
25	C	4.458559	4.473683	7.127203	8.051425	3.566368
26	O	3.278498	3.343524	6.078484	7.398215	2.401590
27	H	5.103807	5.330989	7.938731	9.262588	4.119964
28	H	4.377062	5.043920	7.039108	7.973519	3.288004
29	H	4.463941	4.618854	6.915706	7.476393	3.606439
30	C	5.538153	5.182161	8.158673	9.167922	4.779723
31	H	5.502410	4.903062	7.926725	8.894090	4.915983
32	H	6.472682	6.204183	9.065197	9.869930	5.658890
33	H	5.795221	5.362295	8.500283	9.783524	5.055380

		11	12	13	14	15
11	H	0.000000				
12	H	2.495718	0.000000			
13	H	3.062522	1.769959	0.000000		
14	Br	5.738379	6.446777	5.087567	0.000000	
15	H	3.746343	4.449637	3.439017	2.253081	0.000000
16	C	5.547147	5.939387	5.317669	3.697307	2.724065
17	C	6.604702	6.881746	6.416013	4.863346	4.047893
18	H	5.760081	6.249393	5.353226	2.721106	2.367386
19	H	7.570549	7.862630	7.262566	5.061154	4.707038
20	H	6.711960	6.886071	6.680129	5.814808	4.700456
21	N	2.669720	2.086603	2.161118	6.392399	4.812103
22	H	3.553462	2.331505	2.545280	7.161860	5.622745
23	H	3.106018	2.931246	2.403515	5.929794	4.654593
24	C	4.927658	5.810659	4.603623	4.223100	4.335926
25	C	5.252306	5.544643	4.030263	3.809547	4.055048
26	O	3.946398	4.435715	3.203380	4.263572	3.748836
27	H	5.512465	6.400819	5.317586	5.274056	5.391064
28	H	4.857424	6.111208	4.988925	3.720488	3.967085
29	H	5.363787	5.646654	4.031614	2.818093	3.372864
30	C	6.336000	6.182737	4.637346	5.023114	5.348915
31	H	6.379084	5.805778	4.204411	5.230641	5.362358
32	H	7.291955	7.207291	5.602068	5.164297	5.910379
33	H	6.459531	6.345533	4.990446	5.923173	6.064368

		16	17	18	19	20
16	C	0.000000				

17	C	1.326370	0.000000			
18	H	1.088813	2.142276	0.000000		
19	H	2.076310	1.081398	2.467997	0.000000	
20	H	2.131063	1.083333	3.119367	1.847252	0.000000
21	N	7.009648	8.152585	7.031757	9.050599	8.363136
22	H	7.710279	8.807496	7.762445	9.708370	8.974464
23	H	7.090591	8.310429	6.955617	9.136181	8.645034
24	C	7.019306	8.343639	6.405321	8.870532	9.035407
25	C	6.626027	7.926092	5.978546	8.409157	8.647469
26	O	6.446842	7.761552	5.994798	8.402729	8.346035
27	H	8.087529	9.412740	7.487072	9.950953	10.084724
28	H	6.558710	7.866263	5.911017	8.354950	8.587908
29	H	5.778684	7.053687	5.051997	7.462108	7.838904
30	C	7.799987	9.061115	7.158508	9.516287	9.770852
31	H	7.644422	8.852815	7.077216	9.325669	9.513329
32	H	8.242903	9.476417	7.494658	9.822280	10.263899
33	H	8.622090	9.904679	8.034358	10.419729	10.565702

		21	22	23	24	25
21	N	0.000000				
22	H	1.013071	0.000000			
23	H	1.017757	1.646523	0.000000		
24	C	4.401185	5.103408	3.477362	0.000000	
25	C	4.361197	4.911035	3.466222	1.464613	0.000000
26	O	3.079618	3.768277	2.188917	1.445090	1.455374
27	H	4.731212	5.339612	3.756898	1.087458	2.213920
28	H	4.921666	5.744304	4.110583	1.086005	2.205580
29	H	4.838392	5.436613	4.074906	2.174233	1.088529
30	C	4.860174	5.134201	3.942131	2.599514	1.503848
31	H	4.701768	4.825574	3.915955	3.439591	2.150110
32	H	5.944852	6.225338	5.022708	3.142533	2.138733
33	H	4.740964	4.930241	3.777323	2.737018	2.157169

		26	27	28	29	30
26	O	0.000000				
27	H	2.137583	0.000000			
28	H	2.140358	1.846339	0.000000		
29	H	2.123785	3.111219	2.467728	0.000000	
30	C	2.511879	2.823375	3.532265	2.221132	0.000000
31	H	2.930338	3.777064	4.335702	2.580925	1.093977
32	H	3.417815	3.302430	3.930940	2.569017	1.094234
33	H	2.698622	2.553899	3.793724	3.113391	1.093013

		31	32	33
31	H	0.000000		
32	H	1.766021	0.000000	
33	H	1.775956	1.776574	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.321874	2.490988	-0.250683
2	6	0	-3.319294	1.617115	0.038385
3	7	0	-2.747679	0.351686	0.075589
4	6	0	-1.432056	0.464790	-0.186327
5	7	0	-1.155228	1.753656	-0.390728
6	6	0	0.188358	2.292324	-0.667626
7	6	0	0.821585	2.937503	0.570435
8	1	0	-2.341731	3.559758	-0.376296
9	1	0	-4.366517	1.787301	0.209141
10	1	0	0.810032	1.459923	-0.998092
11	1	0	0.106631	3.018424	-1.477605
12	1	0	0.217231	3.792068	0.892596
13	1	0	0.813158	2.200756	1.387928
14	35	0	-0.096518	-2.561476	-0.153812
15	1	0	-0.748881	-0.405984	-0.221971
16	6	0	-3.368526	-0.909231	0.330056
17	6	0	-4.658860	-1.055269	0.600185
18	1	0	-2.650584	-1.725884	0.273920
19	1	0	-5.044368	-2.049494	0.779966
20	1	0	-5.363825	-0.234447	0.653906
21	7	0	2.147800	3.413691	0.197149
22	1	0	2.538255	4.011683	0.915664
23	1	0	2.774072	2.622622	0.063644
24	6	0	3.482876	-0.556276	-1.154653
25	6	0	3.256396	-0.803606	0.271049
26	8	0	2.894066	0.472356	-0.327909
27	1	0	4.486019	-0.329309	-1.507858
28	1	0	2.806243	-0.999710	-1.879181
29	1	0	2.385511	-1.408205	0.517859
30	6	0	4.372319	-0.770002	1.278593
31	1	0	4.015224	-0.387490	2.239298
32	1	0	4.751696	-1.782679	1.445644
33	1	0	5.197645	-0.139756	0.937558

```
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.4188780           0.2910954           0.1817645
 Standard basis: 6-311++G(d,p) (5D, 7F)
 There are     499 symmetry adapted cartesian basis functions of A      symmetry.
 There are     482 symmetry adapted basis functions of A      symmetry.
    482 basis functions,      760 primitive gaussians,      499 cartesian basis functions
     71 alpha electrons             71 beta electrons
          nuclear repulsion energy           1310.0092143609 Hartrees.
 NAtoms=       33 NActive=       33 NUniq=       33 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      482 RedAO= T EigKep=    3.59D-06    NBF=      482
 NBsUse=      482 1.00D-06 EigRej= -1.00D+00 NBFU=      482
 Initial                guess                from                the                checkpoint                file:
"/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"
 B after Tr=          0.000000        0.000000        0.000000
             Rot=        0.999999        0.000901      -0.000457        0.000465 Ang=      0.13 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn=                5 AccDes=
0.00D+00
 Harris functional with IExCor=    402 and IRadAn=             5 diagonalized for initial guess.
 HarFok:    IExCor=    402 AccDes= 0.00D+00 IRadAn=                5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=    3500011 ScaDFX=    1.000000    1.000000    1.000000    1.000000
 FoFCou: FMM=F IPFlag=                  0 FMFlag=           100000 FMFlg1=                  0
             NFxFlg=                  0 DoJE=T BraDBF=F KetDBF=T FulRan=T
             wScrn=      0.000000  ICntrl=             500  IOpCl=      0  I1Cent=        200000004  NGrid=
0
             NMat0=         1 NMatS0=            1 NMatT0=         0 NMatD0=         1 NMtDS0=         0
NMtDT0=         0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                       energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3205.64834267          A.U. after      10 cycles
                  NFock= 10    Conv=0.88D-08         -V/T= 2.0018
 Calling FoFJK, ICntrl=             2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 ---------------------------------------------------------------------
 Center          Atomic                             Forces (Hartrees/Bohr)
 Number          Number                       X                      Y                      Z
```

1	6	0.000014211	-0.000013986	-0.000079823
2	6	-0.000079356	0.000009492	-0.000030526
3	7	0.000098379	0.000076199	0.000033614
4	6	-0.000173202	-0.000127048	0.000064425
5	7	-0.000001070	-0.000067881	0.000080478
6	6	0.000086883	0.000070662	-0.000013893
7	6	-0.000232826	-0.000104593	0.000060843
8	1	0.000003735	-0.000002332	0.000001475
9	1	0.000002396	-0.000005680	-0.000012351
10	1	0.000017603	0.000000938	0.000036116
11	1	-0.000022241	0.000018522	0.000024826
12	1	-0.000016635	-0.000006170	0.000012655
13	1	0.000058349	0.000052587	-0.000031713
14	35	0.000086492	0.000080276	-0.000018391
15	1	0.000097748	0.000031203	-0.000073292
16	6	0.000027158	0.000057742	0.000039238
17	6	-0.000005334	-0.000041589	0.000020917
18	1	-0.000057910	0.000019129	-0.000035795
19	1	-0.000012634	0.000003126	-0.000012334
20	1	0.000009716	0.000002018	-0.000002859
21	7	0.000112161	0.000042024	-0.000120196
22	1	-0.000009980	0.000008358	0.000059237
23	1	0.000067592	-0.000150863	0.000037272
24	6	-0.000070403	-0.000143110	-0.000104181
25	6	0.000165163	-0.000019677	0.000245317
26	8	-0.000035333	0.000228110	-0.000123887
27	1	0.000002931	0.000035204	-0.000023849
28	1	-0.000009995	-0.000027463	0.000015855
29	1	-0.000077071	0.000034677	-0.000069869
30	6	-0.000055930	-0.000066268	0.000049917
31	1	0.000002535	0.000003271	-0.000009113
32	1	0.000022459	0.000004041	-0.000007539
33	1	-0.000015593	-0.000000919	-0.000012576

Cartesian Forces: Max 0.000245317 RMS 0.000071632

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000501123 RMS 0.000108980
Search for a local minimum.

Step number 34 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 30 31 32 33 34
DE= -4.29D-06 DEPred=-3.97D-06 R= 1.08D+00
TightC=F SS= 1.41D+00 RLast= 4.25D-02 DXNew= 1.7446D+00 1.2749D-01
Trust test= 1.08D+00 RLast= 4.25D-02 DXMaxT set to 1.04D+00
ITU= 1 1 1 1 1 1 1 1 0 0 -1 1 -1 1 1 1 1 1 1 1
ITU= 1 1 0 -1 -1 1 1 1 -1 1 0 0 -1 0
Eigenvalues --- 0.00052 0.00116 0.00221 0.00450 0.00605
Eigenvalues --- 0.00693 0.00729 0.01186 0.01522 0.01888
Eigenvalues --- 0.02004 0.02175 0.02352 0.02375 0.02478
Eigenvalues --- 0.02674 0.02859 0.02869 0.03086 0.03123
Eigenvalues --- 0.03464 0.03526 0.03715 0.03900 0.04060
Eigenvalues --- 0.04408 0.04425 0.05187 0.05329 0.05460
Eigenvalues --- 0.05736 0.05762 0.05938 0.07639 0.08668
Eigenvalues --- 0.08902 0.09562 0.10308 0.11827 0.12286
Eigenvalues --- 0.12762 0.13230 0.14732 0.15886 0.15986
Eigenvalues --- 0.16001 0.16005 0.16019 0.16035 0.16106
Eigenvalues --- 0.16148 0.20193 0.21797 0.22056 0.22497
Eigenvalues --- 0.22987 0.23428 0.24258 0.26034 0.27722
Eigenvalues --- 0.28274 0.29306 0.30353 0.31809 0.32353
Eigenvalues --- 0.33721 0.34278 0.34345 0.34357 0.34546
Eigenvalues --- 0.34661 0.34731 0.35055 0.35096 0.35313
Eigenvalues --- 0.35590 0.35664 0.35843 0.35899 0.36419
Eigenvalues --- 0.36631 0.39429 0.41445 0.41882 0.42630
Eigenvalues --- 0.44809 0.45508 0.46388 0.49486 0.54742
Eigenvalues --- 0.58350 0.60618 1.37231
En-DIIS/RFO-DIIS IScMMF= 0 using points: 34 33 32 31 30
RFO step: Lambda=-2.27693625D-06.
DidBck=F Rises=F RFO-DIIS coefs: 1.33369 -0.19436 -0.13079 -0.06294 0.05440
Iteration 1 RMS(Cart)= 0.01569011 RMS(Int)= 0.00010077
Iteration 2 RMS(Cart)= 0.00014070 RMS(Int)= 0.00005570
Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00005570

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56478	0.00004	0.00000	0.00004	0.00004	2.56482
R2	2.62144	-0.00004	0.00006	0.00001	0.00007	2.62151
R3	2.03393	0.00000	-0.00001	0.00000	-0.00001	2.03392
R4	2.62491	0.00007	-0.00010	0.00003	-0.00007	2.62484
R5	2.03073	0.00000	0.00003	-0.00001	0.00002	2.03075
R6	2.54395	-0.00003	0.00025	-0.00003	0.00022	2.54417

R7	2.69915	-0.00002	0.00007	-0.00005	0.00002	2.69916
R8	2.52092	-0.00014	-0.00015	-0.00010	-0.00025	2.52067
R9	2.09261	0.00006	0.00023	0.00012	0.00035	2.09296
R10	2.78506	-0.00002	-0.00017	0.00010	-0.00007	2.78499
R11	2.89691	-0.00011	0.00006	-0.00011	-0.00005	2.89687
R12	2.06022	0.00000	-0.00006	-0.00005	-0.00010	2.06011
R13	2.06142	0.00000	0.00005	-0.00001	0.00005	2.06147
R14	2.06950	0.00001	0.00008	0.00004	0.00012	2.06961
R15	2.07970	-0.00006	0.00017	-0.00010	0.00007	2.07977
R16	2.75469	0.00009	-0.00055	0.00015	-0.00040	2.75429
R17	4.25771	-0.00004	-0.00170	-0.00286	-0.00456	4.25315
R18	2.50648	0.00002	0.00001	0.00000	0.00002	2.50649
R19	2.05756	-0.00005	0.00005	-0.00015	-0.00010	2.05746
R20	2.04355	0.00000	0.00001	-0.00001	0.00000	2.04354
R21	2.04720	-0.00001	-0.00001	-0.00002	-0.00003	2.04717
R22	1.91443	0.00004	0.00003	0.00011	0.00014	1.91457
R23	1.92328	0.00003	-0.00006	0.00017	0.00009	1.92337
R24	4.13645	-0.00004	-0.00162	-0.00061	-0.00222	4.13424
R25	2.76772	0.00009	-0.00038	-0.00066	-0.00087	2.76685
R26	2.73082	0.00006	-0.00034	0.00042	0.00001	2.73084
R27	2.05500	0.00002	0.00011	0.00013	0.00025	2.05525
R28	2.05225	0.00001	0.00006	-0.00002	0.00005	2.05230
R29	2.75026	0.00009	-0.00056	0.00012	-0.00054	2.74972
R30	2.05702	0.00002	-0.00018	-0.00014	-0.00032	2.05670
R31	2.84186	-0.00003	0.00021	0.00011	0.00033	2.84219
R32	2.06732	-0.00001	-0.00004	0.00003	-0.00001	2.06730
R33	2.06780	0.00000	0.00001	0.00001	0.00003	2.06783
R34	2.06550	-0.00001	-0.00002	-0.00003	-0.00006	2.06544
A1	1.87268	-0.00006	-0.00007	-0.00005	-0.00012	1.87256
A2	2.27925	0.00003	0.00013	0.00008	0.00021	2.27946
A3	2.13121	0.00003	-0.00005	-0.00003	-0.00009	2.13112
A4	1.86487	-0.00002	0.00009	-0.00005	0.00004	1.86490
A5	2.27580	0.00001	-0.00014	-0.00002	-0.00016	2.27564
A6	2.14248	0.00000	0.00005	0.00006	0.00011	2.14259
A7	1.89697	-0.00002	-0.00006	0.00007	0.00001	1.89698
A8	2.25252	-0.00004	-0.00014	-0.00002	-0.00016	2.25236
A9	2.13368	0.00006	0.00019	-0.00005	0.00014	2.13382
A10	1.88997	0.00000	-0.00004	-0.00006	-0.00010	1.88987
A11	2.14495	0.00047	-0.00059	0.00060	0.00002	2.14497
A12	2.24821	-0.00047	0.00062	-0.00057	0.00005	2.24827
A13	1.90027	0.00009	0.00009	0.00009	0.00018	1.90045
A14	2.20359	0.00029	0.00029	0.00020	0.00050	2.20409
A15	2.17864	-0.00038	-0.00042	-0.00030	-0.00072	2.17792
A16	1.95915	0.00013	0.00022	0.00061	0.00082	1.95997

A17	1.87312	-0.00010	-0.00068	-0.00044	-0.00112	1.87200
A18	1.89071	0.00003	0.00027	-0.00005	0.00022	1.89094
A19	1.90773	-0.00009	0.00049	-0.00029	0.00020	1.90794
A20	1.92888	-0.00001	-0.00021	-0.00012	-0.00033	1.92855
A21	1.90272	0.00004	-0.00012	0.00029	0.00017	1.90289
A22	1.91563	0.00010	-0.00063	0.00018	-0.00045	1.91518
A23	1.89126	0.00009	-0.00012	0.00024	0.00012	1.89138
A24	1.88229	-0.00028	0.00000	-0.00072	-0.00071	1.88157
A25	1.87512	-0.00004	0.00005	0.00022	0.00027	1.87539
A26	1.89916	0.00019	-0.00002	0.00029	0.00026	1.89942
A27	1.99970	-0.00006	0.00065	-0.00018	0.00047	2.00016
A28	2.16077	0.00003	-0.00021	0.00015	-0.00006	2.16071
A29	1.94586	0.00000	0.00004	-0.00002	0.00002	1.94588
A30	2.17655	-0.00003	0.00016	-0.00013	0.00004	2.17659
A31	2.07361	0.00002	0.00002	0.00012	0.00013	2.07374
A32	2.16486	-0.00002	-0.00005	-0.00013	-0.00017	2.16469
A33	2.04472	0.00000	0.00003	0.00001	0.00004	2.04476
A34	1.94105	0.00021	-0.00016	-0.00009	-0.00029	1.94076
A35	1.91720	-0.00050	-0.00022	-0.00040	-0.00064	1.91656
A36	1.89091	0.00015	-0.00020	-0.00026	-0.00044	1.89047
A37	2.08755	-0.00005	-0.00093	-0.00003	-0.00111	2.08645
A38	2.07616	0.00005	0.00109	-0.00034	0.00090	2.07706
A39	1.99667	0.00001	0.00034	-0.00031	0.00010	1.99677
A40	2.00255	-0.00002	0.00024	0.00030	0.00051	2.00306
A41	2.03004	0.00001	-0.00036	0.00024	-0.00012	2.02992
A42	2.02442	-0.00010	0.00107	-0.00106	0.00012	2.02454
A43	2.13372	0.00008	-0.00007	0.00048	0.00031	2.13402
A44	1.96177	-0.00009	0.00014	-0.00028	-0.00019	1.96158
A45	2.02737	0.00006	0.00053	0.00022	0.00082	2.02819
A46	2.04225	0.00003	-0.00105	0.00035	-0.00071	2.04154
A47	2.53909	0.00009	0.00044	0.00023	0.00103	2.54012
A48	2.50022	-0.00013	-0.00135	-0.00314	-0.00407	2.49614
A49	1.93259	0.00000	-0.00030	0.00019	-0.00011	1.93248
A50	1.91652	0.00003	-0.00004	0.00007	0.00003	1.91655
A51	1.94352	-0.00004	0.00009	-0.00025	-0.00017	1.94336
A52	1.87832	0.00000	-0.00002	0.00019	0.00018	1.87849
A53	1.89533	0.00001	0.00018	-0.00006	0.00012	1.89545
A54	1.89597	0.00000	0.00009	-0.00013	-0.00004	1.89593
A55	3.48280	-0.00043	0.00077	0.00117	0.00194	3.48474
A56	2.53588	-0.00033	-0.00001	-0.00222	-0.00217	2.53371
A57	2.94143	0.00015	0.00439	0.00886	0.01325	2.95468
A58	3.08701	0.00003	0.00162	0.00411	0.00576	3.09276
D1	0.00296	0.00000	0.00024	-0.00010	0.00014	0.00310
D2	-3.12930	0.00000	0.00066	0.00094	0.00160	-3.12771

D3	3.13369	0.00001	0.00052	-0.00018	0.00034	3.13403
D4	0.00143	0.00001	0.00094	0.00086	0.00180	0.00323
D5	-0.00494	0.00002	-0.00022	0.00000	-0.00022	-0.00516
D6	-3.10822	0.00001	0.00107	-0.00001	0.00106	-3.10716
D7	-3.13679	0.00001	-0.00047	0.00006	-0.00040	-3.13719
D8	0.04311	0.00001	0.00082	0.00006	0.00088	0.04399
D9	-0.00002	-0.00002	-0.00018	0.00017	-0.00001	-0.00003
D10	-3.13471	0.00000	0.00040	0.00093	0.00133	-3.13338
D11	3.13313	-0.00002	-0.00057	-0.00077	-0.00134	3.13179
D12	-0.00156	0.00000	0.00002	-0.00001	0.00001	-0.00155
D13	-0.00306	0.00003	0.00005	-0.00018	-0.00013	-0.00319
D14	-3.13486	0.00002	0.00067	0.00229	0.00296	-3.13191
D15	3.13219	0.00002	-0.00049	-0.00087	-0.00136	3.13083
D16	0.00039	0.00001	0.00013	0.00159	0.00172	0.00211
D17	-0.01610	-0.00002	-0.00485	-0.00658	-0.01143	-0.02753
D18	3.12576	-0.00004	-0.00430	-0.00664	-0.01094	3.11482
D19	3.13322	0.00000	-0.00419	-0.00573	-0.00992	3.12330
D20	-0.00810	-0.00002	-0.00364	-0.00579	-0.00944	-0.01754
D21	0.00493	-0.00003	0.00010	0.00011	0.00021	0.00515
D22	3.10889	-0.00001	-0.00115	0.00013	-0.00101	3.10788
D23	3.13598	-0.00001	-0.00058	-0.00253	-0.00311	3.13287
D24	-0.04325	0.00001	-0.00183	-0.00251	-0.00433	-0.04758
D25	1.32475	0.00010	-0.00139	0.00082	-0.00057	1.32418
D26	-2.86200	0.00000	-0.00110	0.00054	-0.00056	-2.86256
D27	-0.80992	0.00001	-0.00145	0.00061	-0.00084	-0.81076
D28	-1.77268	0.00009	0.00008	0.00080	0.00088	-1.77179
D29	0.32376	-0.00002	0.00037	0.00052	0.00089	0.32465
D30	2.37584	-0.00001	0.00002	0.00059	0.00061	2.37645
D31	-1.09218	-0.00012	-0.00139	-0.00180	-0.00319	-1.09537
D32	0.95064	-0.00006	-0.00175	-0.00130	-0.00305	0.94759
D33	3.12452	-0.00025	-0.00102	-0.00183	-0.00284	3.12168
D34	3.11479	-0.00001	-0.00100	-0.00144	-0.00244	3.11235
D35	-1.12558	0.00005	-0.00136	-0.00094	-0.00230	-1.12788
D36	1.04831	-0.00014	-0.00063	-0.00146	-0.00209	1.04621
D37	1.02069	0.00000	-0.00104	-0.00154	-0.00258	1.01811
D38	3.06350	0.00006	-0.00140	-0.00103	-0.00243	3.06107
D39	-1.04580	-0.00012	-0.00067	-0.00156	-0.00223	-1.04803
D40	2.94071	0.00010	0.00162	0.00012	0.00175	2.94245
D41	-1.24927	0.00009	0.00113	-0.00052	0.00060	-1.24867
D42	0.86370	0.00003	0.00237	0.00016	0.00254	0.86624
D43	2.95690	0.00002	0.00188	-0.00048	0.00139	2.95830
D44	-1.23519	-0.00003	0.00189	-0.00021	0.00169	-1.23351
D45	0.85801	-0.00003	0.00140	-0.00085	0.00054	0.85856
D46	3.14127	-0.00002	-0.00006	-0.00061	-0.00067	3.14059

D47	-0.00033	-0.00001	-0.00031	-0.00073	-0.00104	-0.00137
D48	-0.00063	0.00000	-0.00068	-0.00054	-0.00122	-0.00186
D49	3.14096	0.00001	-0.00093	-0.00066	-0.00159	3.13937
D50	2.31624	0.00001	-0.00659	-0.00684	-0.01348	2.30275
D51	-1.34479	0.00021	-0.00633	-0.01508	-0.02138	-1.36617
D52	-1.96923	-0.00019	-0.00765	-0.00929	-0.01696	-1.98619
D53	0.65292	0.00002	-0.00739	-0.01753	-0.02485	0.62807
D54	-2.71384	-0.00002	0.00047	-0.00002	0.00044	-2.71340
D55	-0.01139	0.00000	0.00009	-0.00052	-0.00044	-0.01182
D56	-0.02989	-0.00001	-0.00011	-0.00028	-0.00038	-0.03027
D57	2.67256	0.00001	-0.00049	-0.00078	-0.00126	2.67130
D58	0.56191	-0.00010	0.00076	-0.00697	-0.00632	0.55560
D59	-1.84933	-0.00010	0.00065	-0.00736	-0.00685	-1.85618
D60	1.85641	0.00002	-0.00237	0.00426	0.00201	1.85841
D61	-0.56212	0.00000	-0.00146	0.00378	0.00240	-0.55971
D62	2.55194	0.00001	0.00120	0.00125	0.00242	2.55436
D63	-1.65944	0.00003	0.00097	0.00165	0.00259	-1.65685
D64	0.44124	0.00002	0.00111	0.00137	0.00246	0.44370
D65	1.35170	-0.00003	0.00090	0.00066	0.00158	1.35328
D66	-2.85967	-0.00001	0.00067	0.00105	0.00175	-2.85792
D67	-0.75899	-0.00002	0.00082	0.00077	0.00161	-0.75738
D68	-1.03300	0.00000	0.00132	0.00041	0.00174	-1.03126
D69	1.03881	0.00002	0.00109	0.00081	0.00191	1.04072
D70	3.13949	0.00001	0.00123	0.00053	0.00177	3.14126

Item	Value	Threshold	Converged?
Maximum Force	0.000501	0.000450	NO
RMS Force	0.000109	0.000300	YES
Maximum Displacement	0.078081	0.001800	NO
RMS Displacement	0.015667	0.001200	NO

Predicted change in Energy=-3.813876D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.639879	2.092411	-0.194000
2	6	0	-3.532581	1.115719	0.108110
3	7	0	-2.827091	-0.080494	0.134458
4	6	0	-1.535330	0.174228	-0.146686
5	7	0	-1.402650	1.485386	-0.352824
6	6	0	-0.128830	2.165536	-0.647328
7	6	0	0.449885	2.874490	0.582480

8	1	0	-2.776753	3.152863	-0.317037
9	1	0	-4.589626	1.171635	0.293459
10	1	0	0.573043	1.404210	-0.988233
11	1	0	-0.299313	2.879131	-1.454631
12	1	0	-0.236606	3.661265	0.912872
13	1	0	0.529809	2.141619	1.399647
14	35	0	0.119778	-2.688166	-0.168606
15	1	0	-0.763044	-0.618060	-0.196766
16	6	0	-3.304664	-1.401317	0.394256
17	6	0	-4.565382	-1.684487	0.693729
18	1	0	-2.505864	-2.136939	0.315651
19	1	0	-4.839364	-2.714832	0.874674
20	1	0	-5.351367	-0.942978	0.770981
21	7	0	1.713282	3.486579	0.190677
22	1	0	2.049661	4.121697	0.904776
23	1	0	2.416507	2.764838	0.047534
24	6	0	3.422478	-0.332542	-1.169882
25	6	0	3.265726	-0.585013	0.263797
26	8	0	2.750330	0.636846	-0.335133
27	1	0	4.385240	-0.003797	-1.554415
28	1	0	2.777446	-0.854951	-1.870225
29	1	0	2.472862	-1.276531	0.542539
30	6	0	4.400563	-0.420272	1.236979
31	1	0	4.032240	-0.068680	2.205220
32	1	0	4.892469	-1.384092	1.399646
33	1	0	5.142137	0.292065	0.866496

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357244	0.000000			
3	N	2.205549	1.389005	0.000000		
4	C	2.213976	2.222687	1.346318	0.000000	
5	N	1.387242	2.210367	2.172201	1.333879	0.000000
6	C	2.552689	3.641198	3.596728	2.488813	1.473754
7	C	3.280429	4.379308	4.435226	3.429894	2.497256
8	H	1.076305	2.214042	3.265115	3.231473	2.161000
9	H	2.210645	1.074628	2.167864	3.243034	3.266946
10	H	3.380428	4.259265	3.876298	2.581916	2.076943
11	H	2.772431	4.000725	4.204075	3.248840	2.091377
12	H	3.076068	4.241568	4.617067	3.868950	2.774184
13	H	3.548106	4.384467	4.219866	3.244468	2.690017
14	Br	5.519988	5.280705	3.946624	3.306534	4.446376
15	H	3.296842	3.281658	2.158467	1.107544	2.204073

16	C	3.604735	2.543481	1.428337	2.430125	3.536784
17	C	4.331348	3.041510	2.430480	3.652716	4.598505
18	H	4.262053	3.417163	2.089254	2.548958	3.845150
19	H	5.393457	4.119275	3.396601	4.506272	5.564134
20	H	4.182933	2.825883	2.742445	4.080735	4.769932
21	N	4.587122	5.757331	5.774266	4.651769	3.742885
22	H	5.226576	6.389992	6.483403	5.435093	4.522183
23	H	5.106617	6.173727	5.966472	4.729270	4.047621
24	C	6.601888	7.218280	6.389206	5.087593	5.220566
25	C	6.500334	7.009544	6.115038	4.878020	5.143977
26	O	5.585064	6.316704	5.642935	4.314673	4.238817
27	H	7.456348	8.167569	7.407827	6.088230	6.095995
28	H	6.390938	6.900275	6.002448	4.757082	5.025225
29	H	6.167039	6.478960	5.448535	4.318024	4.842463
30	C	7.611117	8.158945	7.319152	6.123951	6.311599
31	H	7.412405	7.938966	7.165097	6.048826	6.204574
32	H	8.447606	8.882487	7.930427	6.792356	7.136776
33	H	8.057647	8.746673	8.011447	6.754923	6.763504

		6	7	8	9	10
6	C	0.000000				
7	C	1.532956	0.000000			
8	H	2.845242	3.361223	0.000000		
9	H	4.666006	5.327281	2.753993	0.000000	
10	H	1.090165	2.155002	3.837893	5.324469	0.000000
11	H	1.090881	2.170517	2.739846	4.937423	1.775929
12	H	2.164035	1.095192	2.867664	5.052793	3.060071
13	H	2.150461	1.100568	3.860437	5.326644	2.499522
14	Br	4.883585	5.622832	6.521468	6.106558	4.198187
15	H	2.890266	3.778402	4.276605	4.252771	2.549729
16	C	4.888073	5.693382	4.639524	2.877737	4.981854
17	C	6.025289	6.778610	5.255549	2.884135	6.226753
18	H	5.008883	5.824265	5.334386	3.910143	4.870268
19	H	6.951519	7.700783	6.332803	3.937614	7.052026
20	H	6.240941	6.947166	4.958662	2.297796	6.610805
21	N	2.416771	1.457509	4.530955	6.715368	2.650704
22	H	3.313822	2.053943	5.072054	7.290864	3.626103
23	H	2.705686	2.041027	5.220481	7.189205	2.514455
24	C	4.373242	4.710853	7.162811	8.282374	3.341944
25	C	4.463035	4.471988	7.128859	8.049425	3.574231
26	O	3.274740	3.337830	6.072834	7.386208	2.399159
27	H	5.089759	5.323333	7.923998	9.238208	4.103157
28	H	4.366379	5.034087	7.023111	7.941179	3.277364
29	H	4.475758	4.617900	6.922200	7.478923	3.624768
30	C	5.545486	5.185719	8.166770	9.178665	4.788550

31	H	5.517540	4.912107	7.943708	8.917947	4.932909
32	H	6.481003	6.208045	9.074575	9.882586	5.668689
33	H	5.795226	5.363470	8.502572	9.788218	5.055048

		11	12	13	14	15
11	H	0.000000				
12	H	2.494141	0.000000			
13	H	3.062397	1.770217	0.000000		
14	Br	5.729249	6.450727	5.094543	0.000000	
15	H	3.745346	4.452085	3.440324	2.250668	0.000000
16	C	5.547320	5.942364	5.316615	3.701297	2.724451
17	C	6.606164	6.882107	6.410802	4.868441	4.048213
18	H	5.758795	6.255028	5.356903	2.726235	2.367908
19	H	7.571668	7.863934	7.258700	5.067764	4.707528
20	H	6.714545	6.883311	6.670696	5.819101	4.700512
21	N	2.669563	2.086659	2.161281	6.387160	4.809403
22	H	3.553653	2.332183	2.544712	7.158969	5.620498
23	H	3.105678	2.931109	2.403381	5.920889	4.649002
24	C	4.924191	5.803211	4.592547	4.178438	4.306631
25	C	5.259543	5.542428	4.026154	3.808833	4.055144
26	O	3.947333	4.430171	3.194450	4.243022	3.733326
27	H	5.501479	6.393876	5.309768	5.226898	5.359604
28	H	4.856185	6.101341	4.972260	3.649573	3.923219
29	H	5.379885	5.644483	4.024156	2.834685	3.383968
30	C	6.341897	6.186060	4.644619	5.044217	5.362609
31	H	6.391123	5.814267	4.219169	5.272961	5.391298
32	H	7.299080	7.211102	5.609228	5.190240	5.926226
33	H	6.456773	6.347010	4.997866	5.931045	6.068773

		16	17	18	19	20
16	C	0.000000				
17	C	1.326378	0.000000			
18	H	1.088761	2.142258	0.000000		
19	H	2.076397	1.081396	2.468135	0.000000	
20	H	2.130959	1.083317	3.119255	1.847259	0.000000
21	N	7.008049	8.149515	7.031412	9.047790	8.358647
22	H	7.709287	8.804266	7.763401	9.705550	8.969060
23	H	7.085821	8.304266	6.951909	9.130093	8.637774
24	C	6.988795	8.313045	6.372433	8.838187	9.006660
25	C	6.622190	7.919592	5.976823	8.402486	8.639424
26	O	6.430324	7.743822	5.978710	8.384559	8.328074
27	H	8.055123	9.380432	7.452165	9.916829	10.054404
28	H	6.512945	7.821708	5.859600	8.307191	8.547591
29	H	5.780775	7.051678	5.057617	7.459736	7.834666
30	C	7.813012	9.070917	7.175968	9.527461	9.777040
31	H	7.673700	8.877756	7.113014	9.352958	9.532760

32	H	8.258577	9.488914	7.515128	9.836413	10.272583
33	H	8.627804	9.908205	8.043345	10.424579	10.566365

		21	22	23	24	25
21	N	0.000000				
22	H	1.013146	0.000000			
23	H	1.017804	1.646362	0.000000		
24	C	4.399791	5.101870	3.476758	0.000000	
25	C	4.358129	4.903344	3.462578	1.464155	0.000000
26	O	3.077811	3.764638	2.187744	1.445096	1.455091
27	H	4.729422	5.340623	3.755994	1.087589	2.212921
28	H	4.922260	5.744331	4.112293	1.086029	2.205751
29	H	4.836112	5.426894	4.071961	2.173769	1.088360
30	C	4.855895	5.125094	3.936520	2.599485	1.504020
31	H	4.698491	4.814669	3.910886	3.439876	2.150178
32	H	5.940730	6.216122	5.017192	3.141512	2.138918
33	H	4.734839	4.922495	3.770195	2.737553	2.157181

		26	27	28	29	30
26	O	0.000000				
27	H	2.137757	0.000000			
28	H	2.140725	1.846402	0.000000		
29	H	2.123277	3.110347	2.468184	0.000000	
30	C	2.512430	2.822334	3.532446	2.220689	0.000000
31	H	2.931629	3.776728	4.336126	2.579743	1.093970
32	H	3.417953	3.299844	3.930059	2.569183	1.094249
33	H	2.698801	2.553672	3.794345	3.112952	1.092984

		31	32	33
31	H	0.000000		
32	H	1.766141	0.000000	
33	H	1.776003	1.776537	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.327521	2.485615	-0.255213
2	6	0	-3.322044	1.610664	0.040583
3	7	0	-2.747161	0.346919	0.082906
4	6	0	-1.432316	0.461997	-0.182636

5	7	0	-1.159398	1.750379	-0.394344
6	6	0	0.182684	2.290301	-0.675861
7	6	0	0.817595	2.942787	0.557469
8	1	0	-2.350134	3.553709	-0.385973
9	1	0	-4.369513	1.779058	0.211691
10	1	0	0.804469	1.456833	-1.003236
11	1	0	0.098586	3.012268	-1.489319
12	1	0	0.213922	3.799866	0.874391
13	1	0	0.809490	2.211274	1.379705
14	35	0	-0.088483	-2.559100	-0.166758
15	1	0	-0.747418	-0.407665	-0.218115
16	6	0	-3.364708	-0.914320	0.343784
17	6	0	-4.651917	-1.060834	0.628221
18	1	0	-2.647108	-1.730628	0.279815
19	1	0	-5.035377	-2.055247	0.811308
20	1	0	-5.356135	-0.240033	0.690973
21	7	0	2.143344	3.415452	0.178905
22	1	0	2.535942	4.016494	0.893804
23	1	0	2.768182	2.622581	0.049069
24	6	0	3.456687	-0.572023	-1.137653
25	6	0	3.256257	-0.796576	0.295230
26	8	0	2.880251	0.468639	-0.317258
27	1	0	4.453503	-0.349351	-1.511317
28	1	0	2.768912	-1.028333	-1.843489
29	1	0	2.391402	-1.398645	0.567379
30	6	0	4.389895	-0.745700	1.282323
31	1	0	4.048677	-0.350493	2.243651
32	1	0	4.775235	-1.754877	1.456840
33	1	0	5.207095	-0.118156	0.917651

Rotational constants (GHZ): 0.4192423 0.2914536 0.1820355

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1310.6758441008 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 3.60D-06 NBF= 482

NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999999 0.000920 -0.000638 -0.000930 Ang= 0.17 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3205.64834599 A.U. after 10 cycles
NFock= 10 Conv=0.97D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000055110	-0.000043016	-0.000053346
2	6	-0.000104242	0.000067679	-0.000046619
3	7	0.000131999	0.000051278	-0.000019014
4	6	-0.000312083	-0.000248264	0.000074301
5	7	0.000027023	0.000072517	0.000202020
6	6	0.000056037	0.000044485	-0.000137453
7	6	-0.000462067	-0.000180294	0.000017037
8	1	-0.000015480	-0.000005725	-0.000017828
9	1	0.000009539	-0.000013443	0.000000134
10	1	0.000072277	0.000035918	0.000048462
11	1	-0.000041111	-0.000012688	0.000019385
12	1	0.000028655	-0.000017787	0.000054058
13	1	0.000088242	0.000074804	-0.000049142
14	35	0.000083454	0.000046927	-0.000003752

15	1	0.000101816	0.000064966	-0.000071407
16	6	0.000059947	0.000093637	0.000048157
17	6	0.000012381	-0.000057719	0.000011786
18	1	-0.000050034	0.000018684	-0.000028420
19	1	-0.000008389	0.000004567	-0.000010543
20	1	0.000000397	0.000001905	-0.000004992
21	7	0.000260961	0.000093970	-0.000018962
22	1	-0.000019075	0.000013680	0.000007521
23	1	0.000065365	-0.000127294	0.000041146
24	6	0.000121801	-0.000230332	-0.000495916
25	6	0.000114432	-0.000117633	0.000520398
26	8	0.000069144	0.000343640	-0.000032839
27	1	-0.000052476	0.000089095	0.000006093
28	1	-0.000088067	-0.000067375	0.000177572
29	1	-0.000122478	-0.000030111	-0.000222398
30	6	-0.000130869	-0.000004253	-0.000007226
31	1	0.000036823	0.000030855	0.000013223
32	1	0.000016063	0.000006232	-0.000014285
33	1	-0.000005095	0.000001097	-0.000007150

Cartesian Forces: Max 0.000520398 RMS 0.000126574

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000447039 RMS 0.000108356
Search for a local minimum.
Step number 35 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 30 31 32 33 34
35
DE= -3.32D-06 DEPred=-3.81D-06 R= 8.71D-01
TightC=F SS= 1.41D+00 RLast= 5.03D-02 DXNew= 1.7446D+00 1.5083D-01
Trust test= 8.71D-01 RLast= 5.03D-02 DXMaxT set to 1.04D+00
ITU= 1 1 1 1 1 1 1 1 1 0 0 -1 1 -1 1 1 1 1 1 1
ITU= 1 1 1 0 -1 -1 1 1 1 -1 1 0 0 -1 0
Eigenvalues --- 0.00056 0.00085 0.00220 0.00450 0.00606
Eigenvalues --- 0.00692 0.00729 0.01196 0.01537 0.01888
Eigenvalues --- 0.02020 0.02175 0.02335 0.02377 0.02438
Eigenvalues --- 0.02621 0.02783 0.02862 0.03073 0.03101
Eigenvalues --- 0.03491 0.03511 0.03727 0.03926 0.04061

Eigenvalues --- 0.04406 0.04424 0.05110 0.05320 0.05463
Eigenvalues --- 0.05702 0.05754 0.05933 0.07682 0.08675
Eigenvalues --- 0.08935 0.09573 0.10672 0.12148 0.12308
Eigenvalues --- 0.12675 0.13267 0.15347 0.15818 0.15992
Eigenvalues --- 0.16001 0.16006 0.16015 0.16030 0.16150
Eigenvalues --- 0.16447 0.18973 0.21840 0.22052 0.22260
Eigenvalues --- 0.22987 0.23446 0.24999 0.26747 0.27600
Eigenvalues --- 0.28097 0.29333 0.31125 0.31806 0.32315
Eigenvalues --- 0.33757 0.34287 0.34340 0.34379 0.34547
Eigenvalues --- 0.34672 0.34738 0.35081 0.35116 0.35333
Eigenvalues --- 0.35595 0.35731 0.35856 0.35927 0.36421
Eigenvalues --- 0.36634 0.39436 0.41823 0.42333 0.44202
Eigenvalues --- 0.44961 0.45486 0.46653 0.49544 0.55183
Eigenvalues --- 0.58957 0.60670 1.25408

En-DIIS/RFO-DIIS IScMMF= 0 using points: 35 34 33 32 31

RFO step: Lambda=-2.42264282D-06.

DidBck=F Rises=F RFO-DIIS coefs: 2.39427 -1.92218 0.23292 0.31339 -0.01839

Iteration 1 RMS(Cart)= 0.02368568 RMS(Int)= 0.00022460

Iteration 2 RMS(Cart)= 0.00035223 RMS(Int)= 0.00001232

Iteration 3 RMS(Cart)= 0.00000007 RMS(Int)= 0.00001232

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56482	0.00005	0.00005	0.00002	0.00007	2.56489
R2	2.62151	-0.00005	0.00000	0.00000	0.00000	2.62151
R3	2.03392	0.00000	0.00000	0.00001	0.00000	2.03392
R4	2.62484	0.00010	0.00008	-0.00002	0.00006	2.62490
R5	2.03075	-0.00001	-0.00002	0.00002	0.00000	2.03076
R6	2.54417	-0.00013	-0.00015	0.00004	-0.00012	2.54406
R7	2.69916	-0.00005	-0.00009	0.00000	-0.00009	2.69907
R8	2.52067	-0.00005	-0.00013	0.00007	-0.00006	2.52061
R9	2.09296	0.00006	0.00013	0.00030	0.00043	2.09339
R10	2.78499	0.00000	0.00021	-0.00012	0.00009	2.78508
R11	2.89687	-0.00010	-0.00025	0.00007	-0.00018	2.89669
R12	2.06011	0.00001	-0.00003	-0.00004	-0.00007	2.06004
R13	2.06147	-0.00002	-0.00002	-0.00001	-0.00003	2.06143
R14	2.06961	-0.00001	0.00005	-0.00005	-0.00001	2.06961
R15	2.07977	-0.00008	-0.00021	0.00002	-0.00019	2.07958
R16	2.75429	0.00025	0.00038	0.00010	0.00048	2.75477
R17	4.25315	-0.00001	-0.00428	-0.00124	-0.00552	4.24763
R18	2.50649	0.00001	0.00001	-0.00002	-0.00001	2.50649
R19	2.05746	-0.00005	-0.00026	0.00005	-0.00021	2.05725
R20	2.04354	0.00000	-0.00002	0.00000	-0.00001	2.04353
R21	2.04717	0.00000	-0.00004	0.00002	-0.00002	2.04715

R22	1.91457	0.00001	0.00017	-0.00003	0.00013	1.91470
R23	1.92337	0.00003	0.00028	-0.00006	0.00021	1.92358
R24	4.13424	0.00000	-0.00365	-0.00358	-0.00722	4.12702
R25	2.76685	0.00022	-0.00044	0.00035	-0.00007	2.76678
R26	2.73084	0.00018	0.00048	0.00027	0.00075	2.73158
R27	2.05525	-0.00002	0.00018	-0.00001	0.00017	2.05542
R28	2.05230	-0.00003	-0.00002	-0.00002	-0.00004	2.05226
R29	2.74972	0.00008	0.00025	-0.00070	-0.00047	2.74925
R30	2.05670	0.00005	-0.00013	-0.00018	-0.00031	2.05639
R31	2.84219	-0.00007	0.00005	-0.00011	-0.00006	2.84213
R32	2.06730	0.00001	0.00002	-0.00001	0.00001	2.06731
R33	2.06783	0.00000	0.00002	0.00002	0.00003	2.06786
R34	2.06544	0.00000	-0.00003	-0.00002	-0.00005	2.06539
A1	1.87256	-0.00004	-0.00004	-0.00003	-0.00007	1.87249
A2	2.27946	0.00001	0.00009	0.00003	0.00012	2.27958
A3	2.13112	0.00003	-0.00005	0.00000	-0.00005	2.13107
A4	1.86490	-0.00003	-0.00014	0.00006	-0.00008	1.86483
A5	2.27564	0.00003	0.00003	-0.00002	0.00001	2.27566
A6	2.14259	0.00000	0.00010	-0.00005	0.00005	2.14264
A7	1.89698	0.00000	0.00017	-0.00005	0.00012	1.89710
A8	2.25236	0.00004	-0.00003	0.00010	0.00007	2.25243
A9	2.13382	-0.00004	-0.00014	-0.00006	-0.00021	2.13361
A10	1.88987	0.00002	-0.00011	0.00002	-0.00010	1.88977
A11	2.14497	0.00042	0.00124	-0.00050	0.00074	2.14570
A12	2.24827	-0.00044	-0.00116	0.00047	-0.00069	2.24757
A13	1.90045	0.00005	0.00013	0.00000	0.00013	1.90058
A14	2.20409	0.00029	0.00012	0.00028	0.00040	2.20449
A15	2.17792	-0.00034	-0.00025	-0.00027	-0.00052	2.17740
A16	1.95997	0.00004	0.00091	0.00022	0.00113	1.96110
A17	1.87200	-0.00001	-0.00044	-0.00034	-0.00078	1.87122
A18	1.89094	0.00002	-0.00015	-0.00006	-0.00021	1.89073
A19	1.90794	-0.00014	-0.00048	0.00009	-0.00040	1.90754
A20	1.92855	0.00007	-0.00017	0.00013	-0.00004	1.92851
A21	1.90289	0.00003	0.00032	-0.00005	0.00027	1.90317
A22	1.91518	0.00013	0.00041	-0.00008	0.00032	1.91551
A23	1.89138	0.00007	0.00048	0.00004	0.00052	1.89190
A24	1.88157	-0.00018	-0.00129	0.00011	-0.00117	1.88040
A25	1.87539	-0.00003	0.00037	0.00006	0.00043	1.87582
A26	1.89942	0.00014	0.00059	-0.00027	0.00032	1.89974
A27	2.00016	-0.00011	-0.00052	0.00013	-0.00039	1.99978
A28	2.16071	0.00007	0.00028	-0.00012	0.00016	2.16087
A29	1.94588	-0.00002	-0.00004	-0.00001	-0.00005	1.94583
A30	2.17659	-0.00005	-0.00024	0.00013	-0.00011	2.17648
A31	2.07374	0.00001	0.00021	0.00001	0.00022	2.07397

A32	2.16469	-0.00001	-0.00021	-0.00006	-0.00027	2.16441
A33	2.04476	0.00000	0.00000	0.00004	0.00005	2.04481
A34	1.94076	0.00019	-0.00030	-0.00015	-0.00047	1.94030
A35	1.91656	-0.00045	-0.00067	-0.00035	-0.00102	1.91554
A36	1.89047	0.00015	-0.00030	-0.00003	-0.00032	1.89015
A37	2.08645	0.00004	-0.00038	-0.00016	-0.00055	2.08590
A38	2.07706	-0.00013	0.00012	-0.00092	-0.00080	2.07626
A39	1.99677	-0.00006	-0.00035	0.00016	-0.00017	1.99660
A40	2.00306	0.00001	0.00032	0.00009	0.00038	2.00344
A41	2.02992	0.00010	0.00017	0.00082	0.00099	2.03091
A42	2.02454	-0.00024	-0.00111	-0.00060	-0.00166	2.02288
A43	2.13402	0.00011	0.00024	0.00036	0.00054	2.13457
A44	1.96158	-0.00006	-0.00070	-0.00005	-0.00075	1.96083
A45	2.02819	-0.00006	0.00051	0.00010	0.00062	2.02882
A46	2.04154	0.00014	0.00063	0.00009	0.00072	2.04227
A47	2.54012	0.00010	0.00346	0.00408	0.00764	2.54776
A48	2.49614	-0.00010	-0.00122	0.00024	-0.00100	2.49515
A49	1.93248	0.00006	0.00023	0.00015	0.00038	1.93286
A50	1.91655	0.00001	0.00014	0.00002	0.00016	1.91671
A51	1.94336	-0.00003	-0.00039	-0.00016	-0.00055	1.94280
A52	1.87849	-0.00001	0.00030	0.00011	0.00041	1.87890
A53	1.89545	-0.00002	-0.00011	-0.00009	-0.00019	1.89526
A54	1.89593	0.00000	-0.00015	-0.00002	-0.00017	1.89576
A55	3.48474	-0.00038	0.00074	0.00119	0.00193	3.48667
A56	2.53371	-0.00021	0.00032	-0.00080	-0.00046	2.53325
A57	2.95468	0.00010	0.00945	0.00578	0.01522	2.96990
A58	3.09276	0.00001	0.00517	0.00532	0.01050	3.10327
D1	0.00310	0.00001	-0.00021	0.00047	0.00026	0.00336
D2	-3.12771	0.00000	0.00099	0.00054	0.00153	-3.12617
D3	3.13403	0.00000	-0.00035	0.00025	-0.00010	3.13393
D4	0.00323	-0.00001	0.00084	0.00033	0.00117	0.00440
D5	-0.00516	0.00001	-0.00002	0.00004	0.00003	-0.00513
D6	-3.10716	-0.00001	-0.00012	-0.00021	-0.00033	-3.10749
D7	-3.13719	0.00002	0.00011	0.00024	0.00035	-3.13684
D8	0.04399	0.00000	0.00001	-0.00002	-0.00001	0.04398
D9	-0.00003	-0.00002	0.00036	-0.00082	-0.00046	-0.00049
D10	-3.13338	-0.00001	0.00113	0.00035	0.00148	-3.13190
D11	3.13179	-0.00001	-0.00073	-0.00089	-0.00161	3.13018
D12	-0.00155	0.00000	0.00004	0.00028	0.00032	-0.00123
D13	-0.00319	0.00003	-0.00037	0.00085	0.00048	-0.00271
D14	-3.13191	0.00001	0.00234	0.00162	0.00397	-3.12794
D15	3.13083	0.00002	-0.00108	-0.00022	-0.00130	3.12953
D16	0.00211	0.00000	0.00163	0.00055	0.00219	0.00430
D17	-0.02753	-0.00001	-0.00533	-0.00473	-0.01006	-0.03759

D18	3.11482	-0.00003	-0.00575	-0.00463	-0.01039	3.10443
D19	3.12330	0.00000	-0.00447	-0.00342	-0.00789	3.11541
D20	-0.01754	-0.00002	-0.00489	-0.00332	-0.00822	-0.02576
D21	0.00515	-0.00002	0.00024	-0.00056	-0.00032	0.00483
D22	3.10788	0.00001	0.00036	-0.00029	0.00006	3.10795
D23	3.13287	0.00000	-0.00266	-0.00140	-0.00405	3.12881
D24	-0.04758	0.00004	-0.00255	-0.00113	-0.00367	-0.05126
D25	1.32418	0.00015	0.00258	0.00342	0.00600	1.33019
D26	-2.86256	-0.00001	0.00224	0.00344	0.00568	-2.85688
D27	-0.81076	0.00003	0.00231	0.00316	0.00547	-0.80529
D28	-1.77179	0.00011	0.00245	0.00312	0.00557	-1.76623
D29	0.32465	-0.00004	0.00211	0.00313	0.00524	0.32989
D30	2.37645	-0.00001	0.00218	0.00286	0.00504	2.38148
D31	-1.09537	-0.00010	-0.00196	-0.00118	-0.00314	-1.09850
D32	0.94759	-0.00003	-0.00101	-0.00113	-0.00214	0.94545
D33	3.12168	-0.00024	-0.00215	-0.00087	-0.00302	3.11866
D34	3.11235	-0.00001	-0.00167	-0.00094	-0.00261	3.10974
D35	-1.12788	0.00005	-0.00071	-0.00090	-0.00161	-1.12949
D36	1.04621	-0.00015	-0.00186	-0.00064	-0.00249	1.04372
D37	1.01811	0.00000	-0.00165	-0.00102	-0.00267	1.01544
D38	3.06107	0.00007	-0.00070	-0.00097	-0.00167	3.05940
D39	-1.04803	-0.00014	-0.00184	-0.00071	-0.00255	-1.05058
D40	2.94245	0.00010	0.00038	-0.00089	-0.00051	2.94195
D41	-1.24867	0.00012	-0.00063	-0.00125	-0.00188	-1.25054
D42	0.86624	-0.00003	0.00029	-0.00070	-0.00041	0.86583
D43	2.95830	-0.00001	-0.00071	-0.00106	-0.00178	2.95652
D44	-1.23351	-0.00002	-0.00027	-0.00066	-0.00094	-1.23444
D45	0.85856	0.00000	-0.00128	-0.00102	-0.00230	0.85625
D46	3.14059	-0.00002	-0.00079	-0.00021	-0.00101	3.13959
D47	-0.00137	-0.00001	-0.00075	-0.00042	-0.00117	-0.00254
D48	-0.00186	0.00000	-0.00031	-0.00032	-0.00063	-0.00249
D49	3.13937	0.00002	-0.00027	-0.00053	-0.00080	3.13857
D50	2.30275	-0.00007	-0.01748	-0.02362	-0.04112	2.26163
D51	-1.36617	0.00024	-0.01068	-0.00794	-0.01861	-1.38478
D52	-1.98619	-0.00022	-0.01954	-0.02587	-0.04541	-2.03161
D53	0.62807	0.00010	-0.01274	-0.01019	-0.02290	0.60517
D54	-2.71340	-0.00006	-0.00041	0.00039	-0.00003	-2.71343
D55	-0.01182	0.00000	-0.00087	0.00002	-0.00086	-0.01269
D56	-0.03027	0.00001	-0.00058	-0.00003	-0.00062	-0.03089
D57	2.67130	0.00007	-0.00104	-0.00041	-0.00145	2.66985
D58	0.55560	-0.00010	0.00095	0.00538	0.00633	0.56193
D59	-1.85618	-0.00021	0.00071	0.00375	0.00446	-1.85172
D60	1.85841	0.00010	-0.00437	-0.00777	-0.01208	1.84634
D61	-0.55971	0.00000	-0.00515	-0.00798	-0.01308	-0.57279

D62	2.55436	0.00000	0.00138	0.00076	0.00213	2.55649
D63	-1.65685	0.00003	0.00197	0.00100	0.00296	-1.65389
D64	0.44370	0.00001	0.00162	0.00088	0.00249	0.44619
D65	1.35328	-0.00002	0.00077	0.00039	0.00116	1.35444
D66	-2.85792	0.00001	0.00136	0.00062	0.00199	-2.85593
D67	-0.75738	-0.00001	0.00101	0.00050	0.00152	-0.75586
D68	-1.03126	-0.00003	0.00050	0.00022	0.00073	-1.03054
D69	1.04072	0.00000	0.00110	0.00046	0.00156	1.04228
D70	3.14126	-0.00002	0.00075	0.00034	0.00109	-3.14083

Item	Value	Threshold	Converged?
Maximum Force	0.000447	0.000450	YES
RMS Force	0.000108	0.000300	YES
Maximum Displacement	0.104283	0.001800	NO
RMS Displacement	0.023776	0.001200	NO

Predicted change in Energy=-2.021874D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.643222	2.094488	-0.197813
2	6	0	-3.534811	1.115687	0.100912
3	7	0	-2.827024	-0.079205	0.127292
4	6	0	-1.535245	0.178180	-0.151040
5	7	0	-1.404589	1.489871	-0.354865
6	6	0	-0.131081	2.172156	-0.645993
7	6	0	0.449687	2.873949	0.586833
8	1	0	-2.781691	3.154849	-0.319863
9	1	0	-4.592575	1.169210	0.282846
10	1	0	0.570178	1.412522	-0.991780
11	1	0	-0.302390	2.890336	-1.449019
12	1	0	-0.234474	3.661058	0.921227
13	1	0	0.529058	2.137380	1.400589
14	35	0	0.126922	-2.677449	-0.207385
15	1	0	-0.761373	-0.612674	-0.204263
16	6	0	-3.302786	-1.401511	0.382571
17	6	0	-4.561655	-1.686848	0.687697
18	1	0	-2.504396	-2.136404	0.295052
19	1	0	-4.834626	-2.718318	0.863647
20	1	0	-5.347046	-0.945782	0.774490
21	7	0	1.714519	3.484203	0.195853
22	1	0	2.052965	4.115796	0.912200

23	1	0	2.415399	2.760399	0.050869
24	6	0	3.387930	-0.353862	-1.152177
25	6	0	3.267120	-0.582712	0.288888
26	8	0	2.742701	0.632412	-0.315287
27	1	0	4.342397	-0.036609	-1.566168
28	1	0	2.722262	-0.884486	-1.826522
29	1	0	2.477819	-1.265404	0.597273
30	6	0	4.427426	-0.410182	1.230114
31	1	0	4.086261	-0.043189	2.202586
32	1	0	4.919412	-1.373924	1.393115
33	1	0	5.162043	0.293430	0.830338

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357283	0.000000			
3	N	2.205543	1.389038	0.000000		
4	C	2.214055	2.222760	1.346257	0.000000	
5	N	1.387242	2.210338	2.172050	1.333848	0.000000
6	C	2.552989	3.641342	3.596485	2.488493	1.473801
7	C	3.284709	4.382217	4.434990	3.428058	2.498160
8	H	1.076306	2.214141	3.265135	3.231515	2.160969
9	H	2.210690	1.074630	2.167927	3.243095	3.266919
10	H	3.379556	4.258288	3.875378	2.581327	2.076378
11	H	2.770991	4.000027	4.204369	3.249689	2.091248
12	H	3.083579	4.247829	4.619656	3.869393	2.776982
13	H	3.552476	4.387260	4.218747	3.241506	2.690701
14	Br	5.517714	5.281213	3.948250	3.304631	4.442278
15	H	3.296987	3.282121	2.159035	1.107773	2.203884
16	C	3.604702	2.543512	1.428289	2.429890	3.536532
17	C	4.331630	3.041863	2.430538	3.652529	4.598429
18	H	4.261764	3.416949	2.089090	2.548637	3.844716
19	H	5.393704	4.119573	3.396704	4.506129	5.564062
20	H	4.183213	2.826227	2.742322	4.080407	4.769782
21	N	4.590881	5.759717	5.773058	4.648773	3.742924
22	H	5.231825	6.393910	6.482933	5.432362	4.522788
23	H	5.108320	6.173539	5.962566	4.724004	4.046130
24	C	6.578756	7.187082	6.351231	5.052029	5.196470
25	C	6.506644	7.013284	6.117044	4.882131	5.151202
26	O	5.582081	6.309828	5.632416	4.305128	4.235187
27	H	7.430535	8.133717	7.366833	6.049413	6.068381
28	H	6.349441	6.845922	5.938050	4.697112	4.983397
29	H	6.176253	6.485961	5.456126	4.329964	4.855018
30	C	7.635864	8.185389	7.345258	6.148757	6.335200

31	H	7.457715	7.990042	7.218148	6.098351	6.248220
32	H	8.470795	8.907404	7.955242	6.815867	7.158893
33	H	8.076080	8.766038	8.028594	6.769789	6.779146

		6	7	8	9	10
6	C	0.000000				
7	C	1.532862	0.000000			
8	H	2.845660	3.367909	0.000000		
9	H	4.666216	5.331318	2.754146	0.000000	
10	H	1.090126	2.154601	3.836952	5.323334	0.000000
11	H	1.090863	2.170388	2.737133	4.936327	1.776056
12	H	2.164186	1.095188	2.878345	5.060621	3.059897
13	H	2.150695	1.100469	3.867332	5.330838	2.500107
14	Br	4.876229	5.617203	6.518311	6.108254	4.188032
15	H	2.889234	3.774790	4.276596	4.253292	2.548457
16	C	4.887612	5.692304	4.639544	2.877865	4.980710
17	C	6.025000	6.776769	5.255994	2.884775	6.225950
18	H	5.008181	5.823691	5.334076	3.909952	4.868656
19	H	6.951193	7.698963	6.333192	3.938120	7.051124
20	H	6.240641	6.944614	4.959216	2.298724	6.610207
21	N	2.415867	1.457764	4.537659	6.719092	2.647989
22	H	3.312969	2.053911	5.080876	7.296688	3.623739
23	H	2.704849	2.040632	5.225207	7.190091	2.511719
24	C	4.361242	4.698531	7.146190	8.250303	3.329500
25	C	4.473373	4.469362	7.136389	8.052582	3.590900
26	O	3.277011	3.331099	6.073023	7.379173	2.405425
27	H	5.073201	5.316009	7.905145	9.203618	4.081610
28	H	4.344914	5.011458	6.991405	7.885046	3.256456
29	H	4.490978	4.609519	6.931250	7.484430	3.651777
30	C	5.564911	5.198244	8.190437	9.206097	4.810139
31	H	5.550507	4.934067	7.984921	8.970926	4.968492
32	H	6.499240	6.218758	9.096762	9.908488	5.689275
33	H	5.807437	5.378166	8.521361	9.809144	5.065343

		11	12	13	14	15
11	H	0.000000				
12	H	2.493329	0.000000			
13	H	3.062436	1.770414	0.000000		
14	Br	5.720681	6.448337	5.092138	0.000000	
15	H	3.745820	4.450746	3.435630	2.247749	0.000000
16	C	5.547707	5.944266	5.314427	3.706611	2.724962
17	C	6.607384	6.883251	6.406894	4.874958	4.048652
18	H	5.758362	6.257412	5.356237	2.732948	2.368374
19	H	7.572753	7.865186	7.255013	5.075996	4.708031
20	H	6.716275	6.883524	6.665319	5.824695	4.700778
21	N	2.669495	2.087108	2.161166	6.375658	4.803596

22	H	3.553140	2.332219	2.544592	7.149216	5.614750
23	H	3.106916	2.930962	2.401704	5.905422	4.640538
24	C	4.922540	5.791408	4.571220	4.114105	4.264064
25	C	5.274825	5.538104	4.016436	3.807237	4.058676
26	O	3.956785	4.423261	3.179523	4.220085	3.720363
27	H	5.491337	6.388085	5.298059	5.156604	5.313672
28	H	4.851836	6.079012	4.935186	3.545717	3.852443
29	H	5.402504	5.633073	4.002739	2.857983	3.400130
30	C	6.359429	6.197074	4.660087	5.069639	5.387215
31	H	6.418726	5.833702	4.248738	5.331384	5.442131
32	H	7.316342	7.220545	5.621790	5.218117	5.949995
33	H	6.465246	6.361727	5.018952	5.937629	6.080977

		16	17	18	19	20
16	C	0.000000				
17	C	1.326375	0.000000			
18	H	1.088648	2.142099	0.000000		
19	H	2.076523	1.081389	2.468177	0.000000	
20	H	2.130795	1.083306	3.118991	1.847270	0.000000
21	N	7.005598	8.146904	7.028535	9.044806	8.356152
22	H	7.707480	8.801948	7.761470	9.702906	8.966532
23	H	7.080195	8.298364	6.945695	9.123585	8.632205
24	C	6.943969	8.267883	6.323878	8.790030	8.964498
25	C	6.621395	7.916305	5.976988	8.398181	8.635478
26	O	6.416522	7.729072	5.964132	8.368581	8.313983
27	H	8.006833	9.331953	7.399450	9.864751	10.009525
28	H	6.438059	7.747292	5.778090	8.228396	8.478369
29	H	5.786192	7.052659	5.066798	7.460146	7.833395
30	C	7.839467	9.095476	7.204467	9.552351	9.799733
31	H	7.730169	8.932131	7.173353	9.409107	9.583393
32	H	8.284111	9.512422	7.543211	9.860476	10.293987
33	H	8.644457	9.924321	8.060081	10.440552	10.582047

		21	22	23	24	25
21	N	0.000000				
22	H	1.013217	0.000000			
23	H	1.017912	1.646315	0.000000		
24	C	4.398662	5.101140	3.477320	0.000000	
25	C	4.354195	4.892716	3.458101	1.464116	0.000000
26	O	3.074269	3.757183	2.183924	1.445491	1.454843
27	H	4.733558	5.350353	3.761832	1.087679	2.212619
28	H	4.918434	5.740329	4.111441	1.086010	2.205198
29	H	4.827269	5.407124	4.063193	2.172506	1.088193
30	C	4.857550	5.120900	3.935918	2.599815	1.503990
31	H	4.700492	4.805887	3.909190	3.440730	2.150423
32	H	5.941899	6.211669	5.016406	3.140777	2.139020

33	H	4.740149	4.927834	3.773268	2.738034	2.156740
		26	27	28	29	30
26	O	0.000000				
27	H	2.138065	0.000000			
28	H	2.141315	1.847030	0.000000		
29	H	2.122412	3.109190	2.465691	0.000000	
30	C	2.512681	2.822407	3.532079	2.221004	0.000000
31	H	2.932793	3.777454	4.336126	2.580296	1.093974
32	H	3.417908	3.298290	3.928497	2.570315	1.094266
33	H	2.698255	2.554210	3.794592	3.112770	1.092956
		31	32	33		
31	H	0.000000				
32	H	1.766420	0.000000			
33	H	1.775861	1.776417	0.000000		

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.342031	2.475218	-0.260131
2	6	0	-3.331318	1.596469	0.042074
3	7	0	-2.749182	0.336263	0.091319
4	6	0	-1.435464	0.456987	-0.176969
5	7	0	-1.170065	1.745601	-0.396487
6	6	0	0.168870	2.290657	-0.683290
7	6	0	0.807029	2.946922	0.546237
8	1	0	-2.370679	3.542351	-0.397396
9	1	0	-4.379717	1.759855	0.212351
10	1	0	0.792180	1.458863	-1.011892
11	1	0	0.078804	3.011225	-1.497323
12	1	0	0.203629	3.804148	0.863267
13	1	0	0.803671	2.217565	1.370287
14	35	0	-0.072361	-2.553418	-0.178957
15	1	0	-0.745723	-0.409153	-0.211891
16	6	0	-3.359420	-0.927083	0.358855
17	6	0	-4.643488	-1.078584	0.654638
18	1	0	-2.639282	-1.740532	0.289167
19	1	0	-5.021664	-2.074371	0.841166

20	1	0	-5.350060	-0.260327	0.723654
21	7	0	2.130893	3.419813	0.160444
22	1	0	2.525477	4.023669	0.871971
23	1	0	2.755676	2.626509	0.032146
24	6	0	3.416688	-0.587062	-1.120148
25	6	0	3.260290	-0.782237	0.322448
26	8	0	2.867798	0.471351	-0.302879
27	1	0	4.402175	-0.374373	-1.528343
28	1	0	2.706504	-1.056607	-1.794375
29	1	0	2.402829	-1.376713	0.631515
30	6	0	4.423656	-0.715473	1.273294
31	1	0	4.112945	-0.302101	2.237329
32	1	0	4.813441	-1.721886	1.453902
33	1	0	5.229669	-0.095905	0.872010

Rotational constants (GHZ): 0.4202721 0.2915859 0.1822805

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1311.4676974975 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 3.61D-06 NBF= 482

NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999997 0.000847 -0.001053 -0.002055 Ang= 0.28 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0

NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3205.64835349 A.U. after 11 cycles

NFock= 11 Conv=0.58D-08 -V/T= 2.0018

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000066458	-0.000070291	-0.000029723
2	6	-0.000081777	0.000097407	-0.000023928
3	7	0.000069430	-0.000009921	-0.000085002
4	6	-0.000237056	-0.000177532	0.000080566
5	7	0.000042919	0.000137902	0.000233666
6	6	0.000013419	-0.000023820	-0.000178149
7	6	-0.000377200	-0.000114838	-0.000054162
8	1	-0.000026588	-0.000004572	-0.000019776
9	1	0.000011200	-0.000013751	0.000019625
10	1	0.000075694	0.000061439	0.000043395
11	1	-0.000025483	-0.000030755	0.000006141
12	1	0.000025493	-0.000021345	0.000047702
13	1	0.000063707	0.000043064	-0.000049160
14	35	0.000061704	0.000003769	0.000009098
15	1	0.000046176	0.000067956	-0.000041158
16	6	0.000057778	0.000096037	0.000025902
17	6	0.000011608	-0.000041279	0.000009076
18	1	-0.000017947	-0.000002617	-0.000017904
19	1	0.000000597	0.000003507	-0.000003436
20	1	-0.000007973	0.000000743	-0.000003035
21	7	0.000217426	0.000061484	0.000101240
22	1	-0.000015967	0.000005259	-0.000040464
23	1	0.000044252	-0.000054726	0.000070784
24	6	0.000221821	-0.000307414	-0.000544989
25	6	0.000003355	-0.000043924	0.000374759
26	8	0.000144995	0.000334312	-0.000043129
27	1	-0.000087846	0.000119927	0.000062375
28	1	-0.000148374	-0.000081239	0.000283733
29	1	-0.000067265	-0.000113733	-0.000245706

30	6	-0.000145180	0.000033212	-0.000019165
31	1	0.000047826	0.000038439	0.000027178
32	1	0.000004064	0.000005994	-0.000003171
33	1	0.000008735	0.000001306	0.000006817

Cartesian Forces: Max 0.000544989 RMS 0.000122499

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000286273 RMS 0.000087720
Search for a local minimum.
Step number 36 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 30 31 32 33 34
35 36
DE= -7.49D-06 DEPred=-2.02D-06 R= 3.71D+00
TightC=F SS= 1.41D+00 RLast= 7.87D-02 DXNew= 1.7446D+00 2.3612D-01
Trust test= 3.71D+00 RLast= 7.87D-02 DXMaxT set to 1.04D+00
ITU= 1 1 1 1 1 1 1 1 1 1 0 0 -1 1 -1 1 1 1 1 1
ITU= 1 1 1 1 0 -1 -1 1 1 1 -1 1 0 0 -1 0
Eigenvalues --- 0.00055 0.00056 0.00218 0.00455 0.00617
Eigenvalues --- 0.00697 0.00729 0.01214 0.01472 0.01894
Eigenvalues --- 0.02026 0.02159 0.02258 0.02379 0.02393
Eigenvalues --- 0.02574 0.02742 0.02886 0.03061 0.03102
Eigenvalues --- 0.03493 0.03534 0.03801 0.03953 0.04084
Eigenvalues --- 0.04408 0.04425 0.05027 0.05332 0.05465
Eigenvalues --- 0.05692 0.05757 0.05921 0.07742 0.08644
Eigenvalues --- 0.08886 0.09569 0.10878 0.11887 0.12385
Eigenvalues --- 0.12708 0.13220 0.15287 0.15717 0.15963
Eigenvalues --- 0.16001 0.16002 0.16008 0.16030 0.16150
Eigenvalues --- 0.16462 0.18250 0.21517 0.21913 0.22161
Eigenvalues --- 0.22988 0.23484 0.25734 0.27028 0.28006
Eigenvalues --- 0.29151 0.29575 0.31792 0.32328 0.33174
Eigenvalues --- 0.33793 0.34290 0.34339 0.34470 0.34552
Eigenvalues --- 0.34669 0.34755 0.35097 0.35251 0.35489
Eigenvalues --- 0.35579 0.35715 0.35889 0.36412 0.36603
Eigenvalues --- 0.37085 0.39452 0.41590 0.42458 0.42634
Eigenvalues --- 0.44766 0.45761 0.46839 0.49598 0.55273
Eigenvalues --- 0.58668 0.60672 1.09396
En-DIIS/RFO-DIIS IScMMF= 0 using points: 36 35 34 33 32

RFO step: Lambda=-2.41459807D-06.

DidBck=F Rises=F RFO-DIIS coefs: 1.81197 -0.16558 -1.23681 0.42678 0.16364

Iteration 1 RMS(Cart)= 0.03319820 RMS(Int)= 0.00041965

Iteration 2 RMS(Cart)= 0.00065640 RMS(Int)= 0.00001701

Iteration 3 RMS(Cart)= 0.00000009 RMS(Int)= 0.00001701

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56489	0.00003	0.00008	0.00001	0.00009	2.56498
R2	2.62151	-0.00004	-0.00004	-0.00001	-0.00005	2.62146
R3	2.03392	0.00000	0.00000	0.00001	0.00001	2.03394
R4	2.62490	0.00009	0.00014	0.00004	0.00018	2.62508
R5	2.03076	-0.00001	-0.00002	0.00002	0.00000	2.03076
R6	2.54406	-0.00013	-0.00029	0.00003	-0.00026	2.54380
R7	2.69907	-0.00006	-0.00016	-0.00008	-0.00024	2.69884
R8	2.52061	-0.00002	-0.00001	-0.00008	-0.00008	2.52052
R9	2.09339	0.00003	0.00029	0.00028	0.00057	2.09395
R10	2.78508	0.00000	0.00026	-0.00017	0.00009	2.78517
R11	2.89669	-0.00008	-0.00032	-0.00016	-0.00048	2.89621
R12	2.06004	-0.00001	-0.00004	-0.00014	-0.00018	2.05986
R13	2.06143	-0.00002	-0.00006	-0.00002	-0.00008	2.06135
R14	2.06961	-0.00002	-0.00003	-0.00001	-0.00004	2.06957
R15	2.07958	-0.00006	-0.00033	0.00001	-0.00032	2.07927
R16	2.75477	0.00019	0.00092	-0.00012	0.00081	2.75558
R17	4.24763	0.00002	-0.00560	-0.00090	-0.00650	4.24113
R18	2.50649	0.00000	0.00000	0.00001	0.00001	2.50649
R19	2.05725	-0.00001	-0.00032	0.00008	-0.00024	2.05700
R20	2.04353	0.00000	-0.00002	0.00000	-0.00002	2.04351
R21	2.04715	0.00000	-0.00003	0.00002	-0.00002	2.04713
R22	1.91470	-0.00003	0.00017	-0.00007	0.00010	1.91480
R23	1.92358	0.00000	0.00031	0.00006	0.00035	1.92393
R24	4.12702	0.00005	-0.00795	0.00118	-0.00676	4.12025
R25	2.76678	0.00013	0.00001	-0.00089	-0.00087	2.76590
R26	2.73158	0.00019	0.00093	0.00099	0.00192	2.73350
R27	2.05542	-0.00007	0.00014	-0.00011	0.00002	2.05544
R28	2.05226	-0.00005	-0.00005	-0.00005	-0.00011	2.05215
R29	2.74925	0.00004	0.00012	-0.00040	-0.00029	2.74897
R30	2.05639	0.00005	-0.00020	-0.00019	-0.00039	2.05600
R31	2.84213	-0.00005	-0.00016	-0.00002	-0.00018	2.84195
R32	2.06731	0.00002	0.00003	0.00002	0.00005	2.06736
R33	2.06786	0.00000	0.00002	0.00004	0.00006	2.06793
R34	2.06539	0.00001	-0.00004	-0.00001	-0.00005	2.06533
A1	1.87249	-0.00001	-0.00002	0.00002	0.00001	1.87249
A2	2.27958	-0.00002	0.00006	-0.00008	-0.00002	2.27956

A3	2.13107	0.00003	-0.00005	0.00006	0.00001	2.13108
A4	1.86483	-0.00003	-0.00018	-0.00004	-0.00022	1.86461
A5	2.27566	0.00003	0.00011	0.00004	0.00016	2.27581
A6	2.14264	0.00000	0.00005	-0.00001	0.00004	2.14268
A7	1.89710	0.00000	0.00019	0.00000	0.00019	1.89729
A8	2.25243	0.00008	0.00012	0.00018	0.00030	2.25273
A9	2.13361	-0.00008	-0.00032	-0.00019	-0.00051	2.13310
A10	1.88977	0.00004	-0.00009	0.00001	-0.00008	1.88969
A11	2.14570	0.00024	0.00149	-0.00029	0.00120	2.14690
A12	2.24757	-0.00027	-0.00146	0.00024	-0.00123	2.24635
A13	1.90058	0.00001	0.00009	0.00001	0.00010	1.90069
A14	2.20449	0.00022	0.00017	0.00050	0.00068	2.20517
A15	2.17740	-0.00022	-0.00023	-0.00048	-0.00071	2.17669
A16	1.96110	-0.00010	0.00123	-0.00032	0.00091	1.96200
A17	1.87122	0.00007	-0.00042	-0.00043	-0.00085	1.87037
A18	1.89073	0.00004	-0.00038	0.00029	-0.00009	1.89064
A19	1.90754	-0.00010	-0.00080	-0.00018	-0.00098	1.90656
A20	1.92851	0.00011	-0.00003	0.00036	0.00034	1.92884
A21	1.90317	-0.00001	0.00038	0.00027	0.00065	1.90382
A22	1.91551	0.00008	0.00073	0.00000	0.00073	1.91624
A23	1.89190	-0.00001	0.00070	-0.00034	0.00035	1.89225
A24	1.88040	-0.00002	-0.00154	0.00030	-0.00123	1.87917
A25	1.87582	-0.00001	0.00049	0.00015	0.00064	1.87646
A26	1.89974	0.00007	0.00054	-0.00002	0.00052	1.90026
A27	1.99978	-0.00010	-0.00085	-0.00009	-0.00094	1.99884
A28	2.16087	0.00007	0.00037	0.00001	0.00038	2.16125
A29	1.94583	-0.00003	-0.00007	0.00001	-0.00005	1.94578
A30	2.17648	-0.00005	-0.00030	-0.00002	-0.00033	2.17616
A31	2.07397	-0.00001	0.00027	-0.00003	0.00024	2.07421
A32	2.16441	0.00001	-0.00030	-0.00001	-0.00031	2.16411
A33	2.04481	0.00000	0.00003	0.00004	0.00007	2.04487
A34	1.94030	0.00012	-0.00037	-0.00013	-0.00054	1.93976
A35	1.91554	-0.00027	-0.00093	-0.00021	-0.00116	1.91437
A36	1.89015	0.00011	-0.00030	0.00005	-0.00023	1.88992
A37	2.08590	0.00007	-0.00030	0.00054	0.00024	2.08614
A38	2.07626	-0.00023	-0.00087	-0.00255	-0.00341	2.07285
A39	1.99660	-0.00014	-0.00044	-0.00059	-0.00100	1.99560
A40	2.00344	0.00004	0.00026	-0.00032	-0.00009	2.00336
A41	2.03091	0.00018	0.00098	0.00195	0.00293	2.03384
A42	2.02288	-0.00029	-0.00227	-0.00226	-0.00446	2.01842
A43	2.13457	0.00016	0.00052	0.00167	0.00211	2.13668
A44	1.96083	0.00002	-0.00094	0.00011	-0.00083	1.96000
A45	2.02882	-0.00015	0.00049	-0.00024	0.00026	2.02908
A46	2.04227	0.00013	0.00136	0.00027	0.00162	2.04389

A47	2.54776	0.00015	0.00853	0.00010	0.00871	2.55647
A48	2.49515	-0.00006	0.00039	-0.00612	-0.00580	2.48934
A49	1.93286	0.00008	0.00052	0.00015	0.00067	1.93353
A50	1.91671	0.00000	0.00021	0.00022	0.00042	1.91713
A51	1.94280	-0.00001	-0.00064	-0.00008	-0.00072	1.94208
A52	1.87890	-0.00002	0.00045	0.00004	0.00049	1.87939
A53	1.89526	-0.00004	-0.00029	-0.00020	-0.00049	1.89477
A54	1.89576	-0.00001	-0.00023	-0.00013	-0.00036	1.89540
A55	3.48667	-0.00025	-0.00010	0.00493	0.00483	3.49150
A56	2.53325	-0.00004	0.00107	-0.00507	-0.00396	2.52929
A57	2.96990	0.00003	0.01269	0.01030	0.02299	2.99290
A58	3.10327	-0.00002	0.00922	0.00289	0.01213	3.11539
D1	0.00336	0.00000	-0.00010	0.00002	-0.00009	0.00328
D2	-3.12617	-0.00001	0.00109	0.00057	0.00167	-3.12451
D3	3.13393	-0.00002	-0.00049	-0.00010	-0.00059	3.13334
D4	0.00440	-0.00002	0.00071	0.00046	0.00117	0.00556
D5	-0.00513	0.00000	0.00021	0.00004	0.00025	-0.00488
D6	-3.10749	-0.00002	-0.00085	-0.00086	-0.00170	-3.10920
D7	-3.13684	0.00001	0.00055	0.00014	0.00070	-3.13614
D8	0.04398	-0.00001	-0.00050	-0.00075	-0.00126	0.04272
D9	-0.00049	0.00000	-0.00004	-0.00007	-0.00011	-0.00060
D10	-3.13190	-0.00001	0.00141	0.00062	0.00203	-3.12987
D11	3.13018	0.00001	-0.00112	-0.00057	-0.00169	3.12849
D12	-0.00123	0.00000	0.00033	0.00012	0.00044	-0.00079
D13	-0.00271	0.00000	0.00017	0.00009	0.00026	-0.00245
D14	-3.12794	-0.00001	0.00338	0.00264	0.00604	-3.12191
D15	3.12953	0.00001	-0.00116	-0.00053	-0.00169	3.12784
D16	0.00430	0.00000	0.00206	0.00201	0.00408	0.00838
D17	-0.03759	0.00000	-0.00640	-0.00909	-0.01549	-0.05308
D18	3.10443	-0.00001	-0.00718	-0.00879	-0.01597	3.08846
D19	3.11541	-0.00001	-0.00478	-0.00832	-0.01310	3.10231
D20	-0.02576	-0.00002	-0.00556	-0.00802	-0.01359	-0.03934
D21	0.00483	0.00000	-0.00023	-0.00008	-0.00032	0.00451
D22	3.10795	0.00003	0.00082	0.00082	0.00164	3.10958
D23	3.12881	0.00001	-0.00368	-0.00283	-0.00649	3.12232
D24	-0.05126	0.00005	-0.00262	-0.00192	-0.00454	-0.05579
D25	1.33019	0.00013	0.00659	0.00084	0.00744	1.33763
D26	-2.85688	-0.00002	0.00606	0.00015	0.00621	-2.85067
D27	-0.80529	0.00003	0.00609	0.00039	0.00648	-0.79881
D28	-1.76623	0.00009	0.00536	-0.00020	0.00516	-1.76106
D29	0.32989	-0.00005	0.00483	-0.00090	0.00394	0.33383
D30	2.38148	0.00000	0.00486	-0.00066	0.00420	2.38569
D31	-1.09850	-0.00004	-0.00201	-0.00359	-0.00560	-1.10410
D32	0.94545	-0.00002	-0.00062	-0.00361	-0.00422	0.94123

D33	3.11866	-0.00016	-0.00218	-0.00373	-0.00591	3.11274
D34	3.10974	0.00000	-0.00173	-0.00272	-0.00446	3.10529
D35	-1.12949	0.00003	-0.00033	-0.00275	-0.00308	-1.13257
D36	1.04372	-0.00011	-0.00190	-0.00287	-0.00477	1.03895
D37	1.01544	0.00001	-0.00168	-0.00317	-0.00485	1.01059
D38	3.05940	0.00004	-0.00028	-0.00319	-0.00347	3.05592
D39	-1.05058	-0.00011	-0.00184	-0.00332	-0.00516	-1.05574
D40	2.94195	0.00008	-0.00047	-0.00002	-0.00048	2.94147
D41	-1.25054	0.00011	-0.00168	-0.00018	-0.00186	-1.25241
D42	0.86583	-0.00004	-0.00077	-0.00018	-0.00094	0.86489
D43	2.95652	-0.00001	-0.00198	-0.00034	-0.00233	2.95419
D44	-1.23444	-0.00001	-0.00124	-0.00029	-0.00152	-1.23596
D45	0.85625	0.00002	-0.00245	-0.00045	-0.00290	0.85335
D46	3.13959	-0.00001	-0.00095	-0.00053	-0.00148	3.13810
D47	-0.00254	0.00000	-0.00097	-0.00074	-0.00171	-0.00426
D48	-0.00249	0.00000	-0.00007	-0.00086	-0.00093	-0.00342
D49	3.13857	0.00001	-0.00008	-0.00108	-0.00116	3.13741
D50	2.26163	-0.00011	-0.04111	-0.00605	-0.04720	2.21444
D51	-1.38478	0.00020	-0.01268	-0.02182	-0.03449	-1.41927
D52	-2.03161	-0.00017	-0.04407	-0.00935	-0.05342	-2.08503
D53	0.60517	0.00014	-0.01564	-0.02512	-0.04072	0.56445
D54	-2.71343	-0.00004	-0.00034	0.00047	0.00012	-2.71331
D55	-0.01269	0.00000	-0.00104	-0.00034	-0.00140	-0.01408
D56	-0.03089	0.00006	-0.00053	0.00083	0.00029	-0.03060
D57	2.66985	0.00010	-0.00123	0.00002	-0.00123	2.66863
D58	0.56193	-0.00010	0.00956	-0.01430	-0.00473	0.55720
D59	-1.85172	-0.00027	0.00818	-0.01639	-0.00820	-1.85992
D60	1.84634	0.00011	-0.01455	0.00915	-0.00533	1.84101
D61	-0.57279	0.00004	-0.01619	0.00886	-0.00726	-0.58005
D62	2.55649	0.00001	0.00168	0.00085	0.00252	2.55900
D63	-1.65389	0.00003	0.00268	0.00113	0.00380	-1.65008
D64	0.44619	0.00002	0.00212	0.00106	0.00317	0.44936
D65	1.35444	-0.00002	0.00085	-0.00034	0.00052	1.35496
D66	-2.85593	0.00000	0.00185	-0.00006	0.00180	-2.85413
D67	-0.75586	-0.00001	0.00129	-0.00013	0.00117	-0.75469
D68	-1.03054	-0.00004	0.00012	-0.00056	-0.00045	-1.03098
D69	1.04228	-0.00002	0.00112	-0.00028	0.00084	1.04312
D70	-3.14083	-0.00003	0.00056	-0.00035	0.00020	-3.14063

Item	Value	Threshold	Converged?
Maximum Force	0.000286	0.000450	YES
RMS Force	0.000088	0.000300	YES
Maximum Displacement	0.147610	0.001800	NO
RMS Displacement	0.033255	0.001200	NO

Predicted change in Energy=-6.479419D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.645383	2.097429	-0.201097
2	6	0	-3.535268	1.115462	0.092490
3	7	0	-2.824185	-0.077615	0.117272
4	6	0	-1.532507	0.183866	-0.157016
5	7	0	-1.404788	1.496472	-0.356484
6	6	0	-0.132102	2.181812	-0.644251
7	6	0	0.450953	2.874950	0.592075
8	1	0	-2.786365	3.157714	-0.320954
9	1	0	-4.593894	1.165391	0.270404
10	1	0	0.568827	1.424499	-0.995455
11	1	0	-0.304889	2.905199	-1.442212
12	1	0	-0.229614	3.663315	0.930750
13	1	0	0.528485	2.134050	1.401838
14	35	0	0.136015	-2.663326	-0.269741
15	1	0	-0.756365	-0.604753	-0.216252
16	6	0	-3.296875	-1.402281	0.365212
17	6	0	-4.552409	-1.691419	0.680357
18	1	0	-2.499321	-2.135924	0.262508
19	1	0	-4.823419	-2.724738	0.848224
20	1	0	-5.336844	-0.951419	0.783290
21	7	0	1.718764	3.481200	0.202925
22	1	0	2.059853	4.108403	0.921943
23	1	0	2.416017	2.753943	0.056428
24	6	0	3.336398	-0.385938	-1.126269
25	6	0	3.265260	-0.580608	0.322636
26	8	0	2.725569	0.623594	-0.289539
27	1	0	4.276805	-0.082499	-1.580834
28	1	0	2.644150	-0.930687	-1.761353
29	1	0	2.483652	-1.253241	0.669586
30	6	0	4.456920	-0.393672	1.220802
31	1	0	4.150477	-0.005149	2.196495
32	1	0	4.951666	-1.355567	1.386565
33	1	0	5.179531	0.298906	0.781873

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				

2	C	1.357331	0.000000			
3	N	2.205480	1.389132	0.000000		
4	C	2.214081	2.222875	1.346119	0.000000	
5	N	1.387217	2.210360	2.171838	1.333804	0.000000
6	C	2.553446	3.641625	3.596142	2.488036	1.473849
7	C	3.289522	4.385811	4.435042	3.425957	2.498747
8	H	1.076312	2.214178	3.265092	3.231533	2.160959
9	H	2.210815	1.074632	2.168037	3.243172	3.266956
10	H	3.378607	4.257080	3.873892	2.580263	2.075722
11	H	2.769616	3.999228	4.204286	3.250297	2.091195
12	H	3.093383	4.256945	4.624727	3.871348	2.780866
13	H	3.555865	4.389305	4.216866	3.237426	2.689934
14	Br	5.514134	5.280982	3.949489	3.301996	4.436836
15	H	3.297030	3.282798	2.159859	1.108073	2.203466
16	C	3.604596	2.543666	1.428164	2.429317	3.536044
17	C	4.332329	3.042818	2.430677	3.652081	4.598391
18	H	4.261167	3.416666	2.088844	2.547971	3.843885
19	H	5.394275	4.120389	3.396836	4.505617	5.563899
20	H	4.184310	2.827522	2.742366	4.079954	4.769939
21	N	4.596067	5.763138	5.771558	4.644646	3.742815
22	H	5.238749	6.399303	6.482597	5.428738	4.523306
23	H	5.110293	6.172820	5.956604	4.716110	4.043548
24	C	6.542535	7.138584	6.292395	4.997036	5.158961
25	C	6.510137	7.012618	6.113634	4.881912	5.156046
26	O	5.570201	6.291738	5.608650	4.282773	4.222114
27	H	7.387317	8.078590	7.301208	5.987180	6.022680
28	H	6.291506	6.768211	5.844626	4.610921	4.925308
29	H	6.188059	6.493935	5.464456	4.344892	4.871725
30	C	7.659640	8.211312	7.371035	6.172939	6.357680
31	H	7.506863	8.046942	7.278346	6.153946	6.295517
32	H	8.494645	8.933570	7.981737	6.840833	7.181702
33	H	8.088893	8.780077	8.040083	6.778363	6.788467

		6	7	8	9	10
6	C	0.000000				
7	C	1.532610	0.000000			
8	H	2.846405	3.375471	0.000000		
9	H	4.666615	5.336342	2.754309	0.000000	
10	H	1.090032	2.153591	3.836184	5.321957	0.000000
11	H	1.090819	2.170377	2.734723	4.935135	1.776357
12	H	2.164483	1.095168	2.891257	5.071747	3.059424
13	H	2.150613	1.100300	3.873516	5.334529	2.500421
14	Br	4.866981	5.613770	6.513635	6.109244	4.174242
15	H	2.887530	3.770854	4.276450	4.254042	2.545812
16	C	4.886771	5.691431	4.639504	2.878225	4.978530

17	C	6.024584	6.774448	5.256960	2.886371	6.224496
18	H	5.006874	5.824225	5.333426	3.909729	4.865452
19	H	6.950552	7.696825	6.334020	3.939500	7.049230
20	H	6.240541	6.940912	4.960774	2.301284	6.609529
21	N	2.414916	1.458191	4.547008	6.724372	2.643575
22	H	3.312006	2.053967	5.092587	7.304668	3.619795
23	H	2.703922	2.040352	5.231656	7.190836	2.507187
24	C	4.342370	4.681014	7.119989	8.200418	3.309720
25	C	4.484184	4.464729	7.142229	8.050934	3.609511
26	O	3.274164	3.319597	6.066644	7.360817	2.406512
27	H	5.044081	5.301432	7.872398	9.147328	4.045097
28	H	4.317771	4.983133	6.948401	7.804541	3.231171
29	H	4.513084	4.602156	6.943398	7.490046	3.689066
30	C	5.583069	5.208355	8.213071	9.233156	4.830612
31	H	5.585080	4.955362	8.028763	9.030172	5.006062
32	H	6.517819	6.227753	9.119345	9.935731	5.710697
33	H	5.813141	5.388087	8.534900	9.825082	5.067982

		11	12	13	14	15
11	H	0.000000				
12	H	2.492259	0.000000			
13	H	3.062320	1.770675	0.000000		
14	Br	5.707675	6.449903	5.095392	0.000000	
15	H	3.745207	4.450785	3.430757	2.244309	0.000000
16	C	5.547355	5.948797	5.311648	3.711891	2.725499
17	C	6.608754	6.886395	6.400799	4.881456	4.049037
18	H	5.756260	6.263330	5.357085	2.739788	2.368880
19	H	7.573599	7.868741	7.249633	5.084251	4.708331
20	H	6.719147	6.884861	6.656185	5.830239	4.701069
21	N	2.670847	2.087839	2.160780	6.362681	4.795517
22	H	3.553722	2.332347	2.544300	7.139858	5.607175
23	H	3.110005	2.931000	2.399410	5.886560	4.628088
24	C	4.918371	5.774446	4.541590	4.020272	4.198419
25	C	5.292589	5.531260	4.002997	3.805365	4.057641
26	O	3.964600	4.411589	3.157438	4.184498	3.692976
27	H	5.471515	6.375499	5.278194	5.052304	5.240957
28	H	4.848990	6.050686	4.886147	3.393771	3.749276
29	H	5.433993	5.621615	3.979022	2.895181	3.420958
30	C	6.375658	6.205392	4.674907	5.103260	5.411841
31	H	6.446751	5.851918	4.280944	5.409633	5.500724
32	H	7.333995	7.227905	5.634021	5.257763	5.976149
33	H	6.466698	6.371834	5.038288	5.942875	6.086684

		16	17	18	19	20
16	C	0.000000				
17	C	1.326379	0.000000			

18	H	1.088519	2.141811	0.000000		
19	H	2.076663	1.081376	2.468035	0.000000	
20	H	2.130619	1.083297	3.118622	1.847290	0.000000
21	N	7.002240	8.143190	7.024804	9.040478	8.352637
22	H	7.705331	8.798768	7.759675	9.699314	8.962821
23	H	7.071540	8.289118	6.936412	9.113304	8.623508
24	C	6.874430	8.197650	6.248742	8.715000	8.898950
25	C	6.613515	7.904292	5.971015	8.384526	8.622407
26	O	6.387700	7.698633	5.934575	8.336250	8.284573
27	H	7.930294	9.255087	7.316444	9.782425	9.938127
28	H	6.327754	7.637482	5.657200	8.111295	8.376868
29	H	5.790454	7.049701	5.076895	7.455904	7.827144
30	C	7.865791	9.118347	7.234850	9.575875	9.819385
31	H	7.795424	8.993465	7.245710	9.473374	9.638560
32	H	8.311665	9.536193	7.575597	9.885177	10.314103
33	H	8.655467	9.933900	8.072355	10.450160	10.590442

		21	22	23	24	25
21	N	0.000000				
22	H	1.013268	0.000000			
23	H	1.018099	1.646369	0.000000		
24	C	4.397528	5.101357	3.479185	0.000000	
25	C	4.347903	4.878422	3.451276	1.463654	0.000000
26	O	3.069542	3.748968	2.180344	1.446507	1.454692
27	H	4.735538	5.361197	3.766771	1.087690	2.212360
28	H	4.917264	5.738808	4.114957	1.085952	2.202577
29	H	4.818481	5.384284	4.054388	2.168982	1.087989
30	C	4.852650	5.109200	3.927917	2.600840	1.503895
31	H	4.694910	4.787118	3.898823	3.442162	2.150839
32	H	5.936916	6.199470	5.008678	3.140638	2.139269
33	H	4.736991	4.925878	3.767026	2.739919	2.156125

		26	27	28	29	30
26	O	0.000000				
27	H	2.138304	0.000000			
28	H	2.142115	1.848668	0.000000		
29	H	2.121546	3.106513	2.457492	0.000000	
30	C	2.512675	2.824612	3.530973	2.221820	0.000000
31	H	2.933606	3.780232	4.334767	2.582148	1.093999
32	H	3.417881	3.298727	3.926136	2.572085	1.094300
33	H	2.697272	2.557883	3.795795	3.112802	1.092928

		31	32	33
31	H	0.000000		
32	H	1.766782	0.000000	
33	H	1.775545	1.776192	0.000000

Stoichiometry C10H18BrN3O

Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.355318	2.464434	-0.267438
2	6	0	-3.338716	1.582419	0.044532
3	7	0	-2.748533	0.326295	0.103893
4	6	0	-1.436238	0.452574	-0.168084
5	7	0	-1.179188	1.740775	-0.399378
6	6	0	0.155953	2.290248	-0.695535
7	6	0	0.799050	2.954072	0.527027
8	1	0	-2.390821	3.530037	-0.414670
9	1	0	-4.388051	1.740595	0.213973
10	1	0	0.780499	1.459049	-1.022978
11	1	0	0.058570	3.006523	-1.512452
12	1	0	0.197875	3.813845	0.841307
13	1	0	0.799868	2.230031	1.355533
14	35	0	-0.055362	-2.546665	-0.198423
15	1	0	-0.741174	-0.409711	-0.202365
16	6	0	-3.350273	-0.938788	0.381608
17	6	0	-4.629495	-1.095089	0.695363
18	1	0	-2.628307	-1.749593	0.302646
19	1	0	-5.001536	-2.092179	0.887126
20	1	0	-5.337781	-0.279244	0.774484
21	7	0	2.121995	3.422757	0.131461
22	1	0	2.520034	4.031559	0.836895
23	1	0	2.744962	2.627039	0.007882
24	6	0	3.357128	-0.617187	-1.089831
25	6	0	3.260983	-0.766918	0.362966
26	8	0	2.844971	0.468462	-0.282710
27	1	0	4.324758	-0.419264	-1.545450
28	1	0	2.617387	-1.107333	-1.715795
29	1	0	2.415531	-1.350470	0.721294
30	6	0	4.461392	-0.675079	1.264234
31	1	0	4.190469	-0.233585	2.227830
32	1	0	4.858421	-1.676372	1.457295
33	1	0	5.250489	-0.068237	0.813059

Rotational constants (GHZ): 0.4213554 0.2923053 0.1828017
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 499 symmetry adapted cartesian basis functions of A symmetry.
There are 482 symmetry adapted basis functions of A symmetry.
482 basis functions, 760 primitive gaussians, 499 cartesian basis functions
71 alpha electrons 71 beta electrons
nuclear repulsion energy 1312.9464195282 Hartrees.
NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 482 RedAO= T EigKep= 3.64D-06 NBF= 482
NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999996 0.001416 -0.001402 -0.001936 Ang= 0.32 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3205.64835914 A.U. after 11 cycles
NFock= 11 Conv=0.85D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Atomic Forces (Hartrees/Bohr)
Number Number X Y Z

1	6	0.000063391	-0.000055847	0.000023756
2	6	-0.000019873	0.000079514	-0.000020789
3	7	-0.000023127	-0.000083819	-0.000093871
4	6	-0.000047985	-0.000068190	0.000020843
5	7	0.000018672	0.000199034	0.000186360
6	6	-0.000052089	-0.000088754	-0.000165769
7	6	-0.000130367	-0.000010170	-0.000105954
8	1	-0.000029325	-0.000003607	-0.000017725
9	1	0.000009528	-0.000015439	0.000030334
10	1	0.000052627	0.000066643	0.000000272
11	1	-0.000012335	-0.000048281	-0.000020354
12	1	0.000026484	-0.000012781	0.000034935
13	1	0.000009714	-0.000004911	-0.000013546
14	35	0.000018424	-0.000100532	0.000008223
15	1	-0.000064543	0.000088649	0.000000761
16	6	0.000009595	0.000046874	0.000011406
17	6	0.000008680	0.000004877	-0.000002077
18	1	0.000025363	-0.000023493	-0.000002195
19	1	0.000010227	-0.000000088	0.000003674
20	1	-0.000016200	0.000005439	0.000002160
21	7	0.000118783	0.000000679	0.000206066
22	1	-0.000001882	0.000008799	-0.000079769
23	1	-0.000041968	0.000061576	0.000115447
24	6	0.000378035	-0.000201253	-0.000710505
25	6	-0.000184790	0.000112079	0.000281914
26	8	0.000196563	0.000048331	-0.000086244
27	1	-0.000068787	0.000103817	0.000122085
28	1	-0.000182200	-0.000031974	0.000292435
29	1	0.000002473	-0.000114156	-0.000049495
30	6	-0.000104533	0.000009939	-0.000018671
31	1	0.000031008	0.000025795	0.000029033
32	1	-0.000011229	0.000007329	0.000017120
33	1	0.000011664	-0.000006080	0.000000139

Cartesian Forces: Max 0.000710505 RMS 0.000116609

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000330247 RMS 0.000075256

Search for a local minimum.

Step number 37 out of a maximum of 172

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 31 32 33 34 35
36 37
DE= -5.66D-06 DEPred=-6.48D-06 R= 8.73D-01
TightC=F SS= 1.41D+00 RLast= 1.03D-01 DXNew= 1.7446D+00 3.0791D-01
Trust test= 8.73D-01 RLast= 1.03D-01 DXMaxT set to 1.04D+00
ITU= 1 1 1 1 1 1 1 1 1 1 1 0 0 -1 1 -1 1 1 1 1
ITU= 1 1 1 1 1 0 -1 -1 1 1 1 -1 1 0 0 -1 0
Eigenvalues --- 0.00057 0.00094 0.00217 0.00456 0.00617
Eigenvalues --- 0.00698 0.00729 0.01180 0.01432 0.01895
Eigenvalues --- 0.02053 0.02118 0.02230 0.02379 0.02385
Eigenvalues --- 0.02592 0.02753 0.02896 0.03062 0.03106
Eigenvalues --- 0.03496 0.03570 0.03844 0.03974 0.04146
Eigenvalues --- 0.04414 0.04423 0.04982 0.05402 0.05482
Eigenvalues --- 0.05705 0.05773 0.05914 0.07820 0.08622
Eigenvalues --- 0.08787 0.09540 0.10434 0.11222 0.12289
Eigenvalues --- 0.12922 0.13176 0.13841 0.15746 0.15933
Eigenvalues --- 0.16000 0.16001 0.16009 0.16033 0.16087
Eigenvalues --- 0.16158 0.18498 0.21415 0.22021 0.22170
Eigenvalues --- 0.23006 0.23473 0.25924 0.27329 0.28142
Eigenvalues --- 0.29173 0.29663 0.31723 0.32175 0.33121
Eigenvalues --- 0.33622 0.34289 0.34338 0.34426 0.34549
Eigenvalues --- 0.34669 0.34745 0.35104 0.35281 0.35498
Eigenvalues --- 0.35569 0.35668 0.35891 0.36415 0.36621
Eigenvalues --- 0.36802 0.39465 0.40184 0.41886 0.42469
Eigenvalues --- 0.44883 0.45709 0.46503 0.49524 0.54811
Eigenvalues --- 0.58395 0.60652 1.14319
En-DIIS/RFO-DIIS IScMMF= 0 using points: 37 36 35 34 33
RFO step: Lambda=-1.66401386D-06.
DidBck=T Rises=F RFO-DIIS coefs: 0.78843 0.38759 -0.76676 0.47156
0.11918
Iteration 1 RMS(Cart)= 0.01162737 RMS(Int)= 0.00005472
Iteration 2 RMS(Cart)= 0.00010950 RMS(Int)= 0.00001188
Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00001188

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56498	0.00000	-0.00003	0.00000	-0.00002	2.56496
R2	2.62146	-0.00001	-0.00004	-0.00002	-0.00006	2.62140
R3	2.03394	0.00000	0.00000	0.00000	0.00001	2.03394
R4	2.62508	0.00001	0.00003	0.00005	0.00007	2.62515
R5	2.03076	0.00000	-0.00002	0.00000	-0.00002	2.03075
R6	2.54380	-0.00004	-0.00013	0.00003	-0.00010	2.54370
R7	2.69884	-0.00004	0.00001	-0.00009	-0.00008	2.69876

R8	2.52052	0.00011	0.00019	-0.00004	0.00014	2.52067
R9	2.09395	-0.00002	-0.00029	0.00016	-0.00012	2.09383
R10	2.78517	0.00003	0.00006	0.00001	0.00007	2.78524
R11	2.89621	0.00004	0.00009	-0.00004	0.00005	2.89627
R12	2.05986	-0.00001	0.00009	-0.00008	0.00002	2.05988
R13	2.06135	-0.00002	-0.00002	-0.00002	-0.00004	2.06131
R14	2.06957	-0.00001	-0.00007	0.00002	-0.00005	2.06951
R15	2.07927	-0.00001	-0.00003	-0.00001	-0.00004	2.07922
R16	2.75558	0.00011	0.00025	-0.00003	0.00022	2.75580
R17	4.24113	0.00010	0.00338	-0.00064	0.00274	4.24387
R18	2.50649	0.00000	-0.00001	0.00002	0.00001	2.50650
R19	2.05700	0.00004	0.00007	0.00000	0.00007	2.05707
R20	2.04351	0.00000	0.00000	0.00000	0.00000	2.04351
R21	2.04713	0.00001	0.00002	0.00001	0.00003	2.04716
R22	1.91480	-0.00005	-0.00009	-0.00001	-0.00010	1.91470
R23	1.92393	-0.00003	-0.00009	0.00005	-0.00004	1.92389
R24	4.12025	0.00008	0.00141	-0.00067	0.00073	4.12099
R25	2.76590	0.00028	0.00077	0.00035	0.00110	2.76701
R26	2.73350	0.00014	-0.00027	0.00032	0.00007	2.73357
R27	2.05544	-0.00008	-0.00015	-0.00006	-0.00021	2.05523
R28	2.05215	-0.00004	-0.00001	-0.00002	-0.00003	2.05212
R29	2.74897	-0.00012	0.00040	-0.00057	-0.00017	2.74880
R30	2.05600	0.00005	0.00025	-0.00004	0.00021	2.05621
R31	2.84195	-0.00004	-0.00020	0.00001	-0.00019	2.84176
R32	2.06736	0.00003	0.00000	0.00002	0.00002	2.06738
R33	2.06793	-0.00001	-0.00003	0.00000	-0.00002	2.06790
R34	2.06533	0.00001	0.00004	-0.00001	0.00003	2.06536
A1	1.87249	0.00004	0.00008	0.00003	0.00011	1.87260
A2	2.27956	-0.00005	-0.00012	-0.00008	-0.00021	2.27935
A3	2.13108	0.00001	0.00004	0.00006	0.00010	2.13118
A4	1.86461	0.00000	0.00000	-0.00003	-0.00003	1.86458
A5	2.27581	0.00002	0.00009	0.00009	0.00018	2.27599
A6	2.14268	-0.00002	-0.00008	-0.00006	-0.00014	2.14254
A7	1.89729	0.00000	-0.00003	-0.00001	-0.00003	1.89725
A8	2.25273	0.00005	0.00007	0.00000	0.00007	2.25280
A9	2.13310	-0.00005	-0.00003	0.00001	-0.00003	2.13308
A10	1.88969	0.00003	0.00008	0.00000	0.00009	1.88978
A11	2.14690	-0.00010	-0.00008	0.00011	0.00005	2.14695
A12	2.24635	0.00008	0.00003	-0.00014	-0.00010	2.24624
A13	1.90069	-0.00006	-0.00013	0.00001	-0.00013	1.90056
A14	2.20517	-0.00002	-0.00042	0.00022	-0.00019	2.20497
A15	2.17669	0.00008	0.00057	-0.00023	0.00035	2.17704
A16	1.96200	-0.00029	-0.00052	-0.00054	-0.00105	1.96095
A17	1.87037	0.00016	0.00083	0.00008	0.00091	1.87128

A18	1.89064	0.00005	-0.00019	0.00014	-0.00005	1.89059
A19	1.90656	0.00002	-0.00005	0.00002	-0.00003	1.90653
A20	1.92884	0.00012	0.00014	0.00019	0.00033	1.92917
A21	1.90382	-0.00005	-0.00019	0.00012	-0.00007	1.90375
A22	1.91624	-0.00007	0.00024	-0.00012	0.00011	1.91635
A23	1.89225	-0.00010	-0.00005	-0.00021	-0.00026	1.89199
A24	1.87917	0.00033	0.00050	0.00048	0.00097	1.88015
A25	1.87646	0.00004	-0.00024	-0.00001	-0.00024	1.87622
A26	1.90026	-0.00010	-0.00021	0.00007	-0.00014	1.90012
A27	1.99884	-0.00010	-0.00022	-0.00022	-0.00043	1.99841
A28	2.16125	0.00002	0.00001	0.00006	0.00007	2.16132
A29	1.94578	-0.00001	-0.00001	0.00005	0.00004	1.94581
A30	2.17616	-0.00001	0.00000	-0.00011	-0.00010	2.17605
A31	2.07421	-0.00002	-0.00010	0.00000	-0.00009	2.07411
A32	2.16411	0.00002	0.00013	-0.00004	0.00009	2.16420
A33	2.04487	0.00000	-0.00003	0.00003	0.00000	2.04487
A34	1.93976	-0.00006	0.00026	-0.00037	-0.00006	1.93970
A35	1.91437	0.00015	0.00052	-0.00005	0.00049	1.91487
A36	1.88992	-0.00003	0.00029	0.00001	0.00028	1.89020
A37	2.08614	0.00007	0.00060	0.00001	0.00065	2.08679
A38	2.07285	-0.00024	-0.00002	-0.00104	-0.00111	2.07174
A39	1.99560	-0.00010	0.00009	-0.00035	-0.00026	1.99534
A40	2.00336	0.00002	-0.00028	-0.00045	-0.00073	2.00263
A41	2.03384	0.00021	-0.00035	0.00125	0.00090	2.03474
A42	2.01842	-0.00016	0.00048	-0.00039	0.00008	2.01850
A43	2.13668	0.00016	-0.00054	0.00066	0.00013	2.13681
A44	1.96000	0.00007	0.00018	0.00026	0.00045	1.96045
A45	2.02908	-0.00010	-0.00051	0.00020	-0.00033	2.02875
A46	2.04389	0.00001	0.00031	-0.00046	-0.00015	2.04374
A47	2.55647	0.00010	-0.00095	0.00234	0.00142	2.55789
A48	2.48934	-0.00010	0.00394	-0.00300	0.00086	2.49021
A49	1.93353	0.00005	0.00002	0.00002	0.00004	1.93357
A50	1.91713	0.00000	-0.00008	0.00017	0.00009	1.91722
A51	1.94208	0.00000	0.00016	-0.00009	0.00006	1.94215
A52	1.87939	-0.00002	-0.00015	-0.00002	-0.00017	1.87922
A53	1.89477	-0.00003	-0.00002	-0.00004	-0.00006	1.89471
A54	1.89540	0.00000	0.00007	-0.00004	0.00002	1.89542
A55	3.49150	0.00008	-0.00251	0.00163	-0.00088	3.49061
A56	2.52929	0.00022	0.00238	0.00003	0.00239	2.53168
A57	2.99290	-0.00005	-0.01123	0.00427	-0.00696	2.98593
A58	3.11539	0.00002	-0.00471	0.00081	-0.00392	3.11147
D1	0.00328	-0.00001	-0.00009	-0.00025	-0.00034	0.00293
D2	-3.12451	-0.00002	-0.00121	-0.00011	-0.00132	-3.12582
D3	3.13334	-0.00001	-0.00016	0.00014	-0.00003	3.13332

D4	0.00556	-0.00002	-0.00129	0.00029	-0.00100	0.00456
D5	-0.00488	0.00001	0.00013	0.00032	0.00045	-0.00443
D6	-3.10920	-0.00001	-0.00048	0.00012	-0.00035	-3.10955
D7	-3.13614	0.00001	0.00020	-0.00003	0.00017	-3.13598
D8	0.04272	-0.00001	-0.00041	-0.00023	-0.00063	0.04209
D9	-0.00060	0.00001	0.00002	0.00011	0.00013	-0.00047
D10	-3.12987	-0.00001	-0.00105	-0.00001	-0.00106	-3.13093
D11	3.12849	0.00002	0.00104	-0.00002	0.00101	3.12950
D12	-0.00079	-0.00001	-0.00003	-0.00014	-0.00017	-0.00096
D13	-0.00245	-0.00001	0.00006	0.00009	0.00015	-0.00229
D14	-3.12191	-0.00001	-0.00263	0.00128	-0.00135	-3.12325
D15	3.12784	0.00002	0.00104	0.00020	0.00124	3.12908
D16	0.00838	0.00001	-0.00165	0.00139	-0.00026	0.00812
D17	-0.05308	0.00001	0.00949	-0.00483	0.00466	-0.04841
D18	3.08846	0.00001	0.00918	-0.00455	0.00463	3.09308
D19	3.10231	-0.00002	0.00830	-0.00496	0.00334	3.10565
D20	-0.03934	-0.00001	0.00798	-0.00468	0.00330	-0.03604
D21	0.00451	0.00000	-0.00012	-0.00025	-0.00037	0.00414
D22	3.10958	0.00001	0.00045	-0.00005	0.00040	3.10998
D23	3.12232	0.00000	0.00277	-0.00153	0.00124	3.12357
D24	-0.05579	0.00001	0.00334	-0.00133	0.00201	-0.05378
D25	1.33763	0.00001	-0.00005	-0.00036	-0.00041	1.33721
D26	-2.85067	-0.00003	0.00012	-0.00060	-0.00048	-2.85115
D27	-0.79881	0.00002	0.00024	-0.00035	-0.00011	-0.79892
D28	-1.76106	0.00000	-0.00073	-0.00059	-0.00132	-1.76239
D29	0.33383	-0.00004	-0.00056	-0.00083	-0.00139	0.33244
D30	2.38569	0.00000	-0.00044	-0.00058	-0.00102	2.38467
D31	-1.10410	0.00006	0.00297	-0.00177	0.00120	-1.10291
D32	0.94123	0.00001	0.00279	-0.00197	0.00082	0.94204
D33	3.11274	0.00003	0.00280	-0.00206	0.00074	3.11348
D34	3.10529	0.00003	0.00229	-0.00155	0.00074	3.10603
D35	-1.13257	-0.00002	0.00211	-0.00175	0.00036	-1.13221
D36	1.03895	0.00000	0.00212	-0.00185	0.00028	1.03923
D37	1.01059	0.00001	0.00248	-0.00183	0.00064	1.01124
D38	3.05592	-0.00004	0.00229	-0.00203	0.00027	3.05619
D39	-1.05574	-0.00002	0.00231	-0.00212	0.00019	-1.05556
D40	2.94147	-0.00002	-0.00108	-0.00010	-0.00120	2.94027
D41	-1.25241	-0.00001	-0.00022	-0.00035	-0.00056	-1.25297
D42	0.86489	-0.00007	-0.00153	-0.00026	-0.00180	0.86308
D43	2.95419	-0.00005	-0.00067	-0.00051	-0.00117	2.95303
D44	-1.23596	0.00002	-0.00093	-0.00016	-0.00110	-1.23706
D45	0.85335	0.00004	-0.00006	-0.00041	-0.00047	0.85288
D46	3.13810	0.00001	0.00063	-0.00013	0.00050	3.13860
D47	-0.00426	0.00000	0.00087	-0.00037	0.00050	-0.00375

D48	-0.00342	0.00000	0.00098	-0.00044	0.00054	-0.00288
D49	3.13741	0.00000	0.00123	-0.00069	0.00055	3.13795
D50	2.21444	-0.00005	0.01101	0.00194	0.01299	2.22743
D51	-1.41927	0.00006	0.01875	0.00013	0.01888	-1.40039
D52	-2.08503	0.00000	0.01411	0.00110	0.01520	-2.06982
D53	0.56445	0.00011	0.02185	-0.00071	0.02110	0.58555
D54	-2.71331	-0.00004	-0.00029	-0.00003	-0.00033	-2.71364
D55	-0.01408	-0.00003	0.00044	-0.00065	-0.00021	-0.01430
D56	-0.03060	0.00011	0.00017	0.00080	0.00096	-0.02964
D57	2.66863	0.00012	0.00090	0.00018	0.00108	2.66970
D58	0.55720	0.00000	0.00689	-0.00351	0.00342	0.56062
D59	-1.85992	-0.00023	0.00769	-0.00459	0.00315	-1.85677
D60	1.84101	-0.00004	-0.00285	-0.00131	-0.00416	1.83685
D61	-0.58005	-0.00003	-0.00297	-0.00111	-0.00408	-0.58413
D62	2.55900	0.00001	-0.00179	0.00026	-0.00153	2.55748
D63	-1.65008	0.00001	-0.00201	0.00035	-0.00166	-1.65174
D64	0.44936	0.00001	-0.00188	0.00035	-0.00153	0.44783
D65	1.35496	-0.00002	-0.00096	-0.00024	-0.00120	1.35376
D66	-2.85413	-0.00001	-0.00118	-0.00015	-0.00133	-2.85545
D67	-0.75469	-0.00002	-0.00105	-0.00015	-0.00120	-0.75589
D68	-1.03098	-0.00003	-0.00101	-0.00035	-0.00136	-1.03234
D69	1.04312	-0.00002	-0.00123	-0.00025	-0.00148	1.04163
D70	-3.14063	-0.00003	-0.00110	-0.00025	-0.00136	3.14120

Item	Value	Threshold	Converged?
Maximum Force	0.000330	0.000450	YES
RMS Force	0.000075	0.000300	YES
Maximum Displacement	0.051171	0.001800	NO
RMS Displacement	0.011646	0.001200	NO

Predicted change in Energy=-1.572917D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.645171	2.096974	-0.198070
2	6	0	-3.534886	1.115452	0.097455
3	7	0	-2.824285	-0.077991	0.120628
4	6	0	-1.533126	0.182953	-0.156346
5	7	0	-1.405104	1.495608	-0.355794
6	6	0	-0.132946	2.180720	-0.646616
7	6	0	0.451288	2.874370	0.588900
8	1	0	-2.786111	3.157310	-0.317570

9	1	0	-4.592949	1.165820	0.278513
10	1	0	0.568019	1.423792	-0.998607
11	1	0	-0.307405	2.903644	-1.444601
12	1	0	-0.229580	3.661870	0.928887
13	1	0	0.530547	2.133342	1.398348
14	35	0	0.134339	-2.666539	-0.258689
15	1	0	-0.757225	-0.605776	-0.216084
16	6	0	-3.296729	-1.402298	0.370700
17	6	0	-4.552506	-1.691382	0.684939
18	1	0	-2.498769	-2.135887	0.270415
19	1	0	-4.823036	-2.724465	0.855020
20	1	0	-5.337580	-0.951649	0.785026
21	7	0	1.718321	3.482203	0.199247
22	1	0	2.058538	4.110255	0.917863
23	1	0	2.416734	2.756157	0.052410
24	6	0	3.355173	-0.377613	-1.135584
25	6	0	3.263837	-0.580285	0.311681
26	8	0	2.734255	0.627863	-0.301338
27	1	0	4.301547	-0.072264	-1.576002
28	1	0	2.670213	-0.918040	-1.782132
29	1	0	2.476895	-1.254163	0.644207
30	6	0	4.442914	-0.399310	1.227335
31	1	0	4.123398	-0.014480	2.200308
32	1	0	4.933642	-1.362736	1.396043
33	1	0	5.172862	0.293912	0.801725

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357319	0.000000			
3	N	2.205475	1.389171	0.000000		
4	C	2.214016	2.222839	1.346068	0.000000	
5	N	1.387186	2.210413	2.171926	1.333879	0.000000
6	C	2.553328	3.641653	3.596352	2.488362	1.473887
7	C	3.288120	4.384621	4.434534	3.425934	2.497924
8	H	1.076316	2.214068	3.265064	3.231527	2.160994
9	H	2.210886	1.074624	2.167987	3.243093	3.267026
10	H	3.379146	4.257964	3.875018	2.581452	2.076435
11	H	2.769424	3.999025	4.204138	3.250255	2.091174
12	H	3.090956	4.254476	4.623022	3.870378	2.779379
13	H	3.554583	4.388185	4.216332	3.237257	2.688952
14	Br	5.515470	5.281430	3.949420	3.303107	4.438781
15	H	3.296897	3.282733	2.159785	1.108009	2.203425
16	C	3.604571	2.543707	1.428121	2.429217	3.536085

17	C	4.332352	3.042861	2.430684	3.652061	4.598496
18	H	4.261224	3.416820	2.088860	2.547864	3.843956
19	H	5.394290	4.120461	3.396787	4.505491	5.563932
20	H	4.184453	2.827608	2.742509	4.080120	4.770210
21	N	4.595300	5.762643	5.772038	4.645794	3.743048
22	H	5.236744	6.397524	6.482202	5.429335	4.522764
23	H	5.110787	6.173793	5.958634	4.718723	4.045004
24	C	6.557946	7.156993	6.312967	5.016833	5.174676
25	C	6.507223	7.010282	6.111795	4.879799	5.153044
26	O	5.577381	6.300707	5.619044	4.292961	4.229686
27	H	7.406833	8.100667	7.325030	6.010321	6.042598
28	H	6.312913	6.794939	5.875005	4.639335	4.946549
29	H	6.178601	6.485023	5.455275	4.334334	4.861189
30	C	7.648802	8.198562	7.358004	6.161709	6.347939
31	H	7.484918	8.021724	7.252545	6.130992	6.275218
32	H	8.482288	8.918728	7.966347	6.827749	7.170688
33	H	8.085312	8.774725	8.034710	6.774990	6.786278

		6	7	8	9	10
6	C	0.000000				
7	C	1.532638	0.000000			
8	H	2.846276	3.373796	0.000000		
9	H	4.666639	5.334774	2.754271	0.000000	
10	H	1.090041	2.153597	3.836546	5.322892	0.000000
11	H	1.090796	2.170621	2.734690	4.935083	1.776300
12	H	2.164567	1.095139	2.888613	5.068751	3.059475
13	H	2.150429	1.100278	3.872093	5.332949	2.500051
14	Br	4.870097	5.614315	6.515344	6.109240	4.179278
15	H	2.887845	3.770932	4.276389	4.253935	2.547109
16	C	4.886971	5.690795	4.639448	2.878180	4.979766
17	C	6.024843	6.774458	5.256899	2.886247	6.225626
18	H	5.007112	5.822968	5.333501	3.909851	4.866922
19	H	6.950734	7.696511	6.333981	3.939495	7.050350
20	H	6.240958	6.941750	4.960772	2.301023	6.610611
21	N	2.415891	1.458308	4.545609	6.723395	2.644825
22	H	3.312597	2.053991	5.089698	7.302106	3.620993
23	H	2.705666	2.040777	5.231387	7.191380	2.509498
24	C	4.353290	4.688474	7.133036	8.219155	3.321454
25	C	4.481028	4.463398	7.139149	8.048545	3.605637
26	O	3.278936	3.324343	6.072299	7.369773	2.410864
27	H	5.060081	5.309797	7.889784	9.169740	4.063348
28	H	4.330059	4.992774	6.965981	7.832130	3.243040
29	H	4.502878	4.599014	6.934359	7.481494	3.676151
30	C	5.577342	5.201698	8.203358	9.219367	4.826317
31	H	5.571386	4.942316	8.008825	9.003395	4.994237

32	H	6.511440	6.220615	9.108341	9.919598	5.705940
33	H	5.814579	5.384916	8.532123	9.818608	5.071726

		11	12	13	14	15
11	H	0.000000				
12	H	2.492871	0.000000			
13	H	3.062334	1.770476	0.000000		
14	Br	5.712133	6.449149	5.093290	0.000000	
15	H	3.745347	4.449963	3.430381	2.245761	0.000000
16	C	5.547298	5.946829	5.310824	3.710345	2.725408
17	C	6.608335	6.885093	6.401163	4.879331	4.049017
18	H	5.756756	6.260734	5.354933	2.737663	2.368733
19	H	7.573295	7.867056	7.249437	5.081266	4.708176
20	H	6.718421	6.884542	6.657946	5.828558	4.701224
21	N	2.672177	2.087816	2.160573	6.365982	4.797124
22	H	3.554551	2.331664	2.544368	7.142251	5.608504
23	H	3.111869	2.931127	2.399406	5.891667	4.631274
24	C	4.927132	5.781861	4.550189	4.047456	4.220113
25	C	5.289240	5.529989	4.001936	3.804148	4.055629
26	O	3.967106	4.416217	3.164132	4.196960	3.703994
27	H	5.487781	6.383520	5.285063	5.082440	5.265470
28	H	4.856481	6.060858	4.899444	3.436392	3.781183
29	H	5.422435	5.619023	3.978968	2.880555	3.408817
30	C	6.372934	6.197940	4.663710	5.090424	5.400697
31	H	6.436834	5.837849	4.262025	5.384485	5.478053
32	H	7.330746	7.219679	5.622261	5.241312	5.963045
33	H	6.472249	6.367550	5.028971	5.939316	6.083692

		16	17	18	19	20
16	C	0.000000				
17	C	1.326382	0.000000			
18	H	1.088554	2.141787	0.000000		
19	H	2.076608	1.081376	2.467874	0.000000	
20	H	2.130686	1.083312	3.118669	1.847305	0.000000
21	N	7.002748	8.144025	7.025087	9.041134	8.353916
22	H	7.704967	8.798815	7.759029	9.699145	8.963430
23	H	7.073734	8.291622	6.938428	9.115682	8.626351
24	C	6.896860	8.220200	6.271922	8.738039	8.920887
25	C	6.612127	7.903738	5.969023	8.383928	8.622433
26	O	6.398904	7.710287	5.945567	8.347929	8.296359
27	H	7.955654	9.280498	7.342485	9.808263	9.962958
28	H	6.361886	7.671517	5.693372	8.146565	8.409292
29	H	5.781997	7.043103	5.066990	7.449511	7.821596
30	C	7.851235	9.103912	7.219305	9.560480	9.806059
31	H	7.767355	8.965470	7.216506	9.444178	9.612046
32	H	8.294089	9.518439	7.556821	9.866092	10.297589

33	H	8.648520	9.926622	8.064747	10.441811	10.584002
		21	22	23	24	25
21	N	0.000000				
22	H	1.013217	0.000000			
23	H	1.018079	1.646480	0.000000		
24	C	4.399913	5.102830	3.480304	0.000000	
25	C	4.347995	4.880714	3.452049	1.464238	0.000000
26	O	3.070824	3.751013	2.180731	1.446544	1.454604
27	H	4.739071	5.361336	3.768847	1.087579	2.213204
28	H	4.918749	5.740024	4.114550	1.085935	2.202390
29	H	4.817321	5.387661	4.054196	2.169647	1.088101
30	C	4.852475	5.110499	3.929736	2.601353	1.503794
31	H	4.692061	4.787667	3.899050	3.442414	2.150789
32	H	5.936669	6.200687	5.010534	3.141841	2.139233
33	H	4.739413	4.927167	3.770990	2.740092	2.156094
		26	27	28	29	30
26	O	0.000000				
27	H	2.138071	0.000000			
28	H	2.141651	1.849074	0.000000		
29	H	2.121865	3.107340	2.457127	0.000000	
30	C	2.512258	2.825887	3.531068	2.221721	0.000000
31	H	2.932671	3.780951	4.334512	2.582487	1.094012
32	H	3.417732	3.301198	3.927042	2.571508	1.094288
33	H	2.697235	2.558683	3.795839	3.112810	1.092944
		31	32	33		
31	H	0.000000				
32	H	1.766673	0.000000			
33	H	1.775533	1.776210	0.000000		

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.352549	2.467261	-0.264824
2	6	0	-3.337068	1.585854	0.045267
3	7	0	-2.748603	0.328720	0.101108
4	6	0	-1.436273	0.453933	-0.170937
5	7	0	-1.177377	1.742467	-0.398724

6	6	0	0.158238	2.291209	-0.694290
7	6	0	0.800991	2.951963	0.530149
8	1	0	-2.386810	3.533292	-0.409254
9	1	0	-4.385977	1.745014	0.216370
10	1	0	0.782707	1.460592	-1.023382
11	1	0	0.061215	3.009193	-1.509717
12	1	0	0.199625	3.810723	0.846720
13	1	0	0.801418	2.225668	1.356653
14	35	0	-0.059328	-2.548388	-0.195478
15	1	0	-0.742156	-0.408980	-0.206525
16	6	0	-3.351676	-0.936099	0.376910
17	6	0	-4.631817	-1.091950	0.687135
18	1	0	-2.629891	-1.747284	0.299734
19	1	0	-5.004584	-2.088920	0.878108
20	1	0	-5.340169	-0.275934	0.764084
21	7	0	2.124429	3.422046	0.137472
22	1	0	2.520977	4.029758	0.844610
23	1	0	2.748189	2.627153	0.012763
24	6	0	3.378043	-0.610857	-1.096783
25	6	0	3.258322	-0.769914	0.353858
26	8	0	2.854992	0.470252	-0.290489
27	1	0	4.352690	-0.411082	-1.536081
28	1	0	2.646726	-1.095563	-1.736698
29	1	0	2.406382	-1.354603	0.694887
30	6	0	4.444003	-0.685533	1.274965
31	1	0	4.158412	-0.248507	2.236374
32	1	0	4.835642	-1.688684	1.469314
33	1	0	5.241712	-0.078107	0.839972

Rotational constants (GHZ): 0.4208885 0.2921400 0.1826970

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1312.4911343448 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 3.63D-06 NBF= 482

NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 -0.000360 0.000527 0.000467 Ang= -0.09 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3205.64836331 A.U. after 10 cycles
NFock= 10 Conv=0.69D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000033978	-0.000010636	0.000049649
2	6	0.000007454	0.000023504	-0.000016382
3	7	-0.000022420	-0.000033048	-0.000058417
4	6	0.000042915	-0.000024958	0.000015825
5	7	0.000000508	0.000073851	0.000042362
6	6	-0.000025799	-0.000024903	-0.000047250
7	6	0.000025411	0.000032859	-0.000057897
8	1	-0.000014441	-0.000002459	-0.000012027
9	1	0.000002853	-0.000002708	0.000007407
10	1	0.000022465	0.000010091	-0.000013789
11	1	-0.000001001	-0.000028682	-0.000025003
12	1	0.000009607	-0.000003877	0.000014538
13	1	-0.000015630	-0.000024754	0.000006401
14	35	0.000024387	-0.000053476	0.000006422
15	1	-0.000092945	0.000068914	0.000012090

16	6	-0.000011190	-0.000004262	0.000005122
17	6	0.000005941	0.000021027	0.000004150
18	1	0.000023503	-0.000013588	-0.000002068
19	1	0.000004776	-0.000000525	-0.000002620
20	1	-0.000009672	-0.000000017	0.000002992
21	7	-0.000005159	-0.000035963	0.000125750
22	1	0.000018542	0.000014804	-0.000055538
23	1	-0.000047305	0.000046780	0.000107328
24	6	0.000161796	-0.000161654	-0.000173515
25	6	-0.000103438	0.000095548	0.000081660
26	8	0.000088569	0.000051689	-0.000156465
27	1	-0.000052423	0.000037761	0.000055064
28	1	-0.000082447	-0.000002489	0.000137867
29	1	0.000009059	-0.000077468	-0.000049018
30	6	-0.000012920	0.000008620	-0.000036705
31	1	0.000010963	0.000018425	0.000015701
32	1	-0.000013358	0.000003469	0.000009869
33	1	0.000017421	-0.000001876	0.000006498

Cartesian Forces: Max 0.000173515 RMS 0.000052773

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000137892 RMS 0.000031583
Search for a local minimum.
Step number 38 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 31 32 33 34 35
36 37 38
DE= -4.16D-06 DEPred=-1.57D-06 R= 2.65D+00
TightC=F SS= 1.41D+00 RLast= 3.83D-02 DXNew= 1.7446D+00 1.1486D-01
Trust test= 2.65D+00 RLast= 3.83D-02 DXMaxT set to 1.04D+00
ITU= 1 1 1 1 1 1 1 1 1 1 1 1 0 0 -1 1 -1 1 1 1
ITU= 1 1 1 1 1 1 0 -1 -1 1 1 1 -1 1 0 0 -1 0
Eigenvalues --- 0.00055 0.00108 0.00217 0.00484 0.00613
Eigenvalues --- 0.00676 0.00729 0.01145 0.01334 0.01750
Eigenvalues --- 0.01905 0.02078 0.02218 0.02371 0.02387
Eigenvalues --- 0.02600 0.02741 0.02893 0.03064 0.03107
Eigenvalues --- 0.03445 0.03533 0.03829 0.03916 0.04040

Eigenvalues --- 0.04234 0.04437 0.04575 0.05449 0.05521
Eigenvalues --- 0.05742 0.05760 0.05909 0.07801 0.08695
Eigenvalues --- 0.08770 0.09563 0.10365 0.10972 0.12332
Eigenvalues --- 0.12766 0.13143 0.13590 0.15792 0.15964
Eigenvalues --- 0.16001 0.16002 0.16006 0.16016 0.16079
Eigenvalues --- 0.16175 0.19230 0.21330 0.21986 0.22171
Eigenvalues --- 0.23061 0.23450 0.25697 0.26182 0.28008
Eigenvalues --- 0.29068 0.29632 0.30289 0.31897 0.32456
Eigenvalues --- 0.33697 0.34286 0.34344 0.34361 0.34547
Eigenvalues --- 0.34682 0.34746 0.35041 0.35137 0.35309
Eigenvalues --- 0.35573 0.35713 0.35886 0.35943 0.36419
Eigenvalues --- 0.36628 0.39512 0.40652 0.41878 0.42487
Eigenvalues --- 0.44751 0.45489 0.46453 0.49514 0.54846
Eigenvalues --- 0.58303 0.60635 1.13457
En-DIIS/RFO-DIIS IScMMF= 0 using points: 38 37 36 35 34
RFO step: Lambda=-8.24443588D-07.
DidBck=F Rises=F RFO-DIIS coefs: 1.39925 0.07012 -0.56855 -0.35577 0.45495
Iteration 1 RMS(Cart)= 0.00997301 RMS(Int)= 0.00004634
Iteration 2 RMS(Cart)= 0.00009253 RMS(Int)= 0.00001105
Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00001105

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56496	0.00000	0.00001	0.00000	0.00001	2.56497
R2	2.62140	-0.00001	-0.00008	-0.00002	-0.00010	2.62130
R3	2.03394	0.00000	0.00001	0.00000	0.00001	2.03396
R4	2.62515	0.00000	0.00014	-0.00002	0.00012	2.62527
R5	2.03075	0.00000	-0.00002	0.00000	-0.00001	2.03073
R6	2.54370	-0.00002	-0.00025	0.00006	-0.00019	2.54351
R7	2.69876	0.00000	-0.00014	0.00003	-0.00012	2.69864
R8	2.52067	0.00003	0.00014	0.00002	0.00016	2.52082
R9	2.09383	-0.00006	0.00002	-0.00017	-0.00015	2.09369
R10	2.78524	0.00000	0.00009	-0.00005	0.00004	2.78528
R11	2.89627	0.00003	-0.00016	0.00019	0.00003	2.89629
R12	2.05988	0.00001	-0.00002	0.00000	-0.00002	2.05986
R13	2.06131	0.00000	-0.00007	0.00001	-0.00006	2.06125
R14	2.06951	0.00000	-0.00009	0.00003	-0.00006	2.06945
R15	2.07922	0.00002	-0.00018	0.00014	-0.00004	2.07918
R16	2.75580	-0.00002	0.00060	-0.00038	0.00022	2.75602
R17	4.24387	0.00006	0.00067	0.00042	0.00108	4.24495
R18	2.50650	-0.00001	0.00000	-0.00001	-0.00001	2.50649
R19	2.05707	0.00003	-0.00002	0.00009	0.00007	2.05714
R20	2.04351	0.00000	-0.00001	0.00000	-0.00001	2.04350
R21	2.04716	0.00001	0.00002	0.00001	0.00003	2.04719

R22	1.91470	-0.00002	-0.00007	-0.00002	-0.00010	1.91461
R23	1.92389	-0.00005	0.00009	-0.00011	-0.00002	1.92387
R24	4.12099	0.00005	-0.00116	-0.00111	-0.00227	4.11872
R25	2.76701	0.00001	0.00043	0.00006	0.00048	2.76748
R26	2.73357	0.00005	0.00085	0.00034	0.00120	2.73477
R27	2.05523	-0.00006	-0.00020	-0.00016	-0.00036	2.05486
R28	2.05212	-0.00003	-0.00008	-0.00009	-0.00017	2.05195
R29	2.74880	-0.00004	0.00009	-0.00079	-0.00069	2.74811
R30	2.05621	0.00003	0.00008	0.00001	0.00008	2.05630
R31	2.84176	0.00000	-0.00030	0.00012	-0.00018	2.84158
R32	2.06738	0.00002	0.00004	0.00007	0.00010	2.06749
R33	2.06790	-0.00001	0.00001	-0.00002	-0.00002	2.06789
R34	2.06536	0.00001	0.00002	0.00001	0.00003	2.06539
A1	1.87260	0.00001	0.00011	-0.00003	0.00008	1.87267
A2	2.27935	-0.00002	-0.00020	-0.00005	-0.00025	2.27910
A3	2.13118	0.00001	0.00009	0.00008	0.00017	2.13135
A4	1.86458	0.00001	-0.00012	0.00008	-0.00004	1.86454
A5	2.27599	0.00000	0.00022	-0.00005	0.00017	2.27616
A6	2.14254	-0.00001	-0.00009	-0.00004	-0.00013	2.14242
A7	1.89725	-0.00001	0.00006	-0.00009	-0.00003	1.89722
A8	2.25280	0.00003	0.00024	0.00006	0.00030	2.25310
A9	2.13308	-0.00002	-0.00030	0.00003	-0.00026	2.13281
A10	1.88978	0.00002	0.00005	0.00003	0.00009	1.88987
A11	2.14695	-0.00005	0.00050	-0.00044	0.00006	2.14701
A12	2.24624	0.00003	-0.00057	0.00038	-0.00019	2.24606
A13	1.90056	-0.00002	-0.00010	0.00000	-0.00010	1.90046
A14	2.20497	0.00001	-0.00003	0.00021	0.00018	2.20516
A15	2.17704	0.00001	0.00019	-0.00023	-0.00004	2.17699
A16	1.96095	-0.00008	-0.00048	-0.00036	-0.00084	1.96012
A17	1.87128	0.00004	0.00055	-0.00012	0.00043	1.87171
A18	1.89059	0.00000	-0.00014	0.00001	-0.00013	1.89046
A19	1.90653	0.00001	-0.00053	0.00034	-0.00019	1.90634
A20	1.92917	0.00005	0.00044	0.00035	0.00080	1.92997
A21	1.90375	-0.00002	0.00017	-0.00024	-0.00007	1.90368
A22	1.91635	0.00000	0.00056	-0.00024	0.00032	1.91667
A23	1.89199	-0.00004	-0.00004	-0.00033	-0.00037	1.89162
A24	1.88015	0.00006	0.00025	0.00034	0.00059	1.88074
A25	1.87622	0.00000	0.00004	-0.00008	-0.00004	1.87617
A26	1.90012	-0.00002	0.00004	-0.00006	-0.00003	1.90010
A27	1.99841	0.00000	-0.00079	0.00034	-0.00044	1.99797
A28	2.16132	0.00000	0.00021	-0.00010	0.00012	2.16144
A29	1.94581	-0.00001	-0.00001	-0.00002	-0.00003	1.94578
A30	2.17605	0.00001	-0.00020	0.00012	-0.00008	2.17597
A31	2.07411	-0.00001	-0.00001	-0.00008	-0.00008	2.07403

A32	2.16420	0.00002	0.00000	0.00006	0.00006	2.16425
A33	2.04487	0.00000	0.00001	0.00002	0.00003	2.04490
A34	1.93970	0.00004	-0.00010	0.00060	0.00052	1.94022
A35	1.91487	0.00000	0.00005	-0.00013	-0.00007	1.91479
A36	1.89020	0.00000	0.00023	0.00016	0.00039	1.89059
A37	2.08679	-0.00001	0.00093	-0.00047	0.00049	2.08728
A38	2.07174	-0.00007	-0.00237	-0.00057	-0.00297	2.06877
A39	1.99534	-0.00006	-0.00060	-0.00021	-0.00081	1.99453
A40	2.00263	0.00000	-0.00060	-0.00076	-0.00137	2.00126
A41	2.03474	0.00009	0.00169	0.00134	0.00303	2.03778
A42	2.01850	-0.00010	-0.00195	-0.00027	-0.00220	2.01630
A43	2.13681	0.00006	0.00085	-0.00004	0.00079	2.13760
A44	1.96045	0.00002	-0.00005	0.00062	0.00058	1.96103
A45	2.02875	-0.00005	-0.00045	0.00035	-0.00010	2.02865
A46	2.04374	0.00003	0.00095	-0.00031	0.00064	2.04438
A47	2.55789	0.00013	0.00343	0.00562	0.00906	2.56695
A48	2.49021	-0.00009	-0.00043	-0.00273	-0.00325	2.48695
A49	1.93357	0.00002	0.00034	-0.00002	0.00033	1.93390
A50	1.91722	-0.00001	0.00020	0.00005	0.00025	1.91747
A51	1.94215	0.00002	-0.00018	0.00009	-0.00009	1.94206
A52	1.87922	-0.00001	0.00004	-0.00003	0.00001	1.87923
A53	1.89471	-0.00002	-0.00029	-0.00008	-0.00037	1.89434
A54	1.89542	0.00000	-0.00012	-0.00002	-0.00014	1.89528
A55	3.49061	-0.00002	0.00084	-0.00046	0.00038	3.49100
A56	2.53168	0.00005	0.00013	0.00055	0.00069	2.53237
A57	2.98593	-0.00002	0.00047	0.00278	0.00326	2.98919
A58	3.11147	0.00000	0.00047	0.00281	0.00328	3.11475
D1	0.00293	0.00000	-0.00027	0.00001	-0.00026	0.00267
D2	-3.12582	0.00000	-0.00062	0.00035	-0.00028	-3.12610
D3	3.13332	-0.00001	-0.00043	-0.00037	-0.00080	3.13251
D4	0.00456	-0.00001	-0.00079	-0.00003	-0.00082	0.00374
D5	-0.00443	-0.00001	0.00039	-0.00044	-0.00005	-0.00448
D6	-3.10955	-0.00002	-0.00139	0.00009	-0.00130	-3.11085
D7	-3.13598	0.00000	0.00054	-0.00010	0.00044	-3.13553
D8	0.04209	0.00000	-0.00124	0.00043	-0.00081	0.04128
D9	-0.00047	0.00001	0.00005	0.00043	0.00048	0.00001
D10	-3.13093	-0.00001	-0.00022	-0.00031	-0.00053	-3.13146
D11	3.12950	0.00001	0.00038	0.00012	0.00050	3.12999
D12	-0.00096	-0.00001	0.00010	-0.00062	-0.00051	-0.00147
D13	-0.00229	-0.00001	0.00019	-0.00071	-0.00051	-0.00281
D14	-3.12325	-0.00001	0.00056	0.00038	0.00094	-3.12232
D15	3.12908	0.00000	0.00045	-0.00003	0.00042	3.12950
D16	0.00812	0.00000	0.00081	0.00105	0.00187	0.00999
D17	-0.04841	0.00000	0.00079	-0.00390	-0.00311	-0.05152

D18	3.09308	0.00001	0.00036	-0.00324	-0.00288	3.09020
D19	3.10565	-0.00001	0.00048	-0.00472	-0.00424	3.10141
D20	-0.03604	-0.00001	0.00005	-0.00406	-0.00401	-0.04006
D21	0.00414	0.00002	-0.00036	0.00071	0.00035	0.00449
D22	3.10998	0.00002	0.00138	0.00020	0.00159	3.11157
D23	3.12357	0.00001	-0.00073	-0.00047	-0.00120	3.12236
D24	-0.05378	0.00002	0.00101	-0.00098	0.00003	-0.05375
D25	1.33721	0.00001	0.00299	-0.00152	0.00146	1.33868
D26	-2.85115	0.00000	0.00241	-0.00140	0.00101	-2.85014
D27	-0.79892	-0.00001	0.00284	-0.00174	0.00110	-0.79782
D28	-1.76239	0.00000	0.00094	-0.00092	0.00002	-1.76237
D29	0.33244	-0.00001	0.00036	-0.00080	-0.00043	0.33200
D30	2.38467	-0.00001	0.00079	-0.00114	-0.00035	2.38432
D31	-1.10291	0.00002	-0.00039	-0.00150	-0.00189	-1.10479
D32	0.94204	0.00000	-0.00006	-0.00192	-0.00197	0.94007
D33	3.11348	0.00001	-0.00089	-0.00149	-0.00238	3.11110
D34	3.10603	0.00001	-0.00043	-0.00134	-0.00177	3.10426
D35	-1.13221	-0.00001	-0.00010	-0.00176	-0.00186	-1.13407
D36	1.03923	0.00000	-0.00093	-0.00133	-0.00226	1.03697
D37	1.01124	0.00000	-0.00058	-0.00148	-0.00206	1.00917
D38	3.05619	-0.00001	-0.00025	-0.00190	-0.00215	3.05404
D39	-1.05556	0.00000	-0.00108	-0.00147	-0.00256	-1.05811
D40	2.94027	0.00000	-0.00145	-0.00096	-0.00241	2.93786
D41	-1.25297	0.00002	-0.00119	-0.00047	-0.00165	-1.25462
D42	0.86308	-0.00002	-0.00228	-0.00084	-0.00312	0.85997
D43	2.95303	0.00000	-0.00202	-0.00034	-0.00235	2.95067
D44	-1.23706	-0.00001	-0.00183	-0.00092	-0.00275	-1.23981
D45	0.85288	0.00001	-0.00157	-0.00042	-0.00199	0.85089
D46	3.13860	0.00000	-0.00009	-0.00002	-0.00011	3.13850
D47	-0.00375	0.00000	-0.00001	-0.00021	-0.00022	-0.00398
D48	-0.00288	0.00000	0.00040	-0.00076	-0.00036	-0.00324
D49	3.13795	0.00000	0.00048	-0.00095	-0.00048	3.13747
D50	2.22743	-0.00006	-0.00675	-0.01080	-0.01754	2.20989
D51	-1.40039	0.00000	0.00292	-0.00153	0.00140	-1.39899
D52	-2.06982	-0.00001	-0.00678	-0.01059	-0.01739	-2.08721
D53	0.58555	0.00005	0.00289	-0.00133	0.00155	0.58710
D54	-2.71364	0.00000	-0.00027	0.00077	0.00049	-2.71315
D55	-0.01430	0.00000	-0.00046	-0.00084	-0.00131	-0.01560
D56	-0.02964	0.00007	0.00075	0.00185	0.00259	-0.02705
D57	2.66970	0.00006	0.00057	0.00023	0.00079	2.67049
D58	0.56062	-0.00006	0.00139	0.00118	0.00260	0.56322
D59	-1.85677	-0.00014	0.00008	0.00016	0.00028	-1.85649
D60	1.83685	-0.00004	-0.00388	-0.00775	-0.01160	1.82525
D61	-0.58413	-0.00005	-0.00483	-0.00842	-0.01323	-0.59736

D62	2.55748	0.00001	-0.00074	-0.00021	-0.00096	2.55652
D63	-1.65174	0.00001	-0.00035	-0.00023	-0.00058	-1.65232
D64	0.44783	0.00001	-0.00049	-0.00016	-0.00065	0.44718
D65	1.35376	-0.00001	-0.00107	-0.00073	-0.00179	1.35197
D66	-2.85545	-0.00001	-0.00068	-0.00074	-0.00142	-2.85687
D67	-0.75589	-0.00001	-0.00081	-0.00068	-0.00149	-0.75737
D68	-1.03234	-0.00002	-0.00161	-0.00184	-0.00345	-1.03579
D69	1.04163	-0.00002	-0.00122	-0.00186	-0.00308	1.03855
D70	3.14120	-0.00002	-0.00136	-0.00179	-0.00315	3.13805

Item	Value	Threshold	Converged?
Maximum Force	0.000138	0.000450	YES
RMS Force	0.000032	0.000300	YES
Maximum Displacement	0.046586	0.001800	NO
RMS Displacement	0.010028	0.001200	NO

Predicted change in Energy=-3.227581D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.645876	2.098551	-0.194150
2	6	0	-3.534524	1.115559	0.099731
3	7	0	-2.823230	-0.077637	0.117263
4	6	0	-1.532762	0.185052	-0.160799
5	7	0	-1.405784	1.498505	-0.356173
6	6	0	-0.134706	2.184999	-0.648564
7	6	0	0.452135	2.874190	0.588227
8	1	0	-2.787950	3.159123	-0.310229
9	1	0	-4.592238	1.164601	0.283143
10	1	0	0.565855	1.429746	-1.004900
11	1	0	-0.311875	2.910271	-1.443774
12	1	0	-0.227153	3.661380	0.931962
13	1	0	0.531614	2.130306	1.394998
14	35	0	0.136539	-2.663295	-0.283341
15	1	0	-0.756694	-0.603000	-0.225628
16	6	0	-3.293959	-1.403087	0.364145
17	6	0	-4.547903	-1.694025	0.683921
18	1	0	-2.496265	-2.135988	0.256586
19	1	0	-4.817066	-2.727975	0.850851
20	1	0	-5.332702	-0.955054	0.791688
21	7	0	1.719737	3.481689	0.199471
22	1	0	2.060622	4.108797	0.918525

23	1	0	2.417460	2.755267	0.051276
24	6	0	3.344841	-0.389158	-1.128712
25	6	0	3.262006	-0.577545	0.321246
26	8	0	2.734952	0.627614	-0.298929
27	1	0	4.289181	-0.091990	-1.578515
28	1	0	2.650981	-0.932776	-1.762826
29	1	0	2.474106	-1.245731	0.663011
30	6	0	4.447322	-0.394474	1.228230
31	1	0	4.136050	0.002118	2.199213
32	1	0	4.933642	-1.358906	1.403758
33	1	0	5.178758	0.290241	0.791512

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357326	0.000000			
3	N	2.205499	1.389232	0.000000		
4	C	2.213959	2.222785	1.345968	0.000000	
5	N	1.387132	2.210436	2.171984	1.333962	0.000000
6	C	2.553418	3.641760	3.596411	2.488426	1.473909
7	C	3.288070	4.384616	4.434310	3.425248	2.497251
8	H	1.076324	2.213954	3.265059	3.231552	2.161052
9	H	2.210971	1.074618	2.167962	3.242991	3.267063
10	H	3.379325	4.258173	3.875223	2.581853	2.076762
11	H	2.769118	3.998608	4.203729	3.250140	2.091076
12	H	3.092052	4.255880	4.624240	3.870866	2.779657
13	H	3.552864	4.386446	4.214569	3.235146	2.686873
14	Br	5.515884	5.282348	3.950487	3.303735	4.438992
15	H	3.296723	3.282628	2.159664	1.107930	2.203335
16	C	3.604605	2.543888	1.428060	2.428902	3.536000
17	C	4.332707	3.043350	2.430702	3.651788	4.598582
18	H	4.261087	3.416891	2.088809	2.547503	3.843717
19	H	5.394575	4.120904	3.396737	4.505087	5.563890
20	H	4.185141	2.828372	2.742656	4.080026	4.770557
21	N	4.596367	5.763313	5.771837	4.645036	3.743080
22	H	5.237391	6.398090	6.482303	5.428916	4.522660
23	H	5.111642	6.173905	5.957728	4.717545	4.045078
24	C	6.553686	7.148350	6.300364	5.005755	5.169964
25	C	6.506166	7.007745	6.109141	4.878906	5.153363
26	O	5.579243	6.301060	5.618183	4.292822	4.231717
27	H	7.403375	8.092283	7.311789	5.998474	6.037916
28	H	6.301301	6.776819	5.850896	4.617330	4.934283
29	H	6.175206	6.480480	5.451977	4.333681	4.860362
30	C	7.651915	8.201438	7.361763	6.166576	6.352366

31	H	7.491178	8.030273	7.264465	6.143171	6.283398
32	H	8.482713	8.918144	7.966541	6.829789	7.172899
33	H	8.091132	8.779579	8.038766	6.779562	6.792149

		6	7	8	9	10
6	C	0.000000				
7	C	1.532651	0.000000			
8	H	2.846594	3.374398	0.000000		
9	H	4.666785	5.334929	2.754208	0.000000	
10	H	1.090031	2.153463	3.836838	5.323090	0.000000
11	H	1.090765	2.171184	2.734556	4.934684	1.776225
12	H	2.164789	1.095105	2.890152	5.070388	3.059491
13	H	2.150145	1.100255	3.871146	5.331291	2.500293
14	Br	4.869591	5.614533	6.515667	6.110240	4.178271
15	H	2.887678	3.770209	4.276299	4.253782	2.547246
16	C	4.886801	5.690214	4.639460	2.878387	4.979698
17	C	6.024837	6.773339	5.257263	2.886924	6.225801
18	H	5.006714	5.822794	5.333344	3.909948	4.866456
19	H	6.950543	7.695304	6.334299	3.940176	7.050269
20	H	6.241268	6.940378	4.961495	2.302138	6.611201
21	N	2.416512	1.458424	4.547866	6.724353	2.644319
22	H	3.313040	2.054405	5.091205	7.302913	3.620939
23	H	2.707126	2.040823	5.233553	7.191651	2.510169
24	C	4.354775	4.686690	7.132414	8.210037	3.323628
25	C	4.484399	4.458826	7.138867	8.045226	3.613462
26	O	3.283691	3.323463	6.075452	7.369862	2.418014
27	H	5.061646	5.311866	7.890758	9.161025	4.062988
28	H	4.326910	4.985516	6.959573	7.813399	3.240944
29	H	4.505112	4.589958	6.931030	7.475775	3.685313
30	C	5.583101	5.201470	8.206343	9.221581	4.835332
31	H	5.578006	4.941184	8.012850	9.011420	5.005072
32	H	6.516090	6.218368	9.108969	9.917976	5.714523
33	H	5.822098	5.390648	8.538897	9.823203	5.079807

		11	12	13	14	15
11	H	0.000000				
12	H	2.493084	0.000000			
13	H	3.062425	1.770401	0.000000		
14	Br	5.710720	6.450640	5.094263	0.000000	
15	H	3.744972	4.450322	3.428867	2.246333	0.000000
16	C	5.546752	5.947818	5.308722	3.711560	2.725011
17	C	6.608371	6.885548	6.397861	4.880480	4.048566
18	H	5.755650	6.262146	5.353998	2.738838	2.368267
19	H	7.573101	7.867511	7.246196	5.082202	4.707541
20	H	6.719131	6.884603	6.653843	5.829784	4.700928
21	N	2.674738	2.087873	2.160360	6.363997	4.795634

22	H	3.556075	2.331154	2.545450	7.141975	5.607797
23	H	3.115842	2.930977	2.398454	5.888580	4.629242
24	C	4.935288	5.780344	4.542142	4.022381	4.205220
25	C	5.296488	5.524101	3.992548	3.805840	4.055819
26	O	3.975469	4.415077	3.159457	4.193098	3.702887
27	H	5.495584	6.386514	5.282015	5.053070	5.249027
28	H	4.863057	6.054074	4.883241	3.392048	3.752863
29	H	5.428866	5.607930	3.963169	2.892972	3.411869
30	C	6.380510	6.195841	4.662091	5.100514	5.407307
31	H	6.443039	5.833838	4.262382	5.409583	5.494084
32	H	7.338239	7.215239	5.617163	5.249755	5.967094
33	H	6.481367	6.372455	5.034479	5.941604	6.087861

		16	17	18	19	20
16	C	0.000000				
17	C	1.326378	0.000000			
18	H	1.088589	2.141767	0.000000		
19	H	2.076551	1.081373	2.467735	0.000000	
20	H	2.130728	1.083329	3.118704	1.847331	0.000000
21	N	7.001807	8.142851	7.023975	9.039580	8.352982
22	H	7.704527	8.797749	7.758912	9.697866	8.962138
23	H	7.071782	8.289313	6.936225	9.112827	8.624366
24	C	6.879704	8.202666	6.252118	8.718110	8.905499
25	C	6.607877	7.897642	5.965787	8.377125	8.615848
26	O	6.396185	7.706879	5.942367	8.343557	8.293451
27	H	7.937059	9.261705	7.320369	9.786417	9.947028
28	H	6.331470	7.641336	5.658612	8.113308	8.382436
29	H	5.777946	7.036336	5.065800	7.442682	7.813278
30	C	7.854386	9.104899	7.224290	9.561199	9.805799
31	H	7.781202	8.976862	7.234148	9.456731	9.620529
32	H	8.293139	9.514734	7.558001	9.861864	10.292499
33	H	8.650835	9.927580	8.067138	10.441726	10.584968

		21	22	23	24	25
21	N	0.000000				
22	H	1.013166	0.000000			
23	H	1.018070	1.646663	0.000000		
24	C	4.403236	5.106074	3.484223	0.000000	
25	C	4.344053	4.874614	3.448736	1.464490	0.000000
26	O	3.069985	3.749073	2.179530	1.447179	1.454239
27	H	4.747047	5.371061	3.777093	1.087386	2.213582
28	H	4.919891	5.740699	4.116693	1.085847	2.200659
29	H	4.809620	5.376544	4.047890	2.168448	1.088146
30	C	4.850020	5.106045	3.927649	2.602051	1.503699
31	H	4.684543	4.776229	3.891916	3.442992	2.150981
32	H	5.933872	6.195600	5.008672	3.142945	2.139328

33	H	4.743488	4.931559	3.774794	2.740821	2.155955
		26	27	28	29	30
26	O	0.000000				
27	H	2.137942	0.000000			
28	H	2.141229	1.850565	0.000000		
29	H	2.121978	3.106453	2.452328	0.000000	
30	C	2.511790	2.827423	3.530301	2.222092	0.000000
31	H	2.931729	3.782001	4.333268	2.584396	1.094067
32	H	3.417549	3.303688	3.926752	2.571153	1.094279
33	H	2.697234	2.560171	3.796060	3.113016	1.092957
		31	32	33		
31	H	0.000000				
32	H	1.766716	0.000000			
33	H	1.775352	1.776123	0.000000		

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.355614	2.465689	-0.263811
2	6	0	-3.338344	1.583452	0.049610
3	7	0	-2.748303	0.326959	0.104774
4	6	0	-1.436843	0.453542	-0.170325
5	7	0	-1.179958	1.742220	-0.400049
6	6	0	0.154081	2.291901	-0.701045
7	6	0	0.799841	2.953814	0.521200
8	1	0	-2.391805	3.531489	-0.409527
9	1	0	-4.386967	1.741437	0.223485
10	1	0	0.778507	1.461801	-1.031490
11	1	0	0.053293	3.008882	-1.516857
12	1	0	0.199796	3.813242	0.838352
13	1	0	0.801522	2.228256	1.348318
14	35	0	-0.056031	-2.547615	-0.203191
15	1	0	-0.741973	-0.408579	-0.207912
16	6	0	-3.348700	-0.938387	0.383662
17	6	0	-4.626811	-1.095516	0.701502
18	1	0	-2.626656	-1.748953	0.302042
19	1	0	-4.997474	-2.092941	0.894164

20	1	0	-5.335425	-0.280175	0.783265
21	7	0	2.123111	3.422598	0.125981
22	1	0	2.520585	4.032689	0.830473
23	1	0	2.746515	2.627198	0.002795
24	6	0	3.365122	-0.624602	-1.084831
25	6	0	3.256855	-0.763853	0.368998
26	8	0	2.854350	0.469777	-0.287476
27	1	0	4.336407	-0.434378	-1.535197
28	1	0	2.624209	-1.114545	-1.709384
29	1	0	2.405192	-1.341533	0.722574
30	6	0	4.449895	-0.673429	1.279816
31	1	0	4.174403	-0.221486	2.237330
32	1	0	4.837834	-1.675848	1.485015
33	1	0	5.247476	-0.076366	0.830444

Rotational constants (GHZ): 0.4208092 0.2922874 0.1828021

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1312.6906816393 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 3.64D-06 NBF= 482

NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000535 -0.000301 -0.000378 Ang= 0.08 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0

NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3205.64836636 A.U. after 10 cycles

NFock= 10 Conv=0.68D-08 -V/T= 2.0018

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000008713	0.000020730	0.000042790
2	6	0.000016567	-0.000042977	-0.000019474
3	7	-0.000022401	0.000032259	0.000043634
4	6	0.000100191	0.000053872	-0.000101344
5	7	-0.000001392	-0.000084487	-0.000043675
6	6	-0.000001043	0.000021059	0.000074363
7	6	0.000202089	0.000116572	-0.000009244
8	1	0.000004849	-0.000001513	0.000000531
9	1	-0.000006700	0.000008072	-0.000011513
10	1	-0.000017737	-0.000027837	-0.000008034
11	1	0.000020668	0.000003413	-0.000018861
12	1	-0.000021702	-0.000001080	-0.000009393
13	1	-0.000030571	-0.000030428	0.000018441
14	35	-0.000007427	-0.000023307	0.000005660
15	1	-0.000058068	0.000047395	0.000020737
16	6	-0.000021859	-0.000049323	0.000008651
17	6	-0.000003263	0.000026984	-0.000001705
18	1	0.000007866	0.000000780	0.000004337
19	1	-0.000002469	-0.000002101	-0.000004160
20	1	0.000002427	-0.000001665	0.000002107
21	7	-0.000122226	-0.000105016	0.000020738
22	1	0.000005498	0.000003872	-0.000017698
23	1	-0.000035816	0.000065477	0.000111550
24	6	-0.000052682	-0.000036239	0.000235393
25	6	-0.000060894	0.000071255	-0.000157611
26	8	-0.000011285	-0.000044552	-0.000202168
27	1	0.000011629	-0.000020973	-0.000021629
28	1	0.000030877	0.000001420	-0.000046820
29	1	0.000055646	0.000012445	0.000064773

30	6	0.000051381	0.000000624	0.000017004
31	1	-0.000007841	0.000000558	-0.000002115
32	1	-0.000012893	-0.000006207	0.000007376
33	1	-0.000002705	-0.000009082	-0.000002640

Cartesian Forces: Max 0.000235393 RMS 0.000056175

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000154856 RMS 0.000033387
Search for a local minimum.
Step number 39 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 30 31 32 33 34
35 36 37 38 39
DE= -3.06D-06 DEPred=-3.23D-06 R= 9.47D-01
TightC=F SS= 1.41D+00 RLast= 3.58D-02 DXNew= 1.7446D+00 1.0738D-01
Trust test= 9.47D-01 RLast= 3.58D-02 DXMaxT set to 1.04D+00
ITU= 1 1 1 1 1 1 1 1 1 1 1 1 1 0 0 -1 1 -1 1 1
ITU= 1 1 1 1 1 1 1 0 -1 -1 1 1 1 -1 1 0 0 -1 0

Eigenvalues ---	0.00060	0.00097	0.00221	0.00478	0.00589
Eigenvalues ---	0.00661	0.00742	0.01053	0.01331	0.01635
Eigenvalues ---	0.01901	0.02070	0.02207	0.02372	0.02385
Eigenvalues ---	0.02597	0.02711	0.02914	0.03066	0.03101
Eigenvalues ---	0.03315	0.03547	0.03691	0.03942	0.04011
Eigenvalues ---	0.04209	0.04449	0.04561	0.05383	0.05488
Eigenvalues ---	0.05739	0.05753	0.05905	0.07786	0.08662
Eigenvalues ---	0.08933	0.09556	0.10804	0.11024	0.12323
Eigenvalues ---	0.12657	0.13194	0.13584	0.15749	0.15952
Eigenvalues ---	0.15996	0.16002	0.16008	0.16013	0.16091
Eigenvalues ---	0.16190	0.18551	0.21289	0.21987	0.22156
Eigenvalues ---	0.23071	0.23459	0.25775	0.26784	0.27853
Eigenvalues ---	0.29000	0.29969	0.30208	0.32048	0.32588
Eigenvalues ---	0.33701	0.34288	0.34340	0.34368	0.34549
Eigenvalues ---	0.34688	0.34758	0.35077	0.35169	0.35318
Eigenvalues ---	0.35567	0.35719	0.35868	0.35953	0.36422
Eigenvalues ---	0.36627	0.39533	0.41606	0.42078	0.42670
Eigenvalues ---	0.44563	0.45472	0.46470	0.49509	0.54865
Eigenvalues ---	0.58526	0.60638	1.14573		

En-DIIS/RFO-DIIS IScMMF= 0 using points: 39 38 37 36 35

RFO step: Lambda=-4.92627711D-07.

DidBck=F Rises=F RFO-DIIS coefs: 1.24121 -0.53385 0.38162 -0.48184 0.39287

Iteration 1 RMS(Cart)= 0.00324786 RMS(Int)= 0.00001389

Iteration 2 RMS(Cart)= 0.00001410 RMS(Int)= 0.00001291

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001291

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56497	-0.00001	-0.00001	0.00002	0.00001	2.56498
R2	2.62130	0.00001	-0.00001	0.00001	0.00000	2.62130
R3	2.03396	0.00000	0.00000	-0.00001	-0.00001	2.03395
R4	2.62527	-0.00004	0.00000	0.00000	-0.00001	2.62526
R5	2.03073	0.00001	0.00000	0.00001	0.00001	2.03074
R6	2.54351	0.00004	0.00001	0.00004	0.00005	2.54356
R7	2.69864	0.00004	0.00001	-0.00001	0.00000	2.69865
R8	2.52082	-0.00004	0.00001	-0.00010	-0.00009	2.52074
R9	2.09369	-0.00006	-0.00012	-0.00006	-0.00018	2.09350
R10	2.78528	0.00000	-0.00004	0.00000	-0.00004	2.78525
R11	2.89629	0.00002	0.00002	0.00006	0.00007	2.89636
R12	2.05986	0.00001	0.00000	-0.00003	-0.00003	2.05983
R13	2.06125	0.00001	0.00001	0.00001	0.00002	2.06126
R14	2.06945	0.00001	0.00000	0.00002	0.00002	2.06947
R15	2.07918	0.00003	0.00005	0.00005	0.00009	2.07927
R16	2.75602	-0.00015	-0.00013	-0.00027	-0.00040	2.75562
R17	4.24495	0.00002	0.00105	0.00027	0.00131	4.24627
R18	2.50649	0.00000	0.00000	0.00000	0.00000	2.50649
R19	2.05714	0.00001	0.00006	0.00000	0.00006	2.05720
R20	2.04350	0.00000	0.00000	0.00001	0.00001	2.04351
R21	2.04719	0.00000	0.00001	0.00000	0.00001	2.04720
R22	1.91461	-0.00001	-0.00004	-0.00002	-0.00006	1.91454
R23	1.92387	-0.00005	-0.00004	-0.00006	-0.00009	1.92378
R24	4.11872	0.00003	0.00147	0.00009	0.00156	4.12028
R25	2.76748	-0.00010	-0.00026	0.00005	-0.00018	2.76730
R26	2.73477	-0.00002	0.00015	0.00020	0.00034	2.73511
R27	2.05486	0.00001	-0.00009	0.00002	-0.00007	2.05479
R28	2.05195	0.00001	-0.00003	0.00002	-0.00001	2.05195
R29	2.74811	-0.00003	0.00004	-0.00028	-0.00025	2.74786
R30	2.05630	-0.00003	0.00005	-0.00007	-0.00003	2.05627
R31	2.84158	0.00003	0.00002	0.00004	0.00006	2.84163
R32	2.06749	0.00000	0.00002	0.00001	0.00003	2.06751
R33	2.06789	0.00000	0.00000	-0.00002	-0.00002	2.06787
R34	2.06539	-0.00001	0.00001	-0.00003	-0.00002	2.06537
A1	1.87267	0.00001	0.00002	-0.00001	0.00000	1.87268

A2	2.27910	0.00000	-0.00005	-0.00003	-0.00008	2.27902
A3	2.13135	-0.00001	0.00003	0.00004	0.00007	2.13143
A4	1.86454	0.00000	0.00001	0.00000	0.00001	1.86455
A5	2.27616	-0.00001	0.00000	0.00006	0.00006	2.27622
A6	2.14242	0.00001	-0.00001	-0.00006	-0.00007	2.14235
A7	1.89722	0.00000	-0.00003	-0.00003	-0.00006	1.89716
A8	2.25310	-0.00002	0.00005	-0.00006	-0.00001	2.25309
A9	2.13281	0.00002	-0.00002	0.00009	0.00007	2.13289
A10	1.88987	0.00000	0.00003	0.00003	0.00006	1.88993
A11	2.14701	-0.00007	-0.00018	-0.00011	-0.00029	2.14672
A12	2.24606	0.00007	0.00015	0.00008	0.00023	2.24629
A13	1.90046	0.00000	-0.00003	0.00001	-0.00002	1.90044
A14	2.20516	-0.00004	0.00000	0.00017	0.00017	2.20533
A15	2.17699	0.00005	0.00003	-0.00017	-0.00014	2.17685
A16	1.96012	0.00009	-0.00026	0.00001	-0.00025	1.95987
A17	1.87171	-0.00004	0.00007	-0.00019	-0.00013	1.87158
A18	1.89046	-0.00003	0.00006	0.00015	0.00021	1.89067
A19	1.90634	0.00001	0.00003	0.00005	0.00008	1.90642
A20	1.92997	-0.00004	0.00014	0.00005	0.00019	1.93016
A21	1.90368	0.00001	-0.00004	-0.00008	-0.00012	1.90356
A22	1.91667	0.00001	-0.00002	-0.00010	-0.00012	1.91655
A23	1.89162	0.00000	-0.00019	-0.00007	-0.00026	1.89136
A24	1.88074	-0.00009	0.00021	0.00000	0.00020	1.88094
A25	1.87617	-0.00001	-0.00005	-0.00006	-0.00011	1.87606
A26	1.90010	0.00001	-0.00004	0.00011	0.00007	1.90016
A27	1.99797	0.00007	0.00009	0.00012	0.00021	1.99817
A28	2.16144	-0.00003	-0.00002	-0.00005	-0.00007	2.16136
A29	1.94578	0.00001	0.00000	0.00003	0.00003	1.94581
A30	2.17597	0.00002	0.00002	0.00002	0.00004	2.17601
A31	2.07403	0.00000	-0.00006	0.00000	-0.00006	2.07397
A32	2.16425	0.00000	0.00007	-0.00003	0.00004	2.16429
A33	2.04490	0.00000	-0.00001	0.00003	0.00002	2.04493
A34	1.94022	-0.00001	0.00028	0.00013	0.00043	1.94065
A35	1.91479	0.00005	0.00014	0.00022	0.00037	1.91516
A36	1.89059	0.00000	0.00012	0.00024	0.00035	1.89094
A37	2.08728	-0.00007	0.00016	-0.00035	-0.00021	2.08707
A38	2.06877	0.00010	-0.00038	0.00005	-0.00031	2.06846
A39	1.99453	0.00000	-0.00014	-0.00014	-0.00029	1.99424
A40	2.00126	0.00002	-0.00028	0.00003	-0.00024	2.00102
A41	2.03778	-0.00004	0.00034	0.00032	0.00066	2.03844
A42	2.01630	0.00003	-0.00030	0.00052	0.00019	2.01648
A43	2.13760	0.00000	0.00013	0.00038	0.00054	2.13814
A44	1.96103	0.00001	0.00023	0.00029	0.00052	1.96155
A45	2.02865	0.00001	-0.00015	0.00010	-0.00004	2.02861

A46	2.04438	-0.00004	0.00006	-0.00088	-0.00082	2.04356
A47	2.56695	0.00011	-0.00046	0.00370	0.00323	2.57018
A48	2.48695	-0.00010	-0.00116	-0.00393	-0.00497	2.48198
A49	1.93390	-0.00001	-0.00002	0.00003	0.00000	1.93390
A50	1.91747	-0.00001	0.00001	-0.00006	-0.00005	1.91742
A51	1.94206	0.00000	0.00011	-0.00012	-0.00001	1.94205
A52	1.87923	0.00000	-0.00006	-0.00004	-0.00010	1.87913
A53	1.89434	0.00001	-0.00004	0.00011	0.00007	1.89441
A54	1.89528	0.00001	-0.00001	0.00008	0.00008	1.89536
A55	3.49100	0.00005	0.00002	0.00075	0.00077	3.49177
A56	2.53237	-0.00002	-0.00070	-0.00095	-0.00166	2.53071
A57	2.98919	-0.00003	-0.00111	0.00171	0.00059	2.98978
A58	3.11475	-0.00006	-0.00111	-0.00095	-0.00207	3.11268
D1	0.00267	0.00001	-0.00007	0.00025	0.00018	0.00285
D2	-3.12610	0.00001	-0.00014	0.00019	0.00006	-3.12604
D3	3.13251	0.00001	-0.00020	0.00012	-0.00008	3.13243
D4	0.00374	0.00000	-0.00026	0.00006	-0.00020	0.00354
D5	-0.00448	-0.00001	-0.00013	-0.00011	-0.00024	-0.00472
D6	-3.11085	0.00000	-0.00023	-0.00032	-0.00055	-3.11140
D7	-3.13553	0.00000	-0.00002	0.00001	-0.00001	-3.13554
D8	0.04128	0.00000	-0.00012	-0.00020	-0.00032	0.04096
D9	0.00001	-0.00002	0.00025	-0.00030	-0.00005	-0.00005
D10	-3.13146	-0.00001	-0.00022	-0.00033	-0.00055	-3.13201
D11	3.12999	-0.00001	0.00031	-0.00025	0.00005	3.13005
D12	-0.00147	0.00000	-0.00016	-0.00028	-0.00044	-0.00192
D13	-0.00281	0.00001	-0.00033	0.00024	-0.00010	-0.00290
D14	-3.12232	0.00000	-0.00040	0.00030	-0.00011	-3.12242
D15	3.12950	0.00001	0.00010	0.00026	0.00036	3.12986
D16	0.00999	-0.00001	0.00003	0.00032	0.00035	0.01034
D17	-0.05152	0.00000	0.00046	-0.00213	-0.00167	-0.05319
D18	3.09020	0.00000	0.00061	-0.00190	-0.00129	3.08891
D19	3.10141	0.00001	-0.00007	-0.00216	-0.00223	3.09918
D20	-0.04006	0.00001	0.00009	-0.00193	-0.00185	-0.04190
D21	0.00449	-0.00001	0.00029	-0.00008	0.00021	0.00470
D22	3.11157	-0.00001	0.00038	0.00013	0.00052	3.11209
D23	3.12236	0.00001	0.00036	-0.00015	0.00021	3.12257
D24	-0.05375	0.00001	0.00046	0.00007	0.00052	-0.05323
D25	1.33868	-0.00002	-0.00122	0.00037	-0.00085	1.33782
D26	-2.85014	0.00001	-0.00129	0.00031	-0.00098	-2.85112
D27	-0.79782	-0.00002	-0.00128	0.00020	-0.00108	-0.79890
D28	-1.76237	-0.00002	-0.00134	0.00012	-0.00121	-1.76358
D29	0.33200	0.00001	-0.00141	0.00007	-0.00134	0.33066
D30	2.38432	-0.00001	-0.00139	-0.00005	-0.00144	2.38288
D31	-1.10479	0.00001	-0.00007	-0.00041	-0.00048	-1.10527

D32	0.94007	0.00000	-0.00025	-0.00058	-0.00083	0.93924
D33	3.11110	0.00004	-0.00013	-0.00048	-0.00061	3.11049
D34	3.10426	0.00000	-0.00002	-0.00021	-0.00022	3.10403
D35	-1.13407	-0.00001	-0.00020	-0.00038	-0.00057	-1.13464
D36	1.03697	0.00003	-0.00007	-0.00028	-0.00035	1.03661
D37	1.00917	0.00001	-0.00007	-0.00017	-0.00024	1.00893
D38	3.05404	0.00001	-0.00025	-0.00034	-0.00059	3.05345
D39	-1.05811	0.00004	-0.00013	-0.00025	-0.00037	-1.05849
D40	2.93786	-0.00001	-0.00008	0.00004	-0.00004	2.93782
D41	-1.25462	0.00001	0.00034	0.00056	0.00090	-1.25372
D42	0.85997	0.00002	-0.00015	0.00010	-0.00005	0.85991
D43	2.95067	0.00004	0.00026	0.00063	0.00089	2.95156
D44	-1.23981	-0.00002	-0.00011	0.00002	-0.00009	-1.23991
D45	0.85089	0.00000	0.00030	0.00055	0.00085	0.85175
D46	3.13850	0.00000	0.00009	-0.00002	0.00007	3.13857
D47	-0.00398	0.00000	0.00011	-0.00023	-0.00012	-0.00410
D48	-0.00324	0.00000	-0.00008	-0.00028	-0.00036	-0.00360
D49	3.13747	0.00000	-0.00006	-0.00049	-0.00055	3.13692
D50	2.20989	-0.00002	0.00392	0.00014	0.00409	2.21398
D51	-1.39899	-0.00006	-0.00094	0.00040	-0.00055	-1.39954
D52	-2.08721	0.00004	0.00444	0.00039	0.00484	-2.08237
D53	0.58710	-0.00001	-0.00043	0.00065	0.00020	0.58730
D54	-2.71315	0.00004	0.00024	0.00005	0.00029	-2.71286
D55	-0.01560	0.00002	-0.00004	-0.00012	-0.00015	-0.01575
D56	-0.02705	0.00002	0.00061	0.00020	0.00082	-0.02623
D57	2.67049	-0.00001	0.00034	0.00004	0.00038	2.67088
D58	0.56322	-0.00007	-0.00328	-0.00381	-0.00712	0.55611
D59	-1.85649	-0.00003	-0.00334	-0.00420	-0.00756	-1.86405
D60	1.82525	-0.00010	0.00269	-0.00370	-0.00105	1.82420
D61	-0.59736	-0.00006	0.00250	-0.00274	-0.00029	-0.59765
D62	2.55652	0.00001	-0.00040	-0.00046	-0.00085	2.55566
D63	-1.65232	0.00000	-0.00048	-0.00052	-0.00100	-1.65333
D64	0.44718	0.00001	-0.00041	-0.00054	-0.00094	0.44623
D65	1.35197	-0.00002	-0.00049	-0.00078	-0.00127	1.35070
D66	-2.85687	-0.00002	-0.00057	-0.00084	-0.00142	-2.85829
D67	-0.75737	-0.00002	-0.00050	-0.00086	-0.00136	-0.75873
D68	-1.03579	0.00000	-0.00076	-0.00029	-0.00105	-1.03684
D69	1.03855	0.00000	-0.00085	-0.00036	-0.00120	1.03735
D70	3.13805	0.00000	-0.00077	-0.00037	-0.00114	3.13691

Item	Value	Threshold	Converged?
Maximum Force	0.000155	0.000450	YES
RMS Force	0.000033	0.000300	YES
Maximum Displacement	0.012834	0.001800	NO
RMS Displacement	0.003255	0.001200	NO

Predicted change in Energy=-1.065494D-06
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.644190	2.098476	-0.192704
2	6	0	-3.532681	1.115064	0.100267
3	7	0	-2.821237	-0.078056	0.116559
4	6	0	-1.530831	0.185144	-0.161420
5	7	0	-1.404069	1.498741	-0.355650
6	6	0	-0.133133	2.185403	-0.648175
7	6	0	0.453349	2.874769	0.588738
8	1	0	-2.786517	3.159121	-0.307761
9	1	0	-4.590377	1.163727	0.283915
10	1	0	0.567482	1.430112	-1.004280
11	1	0	-0.310177	2.910436	-1.443644
12	1	0	-0.226039	3.662116	0.931954
13	1	0	0.531953	2.130890	1.395667
14	35	0	0.137188	-2.664311	-0.287651
15	1	0	-0.754897	-0.602847	-0.226948
16	6	0	-3.291686	-1.403735	0.362759
17	6	0	-4.545032	-1.694760	0.684802
18	1	0	-2.494261	-2.136646	0.252978
19	1	0	-4.814028	-2.728865	0.851062
20	1	0	-5.329422	-0.955742	0.795248
21	7	0	1.721140	3.481844	0.200730
22	1	0	2.062034	4.109093	0.919610
23	1	0	2.418785	2.755492	0.052170
24	6	0	3.342475	-0.392051	-1.129952
25	6	0	3.257985	-0.576629	0.320303
26	8	0	2.732299	0.627257	-0.303184
27	1	0	4.287466	-0.096344	-1.579261
28	1	0	2.648689	-0.936861	-1.763117
29	1	0	2.469754	-1.243871	0.663104
30	6	0	4.441953	-0.391918	1.228764
31	1	0	4.129422	0.008041	2.197975
32	1	0	4.926850	-1.356326	1.408242
33	1	0	5.174867	0.290602	0.791114

Distance matrix (angstroms):

	1	2	3	4	5

1	C	0.000000				
2	C	1.357330	0.000000			
3	N	2.205511	1.389228	0.000000		
4	C	2.213908	2.222755	1.345992	0.000000	
5	N	1.387132	2.210444	2.172012	1.333916	0.000000
6	C	2.553512	3.641802	3.596383	2.488278	1.473891
7	C	3.287557	4.384472	4.434528	3.425461	2.497062
8	H	1.076319	2.213914	3.265053	3.231517	2.161092
9	H	2.211009	1.074623	2.167923	3.242957	3.267084
10	H	3.379379	4.258006	3.874825	2.581332	2.076642
11	H	2.769793	3.998944	4.203658	3.249817	2.091222
12	H	3.091485	4.255944	4.624804	3.871341	2.779545
13	H	3.551318	4.385341	4.214196	3.235046	2.686058
14	Br	5.516269	5.282244	3.950238	3.304182	4.439718
15	H	3.296626	3.282434	2.159435	1.107834	2.203329
16	C	3.604618	2.543881	1.428062	2.428973	3.536040
17	C	4.332649	3.043295	2.430658	3.651786	4.598547
18	H	4.261146	3.416908	2.088855	2.547672	3.843825
19	H	5.394521	4.120842	3.396689	4.505103	5.563869
20	H	4.185064	2.828342	2.742616	4.079967	4.770478
21	N	4.596151	5.763192	5.771756	4.644857	3.742885
22	H	5.237210	6.398154	6.482549	5.429059	4.522620
23	H	5.111297	6.173594	5.957430	4.717178	4.044743
24	C	6.551436	7.145110	6.296326	5.002031	5.167621
25	C	6.500387	7.001670	6.103034	4.872895	5.147700
26	O	5.575243	6.296881	5.613859	4.288337	4.227502
27	H	7.401867	8.089687	7.308201	5.995172	6.036148
28	H	6.300321	6.774358	5.847291	4.614403	4.933352
29	H	6.168963	6.473838	5.445403	4.327424	4.854511
30	C	7.644348	8.193857	7.354552	6.159526	6.345150
31	H	7.481116	8.020830	7.256127	6.134865	6.273971
32	H	8.474629	8.909671	7.958346	6.822141	7.165421
33	H	8.085417	8.773734	8.032970	6.773834	6.786535

		6	7	8	9	10
6	C	0.000000				
7	C	1.532690	0.000000			
8	H	2.846833	3.373617	0.000000		
9	H	4.666866	5.334768	2.754194	0.000000	
10	H	1.090016	2.153547	3.837176	5.322961	0.000000
11	H	1.090774	2.171364	2.735752	4.935135	1.776143
12	H	2.164744	1.095116	2.888935	5.070438	3.059496
13	H	2.150024	1.100304	3.869259	5.330071	2.500420
14	Br	4.870603	5.616887	6.516197	6.109864	4.178877
15	H	2.887622	3.770811	4.276261	4.253548	2.546734

16	C	4.886753	5.690514	4.639445	2.878312	4.979223
17	C	6.024728	6.773007	5.257158	2.886817	6.225401
18	H	5.006707	5.823695	5.333385	3.909875	4.865874
19	H	6.950433	7.695114	6.334197	3.940045	7.049825
20	H	6.241129	6.939445	4.961360	2.302130	6.610906
21	N	2.416552	1.458213	4.547712	6.724272	2.644349
22	H	3.313199	2.054483	5.090907	7.303003	3.621046
23	H	2.706985	2.040851	5.233320	7.191368	2.509988
24	C	4.353760	4.687543	7.131014	8.206680	3.322147
25	C	4.479559	4.455355	7.133463	8.039089	3.608371
26	O	3.279868	3.322717	6.071877	7.365736	2.412995
27	H	5.061125	5.313021	7.890247	9.158346	4.061891
28	H	4.327835	4.987912	6.959640	7.810690	3.241885
29	H	4.500487	4.586351	6.925121	7.468986	3.680896
30	C	5.576459	5.195175	8.198876	9.213889	4.828852
31	H	5.568738	4.931662	8.002389	9.001896	4.996413
32	H	6.509695	6.211761	9.101097	9.909207	5.708642
33	H	5.816931	5.386243	8.533438	9.817311	5.074438

		11	12	13	14	15
11	H	0.000000				
12	H	2.493104	0.000000			
13	H	3.062444	1.770377	0.000000		
14	Br	5.710889	6.453142	5.097387	0.000000	
15	H	3.744500	4.451141	3.429604	2.247028	0.000000
16	C	5.546581	5.948531	5.308548	3.710695	2.724788
17	C	6.608487	6.885557	6.396616	4.879434	4.048294
18	H	5.755153	6.263504	5.354958	2.737743	2.368176
19	H	7.573115	7.867708	7.245228	5.080884	4.707292
20	H	6.719583	6.883881	6.651580	5.828868	4.700606
21	N	2.675205	2.087748	2.160352	6.365740	4.795662
22	H	3.556562	2.331356	2.545794	7.144334	5.608215
23	H	3.115879	2.931054	2.399010	5.890282	4.629104
24	C	4.934236	5.781177	4.543459	4.018271	4.200989
25	C	5.291778	5.520824	3.989777	3.803603	4.050111
26	O	3.971173	4.414487	3.160464	4.191571	3.698582
27	H	5.495220	6.387797	5.283432	5.048517	5.245067
28	H	4.864015	6.056241	4.885651	3.386549	3.749104
29	H	5.424451	5.604309	3.959890	2.891790	3.406094
30	C	6.374170	6.189785	4.656234	5.098459	5.401004
31	H	6.433920	5.824527	4.253466	5.409042	5.487260
32	H	7.332460	7.208597	5.610344	5.246689	5.960188
33	H	6.476371	6.368416	5.030785	5.939146	6.082500

		16	17	18	19	20
16	C	0.000000				

17	C	1.326380	0.000000			
18	H	1.088621	2.141821	0.000000		
19	H	2.076520	1.081377	2.467741	0.000000	
20	H	2.130754	1.083334	3.118770	1.847352	0.000000
21	N	7.001683	8.142264	7.024228	9.039041	8.352009
22	H	7.704782	8.797338	7.759735	9.697556	8.961119
23	H	7.071429	8.288529	6.936235	9.112079	8.623232
24	C	6.874866	8.197752	6.246887	8.712844	8.900895
25	C	6.601825	7.891143	5.960413	8.370855	8.608882
26	O	6.391933	7.702430	5.938469	8.339238	8.288775
27	H	7.932481	9.257102	7.315173	9.781300	9.942907
28	H	6.326561	7.636513	5.652792	8.107857	8.378296
29	H	5.771477	7.029295	5.060306	7.435994	7.805615
30	C	7.847478	9.097208	7.218539	9.553908	9.797224
31	H	7.773929	8.968577	7.228823	9.449346	9.610737
32	H	8.284903	9.505496	7.550922	9.852869	10.282381
33	H	8.645044	9.921159	8.062050	10.435459	10.577972

		21	22	23	24	25
21	N	0.000000				
22	H	1.013133	0.000000			
23	H	1.018021	1.646803	0.000000		
24	C	4.405281	5.108868	3.486781	0.000000	
25	C	4.341359	4.872931	3.446619	1.464394	0.000000
26	O	3.070023	3.750688	2.180356	1.447359	1.454106
27	H	4.749508	5.374254	3.779749	1.087350	2.213335
28	H	4.923617	5.744810	4.120873	1.085843	2.200375
29	H	4.806932	5.374593	4.046077	2.168477	1.088132
30	C	4.844142	5.100852	3.922215	2.602382	1.503728
31	H	4.675053	4.767278	3.883201	3.443030	2.151022
32	H	5.928116	6.190052	5.003636	3.143645	2.139311
33	H	4.739284	4.928196	3.770638	2.741199	2.155966

		26	27	28	29	30
26	O	0.000000				
27	H	2.137876	0.000000			
28	H	2.141229	1.850909	0.000000		
29	H	2.122207	3.106300	2.452106	0.000000	
30	C	2.511673	2.827761	3.530455	2.221568	0.000000
31	H	2.931071	3.781982	4.333089	2.584108	1.094081
32	H	3.417549	3.304776	3.927275	2.570059	1.094267
33	H	2.697585	2.560446	3.796358	3.112657	1.092947

		31	32	33
31	H	0.000000		
32	H	1.766654	0.000000	
33	H	1.775402	1.776157	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.351903	2.467716	-0.264188
2	6	0	-3.335384	1.586256	0.049083
3	7	0	-2.746350	0.329304	0.104434
4	6	0	-1.434734	0.454905	-0.170490
5	7	0	-1.176825	1.743301	-0.400383
6	6	0	0.157651	2.291612	-0.701852
7	6	0	0.803458	2.954425	0.519930
8	1	0	-2.387333	3.533523	-0.410011
9	1	0	-4.383914	1.745020	0.222847
10	1	0	0.781419	1.460553	-1.031078
11	1	0	0.057774	3.007570	-1.518685
12	1	0	0.204069	3.814890	0.835545
13	1	0	0.803449	2.229832	1.347960
14	35	0	-0.058054	-2.548637	-0.203618
15	1	0	-0.740777	-0.407842	-0.207747
16	6	0	-3.347705	-0.935469	0.383869
17	6	0	-4.625443	-1.091166	0.703913
18	1	0	-2.626652	-1.746834	0.301009
19	1	0	-4.996908	-2.088236	0.896892
20	1	0	-5.332922	-0.275004	0.787370
21	7	0	2.127374	3.421155	0.125220
22	1	0	2.525307	4.031753	0.828966
23	1	0	2.749998	2.625118	0.002618
24	6	0	3.361830	-0.631189	-1.083555
25	6	0	3.251901	-0.764850	0.370577
26	8	0	2.851906	0.466963	-0.290531
27	1	0	4.333872	-0.443837	-1.533403
28	1	0	2.620528	-1.122269	-1.706745
29	1	0	2.399400	-1.340371	0.725611
30	6	0	4.443673	-0.672763	1.282936
31	1	0	4.167516	-0.216137	2.238051
32	1	0	4.829216	-1.675045	1.493196
33	1	0	5.243143	-0.079265	0.832225

```
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.4205672           0.2926751           0.1829329
 Standard basis: 6-311++G(d,p) (5D, 7F)
 There are     499 symmetry adapted cartesian basis functions of A      symmetry.
 There are     482 symmetry adapted basis functions of A      symmetry.
    482 basis functions,      760 primitive gaussians,      499 cartesian basis functions
     71 alpha electrons             71 beta electrons
          nuclear repulsion energy           1312.9288715160 Hartrees.
 NAtoms=       33 NActive=       33 NUniq=       33 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      482 RedAO= T EigKep=    3.65D-06    NBF=      482
 NBsUse=      482 1.00D-06 EigRej= -1.00D+00 NBFU=      482
 Initial                guess                from                the                checkpoint                file:
"/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"
 B after Tr=          0.000000        0.000000        0.000000
              Rot=        1.000000        0.000216        0.000050        0.000453 Ang=      0.06 deg.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                     energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3205.64836835         A.U. after        8 cycles
                  NFock=    8    Conv=0.64D-08         -V/T= 2.0018
 Calling FoFJK, ICntrl=              2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center         Atomic                             Forces (Hartrees/Bohr)
 Number          Number                       X                       Y                       Z
 -------------------------------------------------------------------
         1               6               -0.000024993        0.000019376        0.000016661
         2               6                0.000017517       -0.000052856        0.000001212
         3               7               -0.000003387        0.000064719        0.000056943
         4               6                0.000041764       -0.000010976       -0.000097591
         5               7               -0.000008964       -0.000062770       -0.000053089
         6               6                0.000004579        0.000033244        0.000078399
         7               6                0.000119847        0.000062975        0.000006084
         8               1                0.000012416        0.000000946       -0.000004728
         9               1               -0.000003534        0.000014101       -0.000016715
        10               1                0.000000805       -0.000026023        0.000003714
        11               1               -0.000000057        0.000012346       -0.000002191
```

12	1	-0.000010255	0.000001936	-0.000002762
13	1	-0.000018515	-0.000013986	0.000017358
14	35	-0.000024056	-0.000021601	0.000003979
15	1	-0.000025663	0.000045383	-0.000000873
16	6	-0.000020233	-0.000050555	0.000017974
17	6	-0.000000369	0.000017857	-0.000001508
18	1	-0.000003978	0.000009313	0.000001833
19	1	-0.000006815	0.000000476	-0.000006387
20	1	0.000004189	-0.000004193	-0.000002184
21	7	-0.000070025	-0.000050421	-0.000031717
22	1	0.000002560	0.000000534	0.000003151
23	1	-0.000025281	0.000047559	0.000100793
24	6	-0.000056690	0.000012070	0.000278094
25	6	-0.000026228	0.000014100	0.000014349
26	8	-0.000030693	-0.000063133	-0.000226364
27	1	0.000009844	-0.000031361	-0.000063616
28	1	0.000060224	0.000005765	-0.000067215
29	1	0.000009995	0.000030068	0.000015657
30	6	0.000077711	0.000001912	-0.000035155
31	1	-0.000014418	0.000004074	-0.000013979
32	1	-0.000000964	-0.000008433	0.000000911
33	1	0.000013664	-0.000002449	0.000008961

Cartesian Forces: Max 0.000278094 RMS 0.000050037

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000235610 RMS 0.000045839
Search for a local minimum.
Step number 40 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 31 32 33 34 35
36 37 38 39 40
DE= -1.99D-06 DEPred=-1.07D-06 R= 1.87D+00
TightC=F SS= 1.41D+00 RLast= 1.55D-02 DXNew= 1.7446D+00 4.6609D-02
Trust test= 1.87D+00 RLast= 1.55D-02 DXMaxT set to 1.04D+00
ITU= 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0 0 -1 1 -1 1
ITU= 1 1 1 1 1 1 1 1 0 -1 -1 1 1 1 -1 1 0 0 -1 0
Eigenvalues --- 0.00060 0.00082 0.00217 0.00375 0.00511

Eigenvalues --- 0.00662 0.00749 0.00850 0.01344 0.01510
Eigenvalues --- 0.01899 0.02056 0.02188 0.02362 0.02381
Eigenvalues --- 0.02600 0.02700 0.02908 0.03059 0.03077
Eigenvalues --- 0.03160 0.03589 0.03622 0.03966 0.04132
Eigenvalues --- 0.04228 0.04479 0.04591 0.05405 0.05503
Eigenvalues --- 0.05733 0.05754 0.05906 0.07991 0.08616
Eigenvalues --- 0.08869 0.09527 0.10230 0.11164 0.12473
Eigenvalues --- 0.13025 0.13295 0.13798 0.15735 0.15948
Eigenvalues --- 0.15999 0.16002 0.16014 0.16014 0.16102
Eigenvalues --- 0.16260 0.18738 0.21622 0.22015 0.22269
Eigenvalues --- 0.23170 0.23656 0.25850 0.27083 0.28707
Eigenvalues --- 0.28928 0.29936 0.30323 0.32000 0.32637
Eigenvalues --- 0.33662 0.34287 0.34340 0.34389 0.34550
Eigenvalues --- 0.34697 0.34775 0.35104 0.35176 0.35322
Eigenvalues --- 0.35535 0.35669 0.35880 0.35958 0.36420
Eigenvalues --- 0.36624 0.39354 0.40993 0.41934 0.42482
Eigenvalues --- 0.44636 0.45476 0.46454 0.49511 0.54847
Eigenvalues --- 0.58433 0.60638 1.35802

En-DIIS/RFO-DIIS IScMMF= 0 using points: 40 39 38 37 36

RFO step: Lambda=-6.55696513D-07.

DidBck=F Rises=F RFO-DIIS coefs: 2.01772 -0.21641 -1.58764 0.49181 0.29453

Iteration 1 RMS(Cart)= 0.01110854 RMS(Int)= 0.00005156

Iteration 2 RMS(Cart)= 0.00008456 RMS(Int)= 0.00001070

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001070

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56498	-0.00002	0.00001	0.00003	0.00005	2.56503
R2	2.62130	0.00002	-0.00002	0.00003	0.00001	2.62131
R3	2.03395	0.00000	-0.00001	-0.00001	-0.00001	2.03394
R4	2.62526	-0.00005	-0.00002	-0.00001	-0.00003	2.62523
R5	2.03074	0.00000	0.00001	0.00001	0.00002	2.03077
R6	2.54356	0.00004	0.00005	0.00005	0.00010	2.54365
R7	2.69865	0.00004	0.00004	0.00000	0.00005	2.69869
R8	2.52074	0.00001	-0.00005	-0.00014	-0.00019	2.52054
R9	2.09350	-0.00005	-0.00038	0.00006	-0.00032	2.09318
R10	2.78525	0.00004	-0.00009	0.00002	-0.00007	2.78518
R11	2.89636	0.00003	0.00019	-0.00005	0.00014	2.89650
R12	2.05983	0.00002	0.00000	-0.00004	-0.00005	2.05979
R13	2.06126	0.00001	0.00003	-0.00001	0.00002	2.06129
R14	2.06947	0.00001	0.00003	0.00001	0.00004	2.06951
R15	2.07927	0.00002	0.00019	0.00002	0.00020	2.07948
R16	2.75562	-0.00005	-0.00064	-0.00015	-0.00078	2.75484
R17	4.24627	0.00001	0.00196	-0.00006	0.00190	4.24817

R18	2.50649	0.00000	-0.00001	0.00000	-0.00001	2.50649
R19	2.05720	-0.00001	0.00013	-0.00004	0.00009	2.05729
R20	2.04351	0.00000	0.00001	0.00000	0.00001	2.04352
R21	2.04720	-0.00001	0.00002	-0.00001	0.00001	2.04721
R22	1.91454	0.00000	-0.00009	-0.00003	-0.00013	1.91442
R23	1.92378	0.00002	-0.00018	0.00000	-0.00020	1.92358
R24	4.12028	0.00004	0.00119	0.00128	0.00247	4.12274
R25	2.76730	-0.00007	-0.00042	0.00025	-0.00015	2.76715
R26	2.73511	-0.00003	0.00069	0.00005	0.00073	2.73584
R27	2.05479	0.00003	-0.00020	0.00009	-0.00011	2.05468
R28	2.05195	0.00000	-0.00008	0.00001	-0.00007	2.05187
R29	2.74786	0.00001	-0.00059	-0.00037	-0.00097	2.74689
R30	2.05627	-0.00002	-0.00001	-0.00012	-0.00013	2.05614
R31	2.84163	0.00004	0.00012	0.00010	0.00021	2.84185
R32	2.06751	-0.00001	0.00008	-0.00002	0.00006	2.06758
R33	2.06787	0.00001	-0.00004	0.00002	-0.00002	2.06785
R34	2.06537	0.00001	-0.00001	-0.00002	-0.00003	2.06534
A1	1.87268	0.00002	-0.00002	0.00001	-0.00001	1.87266
A2	2.27902	0.00000	-0.00012	0.00002	-0.00010	2.27892
A3	2.13143	-0.00002	0.00013	-0.00002	0.00011	2.13154
A4	1.86455	0.00000	0.00007	-0.00003	0.00005	1.86460
A5	2.27622	-0.00001	0.00001	0.00002	0.00003	2.27625
A6	2.14235	0.00001	-0.00008	0.00000	-0.00008	2.14227
A7	1.89716	0.00002	-0.00011	-0.00002	-0.00013	1.89703
A8	2.25309	-0.00004	0.00008	-0.00005	0.00003	2.25313
A9	2.13289	0.00002	0.00004	0.00006	0.00010	2.13299
A10	1.88993	-0.00002	0.00009	0.00004	0.00013	1.89006
A11	2.14672	-0.00007	-0.00063	0.00027	-0.00036	2.14635
A12	2.24629	0.00009	0.00053	-0.00030	0.00023	2.24652
A13	1.90044	-0.00002	-0.00003	0.00000	-0.00003	1.90041
A14	2.20533	-0.00013	0.00027	0.00026	0.00053	2.20586
A15	2.17685	0.00015	-0.00024	-0.00025	-0.00049	2.17636
A16	1.95987	0.00011	-0.00036	0.00018	-0.00019	1.95968
A17	1.87158	-0.00001	-0.00025	-0.00020	-0.00045	1.87113
A18	1.89067	-0.00006	0.00018	0.00019	0.00036	1.89104
A19	1.90642	0.00000	0.00025	-0.00025	0.00000	1.90642
A20	1.93016	-0.00005	0.00047	-0.00010	0.00037	1.93053
A21	1.90356	0.00002	-0.00031	0.00019	-0.00012	1.90344
A22	1.91655	-0.00002	-0.00017	-0.00004	-0.00020	1.91635
A23	1.89136	0.00002	-0.00046	-0.00004	-0.00051	1.89085
A24	1.88094	-0.00003	0.00027	-0.00003	0.00024	1.88118
A25	1.87606	-0.00001	-0.00015	-0.00007	-0.00022	1.87584
A26	1.90016	-0.00003	0.00001	0.00010	0.00011	1.90028
A27	1.99817	0.00006	0.00047	0.00007	0.00055	1.99872

A28	2.16136	-0.00002	-0.00014	-0.00001	-0.00016	2.16121
A29	1.94581	0.00001	-0.00001	0.00005	0.00004	1.94584
A30	2.17601	0.00001	0.00016	-0.00004	0.00012	2.17613
A31	2.07397	0.00001	-0.00012	0.00005	-0.00007	2.07390
A32	2.16429	0.00000	0.00010	-0.00008	0.00002	2.16431
A33	2.04493	0.00000	0.00002	0.00002	0.00005	2.04497
A34	1.94065	-0.00010	0.00106	-0.00032	0.00075	1.94140
A35	1.91516	0.00024	0.00027	0.00032	0.00059	1.91575
A36	1.89094	-0.00007	0.00051	0.00016	0.00067	1.89161
A37	2.08707	-0.00003	-0.00040	-0.00006	-0.00051	2.08657
A38	2.06846	0.00009	-0.00082	-0.00009	-0.00086	2.06760
A39	1.99424	0.00002	-0.00044	-0.00006	-0.00049	1.99375
A40	2.00102	0.00001	-0.00075	0.00025	-0.00050	2.00052
A41	2.03844	-0.00007	0.00154	0.00009	0.00162	2.04007
A42	2.01648	0.00000	-0.00032	0.00011	-0.00020	2.01629
A43	2.13814	-0.00002	0.00046	0.00021	0.00065	2.13879
A44	1.96155	-0.00002	0.00088	0.00006	0.00092	1.96247
A45	2.02861	0.00002	0.00006	0.00010	0.00018	2.02879
A46	2.04356	0.00002	-0.00068	-0.00032	-0.00100	2.04256
A47	2.57018	0.00010	0.00687	0.00422	0.01107	2.58125
A48	2.48198	-0.00008	-0.00663	-0.00436	-0.01093	2.47105
A49	1.93390	-0.00003	0.00004	0.00002	0.00005	1.93396
A50	1.91742	0.00000	-0.00004	-0.00002	-0.00006	1.91736
A51	1.94205	0.00003	0.00008	-0.00003	0.00005	1.94210
A52	1.87913	0.00001	-0.00010	0.00006	-0.00004	1.87908
A53	1.89441	0.00000	-0.00003	-0.00001	-0.00005	1.89437
A54	1.89536	-0.00001	0.00005	-0.00001	0.00004	1.89540
A55	3.49177	0.00012	0.00036	0.00009	0.00045	3.49221
A56	2.53071	0.00014	-0.00186	0.00095	-0.00086	2.52985
A57	2.98978	-0.00004	0.00192	0.00088	0.00280	2.99258
A58	3.11268	0.00001	0.00003	0.00028	0.00031	3.11299
D1	0.00285	0.00000	0.00027	-0.00002	0.00025	0.00310
D2	-3.12604	0.00000	0.00038	0.00005	0.00044	-3.12561
D3	3.13243	0.00000	-0.00053	0.00027	-0.00026	3.13218
D4	0.00354	0.00000	-0.00041	0.00034	-0.00007	0.00347
D5	-0.00472	0.00001	-0.00071	0.00056	-0.00015	-0.00487
D6	-3.11140	0.00000	-0.00082	0.00024	-0.00058	-3.11198
D7	-3.13554	0.00001	0.00001	0.00030	0.00031	-3.13523
D8	0.04096	0.00000	-0.00011	-0.00001	-0.00012	0.04084
D9	-0.00005	-0.00002	0.00026	-0.00053	-0.00027	-0.00032
D10	-3.13201	0.00000	-0.00076	-0.00015	-0.00091	-3.13292
D11	3.13005	-0.00002	0.00015	-0.00059	-0.00044	3.12961
D12	-0.00192	0.00000	-0.00086	-0.00022	-0.00107	-0.00299
D13	-0.00290	0.00002	-0.00071	0.00089	0.00018	-0.00272

D14	-3.12242	0.00001	-0.00008	0.00026	0.00018	-3.12224
D15	3.12986	0.00001	0.00023	0.00054	0.00077	3.13062
D16	0.01034	-0.00001	0.00085	-0.00009	0.00077	0.01110
D17	-0.05319	0.00000	-0.00330	-0.00215	-0.00545	-0.05864
D18	3.08891	-0.00001	-0.00256	-0.00211	-0.00466	3.08425
D19	3.09918	0.00002	-0.00444	-0.00173	-0.00616	3.09301
D20	-0.04190	0.00001	-0.00369	-0.00169	-0.00538	-0.04728
D21	0.00470	-0.00002	0.00087	-0.00090	-0.00002	0.00468
D22	3.11209	-0.00002	0.00100	-0.00057	0.00043	3.11251
D23	3.12257	-0.00001	0.00018	-0.00021	-0.00003	3.12254
D24	-0.05323	-0.00001	0.00031	0.00011	0.00042	-0.05281
D25	1.33782	-0.00004	-0.00156	-0.00022	-0.00178	1.33604
D26	-2.85112	0.00001	-0.00164	-0.00056	-0.00219	-2.85331
D27	-0.79890	-0.00001	-0.00205	-0.00034	-0.00238	-0.80129
D28	-1.76358	-0.00005	-0.00170	-0.00060	-0.00229	-1.76587
D29	0.33066	0.00001	-0.00177	-0.00093	-0.00270	0.32796
D30	2.38288	-0.00001	-0.00218	-0.00071	-0.00289	2.37999
D31	-1.10527	0.00004	-0.00129	-0.00092	-0.00222	-1.10749
D32	0.93924	0.00004	-0.00183	-0.00105	-0.00288	0.93636
D33	3.11049	0.00011	-0.00137	-0.00101	-0.00238	3.10812
D34	3.10403	-0.00001	-0.00091	-0.00062	-0.00153	3.10250
D35	-1.13464	-0.00002	-0.00145	-0.00075	-0.00220	-1.13684
D36	1.03661	0.00005	-0.00099	-0.00070	-0.00169	1.03492
D37	1.00893	0.00000	-0.00098	-0.00064	-0.00162	1.00732
D38	3.05345	-0.00001	-0.00151	-0.00077	-0.00228	3.05117
D39	-1.05849	0.00006	-0.00105	-0.00072	-0.00178	-1.06026
D40	2.93782	-0.00005	-0.00090	0.00037	-0.00053	2.93729
D41	-1.25372	-0.00005	0.00059	0.00058	0.00117	-1.25255
D42	0.85991	0.00001	-0.00086	0.00037	-0.00049	0.85943
D43	2.95156	0.00001	0.00063	0.00058	0.00121	2.95278
D44	-1.23991	0.00000	-0.00099	0.00034	-0.00065	-1.24056
D45	0.85175	-0.00001	0.00050	0.00055	0.00105	0.85279
D46	3.13857	-0.00001	0.00003	-0.00011	-0.00009	3.13848
D47	-0.00410	0.00000	-0.00019	-0.00028	-0.00047	-0.00457
D48	-0.00360	0.00000	-0.00081	-0.00016	-0.00098	-0.00458
D49	3.13692	0.00000	-0.00103	-0.00033	-0.00136	3.13556
D50	2.21398	-0.00002	-0.00620	-0.00142	-0.00764	2.20634
D51	-1.39954	-0.00014	-0.00413	-0.00240	-0.00650	-1.40604
D52	-2.08237	0.00009	-0.00523	-0.00129	-0.00654	-2.08891
D53	0.58730	-0.00003	-0.00315	-0.00227	-0.00539	0.58190
D54	-2.71286	0.00002	0.00091	-0.00011	0.00081	-2.71205
D55	-0.01575	0.00002	-0.00062	-0.00020	-0.00082	-0.01657
D56	-0.02623	-0.00002	0.00207	-0.00023	0.00185	-0.02438
D57	2.67088	-0.00002	0.00054	-0.00031	0.00023	2.67110

D58	0.55611	-0.00006	-0.00646	-0.00423	-0.01073	0.54538
D59	-1.86405	0.00001	-0.00753	-0.00460	-0.01218	-1.87624
D60	1.82420	-0.00009	-0.00552	-0.00408	-0.00959	1.81461
D61	-0.59765	-0.00012	-0.00555	-0.00375	-0.00929	-0.60694
D62	2.55566	0.00000	-0.00118	-0.00069	-0.00187	2.55379
D63	-1.65333	0.00000	-0.00130	-0.00063	-0.00193	-1.65526
D64	0.44623	0.00000	-0.00121	-0.00067	-0.00189	0.44435
D65	1.35070	0.00000	-0.00194	-0.00086	-0.00280	1.34790
D66	-2.85829	0.00000	-0.00207	-0.00079	-0.00286	-2.86115
D67	-0.75873	0.00000	-0.00198	-0.00083	-0.00281	-0.76154
D68	-1.03684	-0.00001	-0.00264	-0.00068	-0.00332	-1.04016
D69	1.03735	-0.00001	-0.00277	-0.00061	-0.00338	1.03398
D70	3.13691	-0.00001	-0.00268	-0.00066	-0.00333	3.13358

Item	Value	Threshold	Converged?
Maximum Force	0.000236	0.000450	YES
RMS Force	0.000046	0.000300	YES
Maximum Displacement	0.046506	0.001800	NO
RMS Displacement	0.011111	0.001200	NO

Predicted change in Energy=-2.406745D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.643407	2.099848	-0.188460
2	6	0	-3.531402	1.115055	0.101472
3	7	0	-2.819794	-0.078012	0.112012
4	6	0	-1.529797	0.186648	-0.166726
5	7	0	-1.403438	1.500955	-0.355649
6	6	0	-0.132746	2.188236	-0.647589
7	6	0	0.454412	2.874883	0.590607
8	1	0	-2.786192	3.160890	-0.299144
9	1	0	-4.588931	1.162717	0.286405
10	1	0	0.567386	1.433319	-1.005357
11	1	0	-0.309842	2.914662	-1.441792
12	1	0	-0.223911	3.662895	0.934464
13	1	0	0.530519	2.129444	1.396481
14	35	0	0.138166	-2.663035	-0.311293
15	1	0	-0.754183	-0.601050	-0.236578
16	6	0	-3.289569	-1.404684	0.354258
17	6	0	-4.540906	-1.696314	0.683467
18	1	0	-2.493320	-2.137572	0.235669

19	1	0	-4.809663	-2.731098	0.845895
20	1	0	-5.323729	-0.957173	0.803815
21	7	0	1.723218	3.480051	0.204502
22	1	0	2.065067	4.106131	0.923853
23	1	0	2.419693	2.753083	0.054188
24	6	0	3.330640	-0.407178	-1.124569
25	6	0	3.255228	-0.573865	0.328272
26	8	0	2.728409	0.623533	-0.305474
27	1	0	4.273433	-0.118825	-1.583041
28	1	0	2.630739	-0.957923	-1.745690
29	1	0	2.468479	-1.235940	0.684025
30	6	0	4.445191	-0.381585	1.227469
31	1	0	4.139832	0.032651	2.193000
32	1	0	4.927286	-1.345422	1.417203
33	1	0	5.178245	0.292044	0.776521

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357354	0.000000			
3	N	2.205553	1.389210	0.000000		
4	C	2.213805	2.222677	1.346043	0.000000	
5	N	1.387137	2.210454	2.172074	1.333815	0.000000
6	C	2.553827	3.641932	3.596262	2.487838	1.473853
7	C	3.286960	4.384399	4.434981	3.425966	2.496935
8	H	1.076313	2.213881	3.265067	3.231436	2.161154
9	H	2.211057	1.074635	2.167872	3.242891	3.267110
10	H	3.379463	4.257514	3.873709	2.579858	2.076257
11	H	2.771333	3.999837	4.203601	3.249022	2.091465
12	H	3.091607	4.257330	4.627031	3.873274	2.780226
13	H	3.547776	4.382377	4.212756	3.234652	2.684240
14	Br	5.517000	5.282998	3.951083	3.305101	4.440419
15	H	3.296412	3.282109	2.159127	1.107666	2.203210
16	C	3.604693	2.543909	1.428087	2.429108	3.536128
17	C	4.332621	3.043290	2.430575	3.651733	4.598478
18	H	4.261237	3.416900	2.088939	2.547999	3.844006
19	H	5.394496	4.120802	3.396620	4.505126	5.563843
20	H	4.184986	2.828401	2.742482	4.079730	4.770265
21	N	4.596389	5.763233	5.771249	4.643966	3.742535
22	H	5.237571	6.398696	6.482901	5.429066	4.522676
23	H	5.110830	6.172593	5.955725	4.715280	4.043776
24	C	6.546046	7.134983	6.282143	4.989382	5.161754
25	C	6.496896	6.997302	6.099060	4.870305	5.145464
26	O	5.572218	6.292252	5.607942	4.282807	4.224281

27	H	7.396624	8.079325	7.293061	5.981366	6.029681
28	H	6.292181	6.758789	5.825256	4.594913	4.924721
29	H	6.166043	6.470326	5.443696	4.328250	4.854200
30	C	7.642681	8.193524	7.356385	6.161748	6.344815
31	H	7.480440	8.024582	7.264925	6.143021	6.275298
32	H	8.471330	8.906992	7.957832	6.822755	7.164003
33	H	8.085641	8.774451	8.034123	6.774854	6.786887

		6	7	8	9	10
6	C	0.000000				
7	C	1.532764	0.000000			
8	H	2.847498	3.372680	0.000000		
9	H	4.667079	5.334731	2.754166	0.000000	
10	H	1.089992	2.153594	3.837932	5.322544	0.000000
11	H	1.090787	2.171707	2.738354	4.936252	1.776058
12	H	2.164676	1.095136	2.887747	5.071910	3.059422
13	H	2.149790	1.100411	3.865178	5.326875	2.500954
14	Br	4.870454	5.619784	6.516910	6.110570	4.176850
15	H	2.887081	3.771876	4.276116	4.253196	2.544843
16	C	4.886544	5.691041	4.639482	2.878280	4.977843
17	C	6.024394	6.771829	5.257088	2.886871	6.224258
18	H	5.006503	5.825788	5.333432	3.909740	4.864086
19	H	6.950100	7.694327	6.334119	3.939993	7.048557
20	H	6.240711	6.936643	4.961255	2.302515	6.610052
21	N	2.416495	1.457798	4.548660	6.724580	2.643637
22	H	3.313327	2.054565	5.091554	7.303816	3.620611
23	H	2.706749	2.040812	5.233775	7.190550	2.509074
24	C	4.354162	4.688970	7.129381	8.196037	3.322231
25	C	4.478826	4.450534	7.130274	8.034196	3.609966
26	O	3.278956	3.323041	6.070342	7.361013	2.411558
27	H	5.060832	5.317138	7.889439	9.147606	4.059269
28	H	4.329087	4.988495	6.957029	7.794239	3.244003
29	H	4.501617	4.578652	6.921727	7.464496	3.686884
30	C	5.574704	5.190038	8.195888	9.213351	4.828743
31	H	5.565107	4.922221	7.997904	9.005746	4.995371
32	H	6.507998	6.204904	9.096727	9.905951	5.709547
33	H	5.816379	5.387042	8.533440	9.818148	5.073226

		11	12	13	14	15
11	H	0.000000				
12	H	2.492755	0.000000			
13	H	3.062444	1.770338	0.000000		
14	Br	5.708717	6.457585	5.102772	0.000000	
15	H	3.743022	4.453511	3.431172	2.248033	0.000000
16	C	5.546289	5.951072	5.307482	3.711573	2.724536
17	C	6.609065	6.886260	6.392509	4.880350	4.047883

18	H	5.753827	6.267691	5.357099	2.738612	2.368230
19	H	7.573408	7.868933	7.241930	5.081803	4.706991
20	H	6.721080	6.882604	6.644597	5.829727	4.699998
21	N	2.676430	2.087484	2.160437	6.365214	4.794524
22	H	3.557537	2.331521	2.546666	7.145638	5.608238
23	H	3.116797	2.931090	2.399929	5.888402	4.626905
24	C	4.938457	5.782728	4.542116	3.992769	4.184722
25	C	5.292700	5.515616	3.984092	3.806541	4.049096
26	O	3.971330	4.414902	3.161509	4.184605	3.692262
27	H	5.498037	6.392601	5.285989	5.019042	5.227087
28	H	4.871990	6.056749	4.880163	3.343325	3.723235
29	H	5.428228	5.595558	3.948302	2.908199	3.411180
30	C	6.371855	6.184188	4.653868	5.111092	5.406024
31	H	6.427853	5.814193	4.249485	5.436132	5.500528
32	H	7.331417	7.200772	5.604167	5.259227	5.963906
33	H	6.474422	6.369527	5.036045	5.942914	6.084217

		16	17	18	19	20
16	C	0.000000				
17	C	1.326375	0.000000			
18	H	1.088669	2.141924	0.000000		
19	H	2.076478	1.081383	2.467811	0.000000	
20	H	2.130768	1.083339	3.118869	1.847388	0.000000
21	N	7.000793	8.140235	7.024091	9.037051	8.349107
22	H	7.704911	8.795740	7.761207	9.696169	8.958000
23	H	7.069141	8.285112	6.934634	9.108602	8.619079
24	C	6.856320	8.178760	6.225996	8.691827	8.883651
25	C	6.597372	7.884527	5.958151	8.364452	8.600673
26	O	6.384746	7.694325	5.931526	8.330770	8.280464
27	H	7.912369	9.236781	7.291914	9.758398	9.924990
28	H	6.297574	7.607794	5.619016	8.075892	8.353055
29	H	5.769952	7.024488	5.062946	7.431894	7.798113
30	C	7.850843	9.098043	7.225655	9.556051	9.795028
31	H	7.787355	8.979044	7.248429	9.462899	9.616057
32	H	8.285534	9.503061	7.555721	9.851632	10.276686
33	H	8.646449	9.920894	8.065263	10.435636	10.576046

		21	22	23	24	25
21	N	0.000000				
22	H	1.013067	0.000000			
23	H	1.017917	1.647063	0.000000		
24	C	4.411438	5.115434	3.493785	0.000000	
25	C	4.335506	4.865549	3.441195	1.464315	0.000000
26	O	3.070860	3.752301	2.181661	1.447744	1.453593
27	H	4.759288	5.386247	3.790083	1.087292	2.212898
28	H	4.931780	5.752485	4.129850	1.085805	2.199728

29	H	4.798534	5.362647	4.038734	2.168220	1.088061
30	C	4.834029	5.088886	3.912208	2.602875	1.503841
31	H	4.656041	4.744325	3.864472	3.443036	2.151185
32	H	5.917930	6.176983	4.994354	3.144867	2.139357
33	H	4.735801	4.925530	3.766708	2.741660	2.156089

		26	27	28	29	30
26	O	0.000000				
27	H	2.137843	0.000000			
28	H	2.141206	1.851751	0.000000		
29	H	2.122336	3.105703	2.450946	0.000000	
30	C	2.511476	2.827987	3.530449	2.220955	0.000000
31	H	2.929782	3.781439	4.332652	2.584520	1.094114
32	H	3.417522	3.306589	3.927872	2.568125	1.094257
33	H	2.698573	2.560280	3.796545	3.112253	1.092931

		31	32	33
31	H	0.000000		
32	H	1.766644	0.000000	
33	H	1.775387	1.776161	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.350947	2.468350	-0.264447
2	6	0	-3.333957	1.587163	0.051166
3	7	0	-2.744957	0.330213	0.106490
4	6	0	-1.433833	0.455610	-0.171110
5	7	0	-1.176209	1.743707	-0.402402
6	6	0	0.157918	2.290864	-0.707307
7	6	0	0.805426	2.956898	0.511913
8	1	0	-2.386715	3.534010	-0.411207
9	1	0	-4.382227	1.746061	0.226446
10	1	0	0.780754	1.458394	-1.034646
11	1	0	0.057508	3.004188	-1.526394
12	1	0	0.207650	3.819642	0.824419
13	1	0	0.803405	2.235112	1.342530
14	35	0	-0.057850	-2.549209	-0.208852
15	1	0	-0.740373	-0.407291	-0.209046

16	6	0	-3.345739	-0.934200	0.388895
17	6	0	-4.621299	-1.088569	0.718118
18	1	0	-2.626075	-1.746288	0.300595
19	1	0	-4.992615	-2.085406	0.912622
20	1	0	-5.326987	-0.271540	0.808072
21	7	0	2.129882	3.419417	0.115596
22	1	0	2.529449	4.032192	0.816423
23	1	0	2.750996	2.622082	-0.005358
24	6	0	3.347116	-0.651014	-1.072140
25	6	0	3.249342	-0.760409	0.384806
26	8	0	2.847261	0.461492	-0.292115
27	1	0	4.315890	-0.473535	-1.532770
28	1	0	2.598388	-1.149922	-1.679981
29	1	0	2.398986	-1.328531	0.756302
30	6	0	4.448756	-0.657416	1.286102
31	1	0	4.182181	-0.182602	2.235088
32	1	0	4.831502	-1.657531	1.511212
33	1	0	5.247239	-0.075661	0.818680

Rotational constants (GHZ): 0.4203897 0.2929806 0.1830727

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1313.2194569955 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 3.66D-06 NBF= 482

NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000837 -0.000293 0.000111 Ang= 0.10 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3205.64837096 A.U. after 10 cycles
NFock= 10 Conv=0.66D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000043662	0.000021684	-0.000012211
2	6	0.000011717	-0.000048203	0.000034152
3	7	0.000048061	0.000110457	0.000044029
4	6	-0.000071595	-0.000133777	-0.000041215
5	7	-0.000019441	-0.000039760	-0.000075901
6	6	0.000036747	0.000050045	0.000075687
7	6	-0.000074260	-0.000037275	0.000054302
8	1	0.000019920	0.000004620	-0.000008747
9	1	0.000002511	0.000021401	-0.000020779
10	1	0.000030771	-0.000020947	0.000006275
11	1	-0.000020503	0.000019528	0.000016891
12	1	0.000004026	0.000005834	0.000008607
13	1	0.000023143	0.000025782	0.000004136
14	35	-0.000060538	0.000009693	0.000010005
15	1	0.000062654	0.000018911	-0.000032902
16	6	0.000002563	-0.000036526	0.000014815
17	6	0.000001182	-0.000009473	-0.000004595
18	1	-0.000025275	0.000027523	0.000007979
19	1	-0.000012834	0.000005711	-0.000006590
20	1	0.000007679	-0.000006217	-0.000010325
21	7	0.000005710	0.000041094	-0.000125288
22	1	0.000007440	-0.000004371	0.000038848
23	1	0.000019819	0.000007519	0.000088760
24	6	-0.000072474	0.000063014	0.000336981
25	6	0.000075038	-0.000086381	0.000131100

26	8	-0.000087185	-0.000019090	-0.000231634
27	1	0.000018726	-0.000034637	-0.000107061
28	1	0.000086306	-0.000004884	-0.000089523
29	1	-0.000057422	0.000057657	-0.000027953
30	6	0.000065911	-0.000005936	-0.000061975
31	1	-0.000016982	0.000003541	-0.000018871
32	1	0.000019810	-0.000008893	-0.000007763
33	1	0.000012435	0.000002358	0.000010767

Cartesian Forces: Max 0.000336981 RMS 0.000061965

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000286236 RMS 0.000058975
Search for a local minimum.
Step number 41 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 31 32 33 34 35
36 37 38 39 40
41
DE= -2.60D-06 DEPred=-2.41D-06 R= 1.08D+00
TightC=F SS= 1.41D+00 RLast= 3.41D-02 DXNew= 1.7446D+00 1.0242D-01
Trust test= 1.08D+00 RLast= 3.41D-02 DXMaxT set to 1.04D+00
ITU= 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0 0 -1 1 -1
ITU= 1 1 1 1 1 1 1 1 1 0 -1 -1 1 1 1 -1 1 0 0 -1
ITU= 0

Eigenvalues ---	0.00064	0.00110	0.00216	0.00291	0.00496
Eigenvalues ---	0.00646	0.00754	0.00803	0.01351	0.01483
Eigenvalues ---	0.01898	0.02057	0.02180	0.02352	0.02382
Eigenvalues ---	0.02608	0.02689	0.02913	0.03053	0.03086
Eigenvalues ---	0.03142	0.03573	0.03625	0.03967	0.04162
Eigenvalues ---	0.04259	0.04477	0.04623	0.05487	0.05594
Eigenvalues ---	0.05744	0.05795	0.05911	0.07972	0.08688
Eigenvalues ---	0.08890	0.09527	0.10213	0.11291	0.12478
Eigenvalues ---	0.13024	0.13191	0.14271	0.15758	0.15954
Eigenvalues ---	0.16001	0.16002	0.16014	0.16019	0.16107
Eigenvalues ---	0.16272	0.19106	0.21542	0.21940	0.22258
Eigenvalues ---	0.23169	0.23634	0.26064	0.27245	0.28305
Eigenvalues ---	0.29154	0.30072	0.30373	0.31934	0.32543

Eigenvalues --- 0.33634 0.34286 0.34344 0.34393 0.34550
Eigenvalues --- 0.34712 0.34768 0.35120 0.35192 0.35329
Eigenvalues --- 0.35527 0.35654 0.35892 0.35990 0.36418
Eigenvalues --- 0.36629 0.39325 0.40566 0.41908 0.42454
Eigenvalues --- 0.44753 0.45497 0.46438 0.49514 0.54883
Eigenvalues --- 0.58281 0.60634 1.30574
En-DIIS/RFO-DIIS IScMMF= 0 using points: 41 40 39 38 37
RFO step: Lambda=-7.07608998D-07.
DidBck=F Rises=F RFO-DIIS coefs: 1.37083 -0.24221 -0.33907 0.27549 -0.06505
Iteration 1 RMS(Cart)= 0.00360974 RMS(Int)= 0.00001175
Iteration 2 RMS(Cart)= 0.00001714 RMS(Int)= 0.00000618
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000618

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56503	-0.00004	0.00001	-0.00002	-0.00001	2.56502
R2	2.62131	0.00002	0.00002	-0.00002	0.00000	2.62130
R3	2.03394	0.00000	-0.00001	0.00001	0.00000	2.03393
R4	2.62523	-0.00004	-0.00003	0.00000	-0.00003	2.62520
R5	2.03077	0.00000	0.00001	-0.00001	0.00000	2.03077
R6	2.54365	0.00000	0.00007	-0.00006	0.00002	2.54367
R7	2.69869	0.00003	0.00004	0.00003	0.00007	2.69876
R8	2.52054	0.00008	-0.00011	0.00009	-0.00002	2.52053
R9	2.09318	-0.00002	-0.00012	-0.00008	-0.00020	2.09299
R10	2.78518	0.00008	-0.00003	0.00007	0.00003	2.78521
R11	2.89650	0.00002	0.00006	-0.00001	0.00005	2.89656
R12	2.05979	0.00003	-0.00002	0.00007	0.00005	2.05984
R13	2.06129	0.00000	0.00002	-0.00001	0.00001	2.06130
R14	2.06951	0.00000	0.00003	-0.00001	0.00002	2.06953
R15	2.07948	-0.00001	0.00009	-0.00003	0.00006	2.07954
R16	2.75484	0.00010	-0.00037	0.00016	-0.00022	2.75462
R17	4.24817	-0.00003	0.00082	0.00077	0.00159	4.24976
R18	2.50649	0.00000	0.00000	0.00001	0.00001	2.50649
R19	2.05729	-0.00004	0.00003	-0.00003	0.00000	2.05729
R20	2.04352	0.00000	0.00001	0.00000	0.00000	2.04352
R21	2.04721	-0.00001	0.00000	-0.00001	-0.00001	2.04721
R22	1.91442	0.00003	-0.00004	0.00002	-0.00002	1.91440
R23	1.92358	0.00008	-0.00008	0.00003	-0.00006	1.92353
R24	4.12274	0.00003	0.00164	0.00076	0.00240	4.12515
R25	2.76715	-0.00007	-0.00011	-0.00012	-0.00022	2.76693
R26	2.73584	-0.00003	0.00007	-0.00001	0.00005	2.73589
R27	2.05468	0.00005	0.00001	0.00004	0.00005	2.05474
R28	2.05187	0.00000	0.00001	0.00000	0.00001	2.05188
R29	2.74689	0.00008	-0.00026	0.00032	0.00006	2.74695

R30	2.05614	0.00000	-0.00006	0.00004	-0.00001	2.05612
R31	2.84185	0.00002	0.00011	-0.00004	0.00007	2.84192
R32	2.06758	-0.00001	0.00001	-0.00002	-0.00001	2.06756
R33	2.06785	0.00001	-0.00001	0.00001	0.00000	2.06784
R34	2.06534	0.00001	-0.00002	0.00002	0.00000	2.06534
A1	1.87266	0.00002	-0.00001	-0.00003	-0.00004	1.87262
A2	2.27892	0.00001	-0.00001	0.00005	0.00005	2.27896
A3	2.13154	-0.00003	0.00002	-0.00003	-0.00001	2.13153
A4	1.86460	0.00000	0.00002	0.00001	0.00004	1.86464
A5	2.27625	-0.00002	0.00000	-0.00001	-0.00002	2.27623
A6	2.14227	0.00003	-0.00002	0.00000	-0.00002	2.14225
A7	1.89703	0.00005	-0.00005	0.00004	-0.00001	1.89702
A8	2.25313	-0.00004	-0.00005	-0.00011	-0.00015	2.25298
A9	2.13299	-0.00001	0.00010	0.00007	0.00017	2.13316
A10	1.89006	-0.00004	0.00004	-0.00006	-0.00002	1.89004
A11	2.14635	-0.00006	-0.00018	0.00032	0.00013	2.14649
A12	2.24652	0.00010	0.00015	-0.00025	-0.00010	2.24643
A13	1.90041	-0.00002	0.00000	0.00003	0.00003	1.90044
A14	2.20586	-0.00022	0.00017	-0.00025	-0.00008	2.20578
A15	2.17636	0.00024	-0.00017	0.00022	0.00005	2.17641
A16	1.95968	0.00012	0.00001	0.00011	0.00011	1.95979
A17	1.87113	0.00003	-0.00021	0.00025	0.00003	1.87116
A18	1.89104	-0.00009	0.00019	-0.00027	-0.00009	1.89095
A19	1.90642	-0.00003	0.00005	0.00004	0.00009	1.90651
A20	1.93053	-0.00005	0.00002	-0.00015	-0.00014	1.93040
A21	1.90344	0.00003	-0.00005	0.00005	-0.00001	1.90343
A22	1.91635	-0.00001	-0.00015	0.00011	-0.00004	1.91631
A23	1.89085	0.00005	-0.00016	0.00023	0.00007	1.89093
A24	1.88118	-0.00003	0.00006	-0.00015	-0.00010	1.88108
A25	1.87584	-0.00001	-0.00010	0.00000	-0.00010	1.87574
A26	1.90028	-0.00004	0.00005	-0.00011	-0.00006	1.90022
A27	1.99872	0.00004	0.00029	-0.00007	0.00022	1.99894
A28	2.16121	0.00000	-0.00009	-0.00003	-0.00012	2.16109
A29	1.94584	0.00000	0.00003	0.00002	0.00004	1.94589
A30	2.17613	0.00000	0.00006	0.00001	0.00008	2.17621
A31	2.07390	0.00002	-0.00002	0.00005	0.00002	2.07392
A32	2.16431	-0.00001	0.00001	-0.00003	-0.00002	2.16429
A33	2.04497	-0.00001	0.00001	-0.00001	0.00000	2.04497
A34	1.94140	-0.00014	0.00022	0.00000	0.00022	1.94162
A35	1.91575	0.00029	0.00031	0.00003	0.00034	1.91609
A36	1.89161	-0.00009	0.00023	-0.00004	0.00019	1.89180
A37	2.08657	0.00001	-0.00028	0.00008	-0.00022	2.08635
A38	2.06760	0.00008	0.00020	0.00019	0.00041	2.06802
A39	1.99375	0.00005	-0.00007	-0.00004	-0.00011	1.99364

A40	2.00052	0.00000	0.00003	0.00007	0.00010	2.00062
A41	2.04007	-0.00010	0.00011	-0.00026	-0.00015	2.03991
A42	2.01629	-0.00002	0.00042	0.00007	0.00049	2.01678
A43	2.13879	-0.00005	0.00015	-0.00011	0.00005	2.13884
A44	1.96247	-0.00007	0.00032	-0.00024	0.00007	1.96253
A45	2.02879	0.00003	0.00006	0.00011	0.00018	2.02897
A46	2.04256	0.00007	-0.00062	0.00010	-0.00053	2.04203
A47	2.58125	0.00007	0.00271	0.00366	0.00633	2.58758
A48	2.47105	-0.00003	-0.00395	-0.00277	-0.00668	2.46437
A49	1.93396	-0.00004	-0.00005	-0.00014	-0.00019	1.93377
A50	1.91736	0.00001	-0.00008	0.00008	0.00000	1.91737
A51	1.94210	0.00002	0.00004	0.00005	0.00009	1.94219
A52	1.87908	0.00002	-0.00004	0.00004	0.00000	1.87908
A53	1.89437	0.00000	0.00007	-0.00001	0.00006	1.89443
A54	1.89540	-0.00002	0.00006	-0.00002	0.00004	1.89544
A55	3.49221	0.00020	0.00013	-0.00029	-0.00016	3.49205
A56	2.52985	0.00017	-0.00052	-0.00068	-0.00119	2.52866
A57	2.99258	-0.00007	-0.00002	-0.00259	-0.00261	2.98996
A58	3.11299	-0.00001	-0.00109	-0.00005	-0.00114	3.11185
D1	0.00310	-0.00001	0.00015	-0.00013	0.00001	0.00312
D2	-3.12561	0.00000	0.00014	-0.00010	0.00004	-3.12557
D3	3.13218	0.00000	0.00006	-0.00005	0.00001	3.13219
D4	0.00347	0.00001	0.00005	-0.00002	0.00004	0.00351
D5	-0.00487	0.00002	-0.00005	0.00007	0.00002	-0.00484
D6	-3.11198	0.00001	-0.00003	0.00010	0.00007	-3.11191
D7	-3.13523	0.00001	0.00003	-0.00001	0.00002	-3.13521
D8	0.04084	0.00000	0.00004	0.00003	0.00007	0.04091
D9	-0.00032	-0.00001	-0.00020	0.00015	-0.00005	-0.00037
D10	-3.13292	0.00001	-0.00037	-0.00001	-0.00038	-3.13330
D11	3.12961	-0.00002	-0.00019	0.00012	-0.00007	3.12954
D12	-0.00299	0.00000	-0.00036	-0.00004	-0.00040	-0.00339
D13	-0.00272	0.00002	0.00017	-0.00011	0.00006	-0.00266
D14	-3.12224	0.00001	-0.00023	-0.00059	-0.00082	-3.12307
D15	3.13062	0.00000	0.00032	0.00004	0.00037	3.13099
D16	0.01110	-0.00001	-0.00008	-0.00044	-0.00052	0.01058
D17	-0.05864	0.00001	-0.00128	0.00209	0.00081	-0.05783
D18	3.08425	0.00000	-0.00099	0.00195	0.00096	3.08521
D19	3.09301	0.00003	-0.00146	0.00191	0.00044	3.09346
D20	-0.04728	0.00002	-0.00117	0.00176	0.00059	-0.04669
D21	0.00468	-0.00002	-0.00008	0.00002	-0.00005	0.00462
D22	3.11251	-0.00002	-0.00008	-0.00002	-0.00010	3.11241
D23	3.12254	-0.00002	0.00035	0.00055	0.00090	3.12344
D24	-0.05281	-0.00002	0.00035	0.00051	0.00085	-0.05196
D25	1.33604	-0.00004	-0.00111	0.00084	-0.00027	1.33577

D26	-2.85331	0.00001	-0.00118	0.00111	-0.00007	-2.85339
D27	-0.80129	0.00001	-0.00126	0.00115	-0.00011	-0.80140
D28	-1.76587	-0.00005	-0.00110	0.00088	-0.00022	-1.76609
D29	0.32796	0.00001	-0.00117	0.00115	-0.00002	0.32794
D30	2.37999	0.00001	-0.00125	0.00120	-0.00006	2.37993
D31	-1.10749	0.00006	-0.00041	0.00126	0.00085	-1.10664
D32	0.93636	0.00008	-0.00071	0.00145	0.00075	0.93711
D33	3.10812	0.00014	-0.00041	0.00141	0.00100	3.10912
D34	3.10250	-0.00003	-0.00018	0.00086	0.00068	3.10318
D35	-1.13684	-0.00001	-0.00047	0.00105	0.00058	-1.13626
D36	1.03492	0.00005	-0.00018	0.00101	0.00083	1.03575
D37	1.00732	-0.00001	-0.00015	0.00087	0.00072	1.00803
D38	3.05117	0.00000	-0.00045	0.00107	0.00061	3.05178
D39	-1.06026	0.00006	-0.00016	0.00103	0.00087	-1.05939
D40	2.93729	-0.00005	0.00023	-0.00025	-0.00002	2.93726
D41	-1.25255	-0.00006	0.00086	-0.00028	0.00058	-1.25197
D42	0.85943	0.00001	0.00035	-0.00024	0.00011	0.85954
D43	2.95278	-0.00001	0.00098	-0.00026	0.00072	2.95349
D44	-1.24056	0.00002	0.00025	-0.00011	0.00014	-1.24041
D45	0.85279	0.00000	0.00089	-0.00014	0.00075	0.85354
D46	3.13848	-0.00001	0.00003	0.00003	0.00006	3.13855
D47	-0.00457	0.00000	-0.00011	0.00017	0.00006	-0.00450
D48	-0.00458	0.00000	-0.00030	0.00019	-0.00010	-0.00468
D49	3.13556	0.00001	-0.00044	0.00033	-0.00011	3.13545
D50	2.20634	-0.00001	0.00223	-0.00064	0.00158	2.20791
D51	-1.40604	-0.00015	-0.00155	0.00239	0.00085	-1.40518
D52	-2.08891	0.00009	0.00285	-0.00084	0.00200	-2.08691
D53	0.58190	-0.00004	-0.00093	0.00219	0.00127	0.58317
D54	-2.71205	0.00000	0.00021	-0.00037	-0.00015	-2.71221
D55	-0.01657	0.00003	-0.00006	-0.00019	-0.00025	-0.01681
D56	-0.02438	-0.00006	0.00031	-0.00041	-0.00010	-0.02448
D57	2.67110	-0.00004	0.00004	-0.00024	-0.00019	2.67091
D58	0.54538	-0.00007	-0.00522	-0.00226	-0.00750	0.53787
D59	-1.87624	0.00005	-0.00534	-0.00187	-0.00724	-1.88347
D60	1.81461	-0.00005	-0.00152	-0.00418	-0.00572	1.80890
D61	-0.60694	-0.00013	-0.00096	-0.00418	-0.00516	-0.61209
D62	2.55379	-0.00001	-0.00070	-0.00046	-0.00116	2.55263
D63	-1.65526	0.00000	-0.00083	-0.00045	-0.00128	-1.65654
D64	0.44435	0.00000	-0.00078	-0.00039	-0.00117	0.44317
D65	1.34790	0.00001	-0.00090	-0.00044	-0.00134	1.34656
D66	-2.86115	0.00002	-0.00103	-0.00043	-0.00146	-2.86261
D67	-0.76154	0.00002	-0.00098	-0.00037	-0.00135	-0.76289
D68	-1.04016	-0.00001	-0.00073	-0.00029	-0.00102	-1.04118
D69	1.03398	0.00000	-0.00086	-0.00028	-0.00114	1.03284

D70 3.13358 0.00000 -0.00081 -0.00022 -0.00103 3.13255

Item	Value	Threshold	Converged?
Maximum Force	0.000286	0.000450	YES
RMS Force	0.000059	0.000300	YES
Maximum Displacement	0.020954	0.001800	NO
RMS Displacement	0.003614	0.001200	NO

Predicted change in Energy=-1.013123D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.642352	2.099769	-0.187155
2	6	0	-3.530684	1.114984	0.101750
3	7	0	-2.819520	-0.078338	0.111170
4	6	0	-1.529415	0.186137	-0.167287
5	7	0	-1.402597	1.500583	-0.354865
6	6	0	-0.131663	2.187806	-0.645976
7	6	0	0.455551	2.873345	0.592840
8	1	0	-2.784733	3.160972	-0.296801
9	1	0	-4.588211	1.162827	0.286644
10	1	0	0.568340	1.433055	-1.004433
11	1	0	-0.308549	2.915029	-1.439503
12	1	0	-0.223040	3.660693	0.937718
13	1	0	0.532120	2.127110	1.397978
14	35	0	0.137941	-2.664751	-0.308557
15	1	0	-0.753903	-0.601512	-0.237153
16	6	0	-3.289937	-1.404984	0.352532
17	6	0	-4.541593	-1.696146	0.680951
18	1	0	-2.493901	-2.138137	0.234149
19	1	0	-4.810957	-2.730861	0.842825
20	1	0	-5.324106	-0.956661	0.801169
21	7	0	1.723783	3.479551	0.206906
22	1	0	2.065776	4.105062	0.926668
23	1	0	2.420635	2.753342	0.054880
24	6	0	3.328978	-0.411772	-1.125595
25	6	0	3.253966	-0.571565	0.327921
26	8	0	2.727950	0.623375	-0.311176
27	1	0	4.271985	-0.126399	-1.585557
28	1	0	2.628505	-0.964585	-1.744236
29	1	0	2.466827	-1.231056	0.687569
30	6	0	4.444490	-0.376441	1.225823

31	1	0	4.139890	0.043740	2.189014
32	1	0	4.924789	-1.340099	1.420947
33	1	0	5.178750	0.293294	0.771056

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357350	0.000000			
3	N	2.205569	1.389194	0.000000		
4	C	2.213823	2.222660	1.346052	0.000000	
5	N	1.387135	2.210416	2.172062	1.333806	0.000000
6	C	2.553787	3.641893	3.596283	2.487877	1.473870
7	C	3.286916	4.384413	4.435147	3.426218	2.497065
8	H	1.076312	2.213899	3.265085	3.231446	2.161149
9	H	2.211043	1.074635	2.167845	3.242871	3.267071
10	H	3.379496	4.257558	3.873819	2.579960	2.076316
11	H	2.771221	3.999722	4.203547	3.248984	2.091420
12	H	3.091099	4.256757	4.626579	3.873008	2.779964
13	H	3.548332	4.383033	4.213474	3.235329	2.684795
14	Br	5.517737	5.283329	3.951239	3.305692	4.441330
15	H	3.296309	3.282031	2.159124	1.107560	2.203058
16	C	3.604708	2.543834	1.428124	2.429263	3.536211
17	C	4.332401	3.043003	2.430533	3.651810	4.598402
18	H	4.261382	3.416906	2.089001	2.548261	3.844238
19	H	5.394320	4.120536	3.396619	4.505299	5.563857
20	H	4.184537	2.827944	2.742353	4.079654	4.769979
21	N	4.595891	5.762955	5.771424	4.644340	3.742479
22	H	5.237201	6.398548	6.483208	5.429559	4.522748
23	H	5.110731	6.172893	5.956577	4.716227	4.044057
24	C	6.545632	7.133886	6.280510	4.987969	5.161292
25	C	6.493681	6.994789	6.097334	4.868272	5.142331
26	O	5.570930	6.291477	5.607603	4.282177	4.222893
27	H	7.397257	8.078965	7.291820	5.980419	6.030137
28	H	6.292591	6.757802	5.823139	4.593390	4.925159
29	H	6.161432	6.466624	5.441182	4.325410	4.849842
30	C	7.638812	8.190927	7.355077	6.159934	6.341153
31	H	7.474774	8.021343	7.264003	6.141128	6.269998
32	H	8.466422	8.902962	7.954991	6.819724	7.159525
33	H	8.084006	8.773675	8.034045	6.774322	6.785231

		6	7	8	9	10
6	C	0.000000				
7	C	1.532792	0.000000			
8	H	2.847413	3.372482	0.000000		
9	H	4.667032	5.334714	2.754183	0.000000	

10	H	1.090020	2.153703	3.837908	5.322586	0.000000
11	H	1.090792	2.171636	2.738201	4.936123	1.776081
12	H	2.164679	1.095146	2.887218	5.071287	3.059510
13	H	2.149893	1.100444	3.865573	5.327541	2.500920
14	Br	4.871740	5.619956	6.517762	6.110740	4.178697
15	H	2.886973	3.771776	4.275993	4.253137	2.544898
16	C	4.886702	5.691268	4.639485	2.878109	4.978165
17	C	6.024393	6.771962	5.256820	2.886413	6.224455
18	H	5.006852	5.826052	5.333578	3.909636	4.864650
19	H	6.950223	7.694526	6.333879	3.939513	7.048929
20	H	6.240462	6.936627	4.960731	2.301849	6.609982
21	N	2.416339	1.457684	4.547739	6.724198	2.643962
22	H	3.313279	2.054602	5.090738	7.303555	3.620923
23	H	2.706521	2.040920	5.233135	7.190784	2.509243
24	C	4.354753	4.690586	7.129437	8.194857	3.322528
25	C	4.474940	4.446202	7.126570	8.031785	3.606419
26	O	3.276724	3.323162	6.068714	7.360341	2.408341
27	H	5.062654	5.320624	7.890816	9.147148	4.060368
28	H	4.331544	4.991329	6.958336	7.793033	3.246578
29	H	4.496567	4.571686	6.916486	7.460897	3.683017
30	C	5.569575	5.183957	8.191052	9.210923	4.824195
31	H	5.557010	4.912107	7.990421	9.002840	4.988414
32	H	6.502768	6.197819	9.091041	9.901942	5.705392
33	H	5.813573	5.384889	8.531175	9.817549	5.070236

		11	12	13	14	15
11	H	0.000000				
12	H	2.492891	0.000000			
13	H	3.062488	1.770305	0.000000		
14	Br	5.710721	6.457147	5.101919	0.000000	
15	H	3.742999	4.452923	3.431163	2.248876	0.000000
16	C	5.546402	5.950578	5.308179	3.711388	2.724842
17	C	6.608928	6.885605	6.393276	4.880099	4.048177
18	H	5.754247	6.267236	5.357577	2.738329	2.368742
19	H	7.573426	7.868287	7.242689	5.081500	4.707459
20	H	6.720596	6.881822	6.645390	5.829497	4.700107
21	N	2.675765	2.087347	2.160512	6.366557	4.794913
22	H	3.557016	2.331580	2.546867	7.146517	5.608645
23	H	3.115729	2.931161	2.400535	5.890545	4.627961
24	C	4.939407	5.784381	4.542770	3.990762	4.182732
25	C	5.288821	5.511209	3.979487	3.807380	4.047619
26	O	3.968013	4.415130	3.162925	4.185682	3.691765
27	H	5.500264	6.396423	5.288324	5.016401	5.225273
28	H	4.875505	6.059487	4.881283	3.339858	3.720727
29	H	5.423759	5.588128	3.940185	2.910577	3.409478

30	C	6.366248	6.177968	4.648015	5.112440	5.405020
31	H	6.418648	5.803728	4.240540	5.439612	5.500168
32	H	7.326398	7.193161	5.596214	5.259258	5.961740
33	H	6.470742	6.367612	5.034589	5.943513	6.083874

		16	17	18	19	20
16	C	0.000000				
17	C	1.326378	0.000000			
18	H	1.088670	2.141969	0.000000		
19	H	2.076497	1.081385	2.467905	0.000000	
20	H	2.130754	1.083337	3.118888	1.847389	0.000000
21	N	7.001234	8.140485	7.024815	9.037502	8.349004
22	H	7.705446	8.796120	7.761944	9.696717	8.958077
23	H	7.070425	8.286286	6.936236	9.110064	8.619866
24	C	6.854296	8.176743	6.223758	8.689729	8.881734
25	C	6.596807	7.884165	5.958264	8.364847	8.599743
26	O	6.385117	7.694853	5.932206	8.331731	8.280667
27	H	7.910350	9.234735	7.289419	9.756029	9.923244
28	H	6.294311	7.604409	5.615183	8.072064	8.350041
29	H	5.769128	7.023839	5.063320	7.432339	7.796592
30	C	7.851235	9.098802	7.226912	9.557891	9.795022
31	H	7.789339	8.981627	7.251846	9.467223	9.617388
32	H	8.284169	9.501935	7.555284	9.851558	10.274775
33	H	8.647425	9.922251	8.066579	10.437667	10.577016

		21	22	23	24	25
21	N	0.000000				
22	H	1.013055	0.000000			
23	H	1.017887	1.647145	0.000000		
24	C	4.415270	5.119498	3.498079	0.000000	
25	C	4.332164	4.862215	3.438605	1.464196	0.000000
26	O	3.071563	3.754048	2.182934	1.447772	1.453623
27	H	4.765410	5.392949	3.796240	1.087320	2.212676
28	H	4.937188	5.757753	4.135579	1.085809	2.199886
29	H	4.793013	5.356507	4.034583	2.168431	1.088054
30	C	4.827952	5.082484	3.906743	2.602841	1.503878
31	H	4.644473	4.731787	3.853870	3.442630	2.151077
32	H	5.911798	6.169931	4.989307	3.145358	2.139392
33	H	4.733634	4.923860	3.764564	2.741543	2.156187

		26	27	28	29	30
26	O	0.000000				
27	H	2.137815	0.000000			
28	H	2.141301	1.851691	0.000000		
29	H	2.122403	3.105795	2.451698	0.000000	
30	C	2.511674	2.827745	3.530576	2.220638	0.000000
31	H	2.929249	3.780712	4.332605	2.584295	1.094107

32	H	3.417832	3.307308	3.928398	2.567355	1.094256
33	H	2.699369	2.559686	3.796406	3.112095	1.092930

		31	32	33
31	H	0.000000		
32	H	1.766636	0.000000	
33	H	1.775418	1.776183	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.347698	2.470637	-0.264148
2	6	0	-3.331816	1.590370	0.050560
3	7	0	-2.744368	0.332676	0.105050
4	6	0	-1.433034	0.456698	-0.172219
5	7	0	-1.173820	1.744665	-0.402412
6	6	0	0.161027	2.290552	-0.706524
7	6	0	0.808990	2.955183	0.513254
8	1	0	-2.382123	3.536454	-0.410085
9	1	0	-4.379937	1.750388	0.225709
10	1	0	0.783051	1.457634	-1.034360
11	1	0	0.061563	3.004595	-1.525106
12	1	0	0.211605	3.817906	0.826599
13	1	0	0.806684	2.232702	1.343310
14	35	0	-0.060386	-2.550343	-0.205963
15	1	0	-0.740415	-0.406750	-0.209963
16	6	0	-3.346890	-0.931100	0.386786
17	6	0	-4.622867	-1.083831	0.715167
18	1	0	-2.628162	-1.744063	0.298898
19	1	0	-4.995649	-2.080197	0.909289
20	1	0	-5.327510	-0.265867	0.804782
21	7	0	2.133398	3.417574	0.117047
22	1	0	2.533541	4.029576	0.818202
23	1	0	2.754286	2.620337	-0.005451
24	6	0	3.344560	-0.658108	-1.073127
25	6	0	3.247705	-0.760291	0.384284
26	8	0	2.847290	0.459118	-0.298160
27	1	0	4.313430	-0.484592	-1.535131

28	1	0	2.594645	-1.158404	-1.678365
29	1	0	2.396694	-1.324863	0.759653
30	6	0	4.448011	-0.655428	1.284238
31	1	0	4.183162	-0.174439	2.230585
32	1	0	4.828090	-1.655286	1.514932
33	1	0	5.247845	-0.078578	0.813062

Rotational constants (GHZ): 0.4203458 0.2930674 0.1830775

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1313.2470813779 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 3.66D-06 NBF= 482

NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000238 -0.000008 0.000443 Ang= 0.06 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3205.64837289 A.U. after 9 cycles

NFock= 9 Conv=0.38D-08 -V/T= 2.0018

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000037896	0.000005555	-0.000014561
2	6	0.000001249	-0.000038024	0.000031578
3	7	0.000044580	0.000092637	0.000047927
4	6	-0.000092177	-0.000114810	-0.000018867
5	7	-0.000001746	-0.000013210	-0.000068830
6	6	0.000022416	0.000037569	0.000051547
7	6	-0.000136356	-0.000065033	0.000056302
8	1	0.000019134	0.000003959	-0.000009646
9	1	0.000004264	0.000021815	-0.000018585
10	1	0.000027974	-0.000000429	0.000018721
11	1	-0.000017101	0.000020266	0.000018977
12	1	0.000005162	0.000001626	0.000006827
13	1	0.000031575	0.000031865	-0.000008698
14	35	-0.000065603	0.000034548	0.000012892
15	1	0.000070112	-0.000022119	-0.000040194
16	6	0.000006936	-0.000019844	0.000010560
17	6	0.000007866	-0.000016398	-0.000007480
18	1	-0.000021997	0.000026167	0.000007243
19	1	-0.000010666	0.000006992	-0.000005440
20	1	0.000004054	-0.000008859	-0.000010596
21	7	0.000056329	0.000073850	-0.000131230
22	1	0.000008024	-0.000010279	0.000046490
23	1	0.000021031	-0.000003872	0.000074141
24	6	-0.000054553	0.000077507	0.000251451
25	6	0.000069456	-0.000111896	0.000220510
26	8	-0.000053647	-0.000022956	-0.000197248
27	1	0.000006777	-0.000035097	-0.000100831
28	1	0.000074731	-0.000012640	-0.000057355
29	1	-0.000065470	0.000039522	-0.000082214
30	6	0.000050005	0.000017695	-0.000077419
31	1	-0.000004143	0.000005983	-0.000004735
32	1	0.000018248	-0.000006965	-0.000016789
33	1	0.000011432	0.000004876	0.000015552

Cartesian Forces: Max 0.000251451 RMS 0.000059719

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000305971 RMS 0.000058429
Search for a local minimum.
Step number 42 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 31 32 33 34 35
36 37 38 39 40
41 42
DE= -1.93D-06 DEPred=-1.01D-06 R= 1.91D+00
TightC=F SS= 1.41D+00 RLast= 1.75D-02 DXNew= 1.7446D+00 5.2538D-02
Trust test= 1.91D+00 RLast= 1.75D-02 DXMaxT set to 1.04D+00
ITU= 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0 0 -1 1
ITU= -1 1 1 1 1 1 1 1 1 1 0 -1 -1 1 1 1 -1 1 0 0
ITU= -1 0
Eigenvalues --- 0.00064 0.00097 0.00203 0.00221 0.00483
Eigenvalues --- 0.00657 0.00750 0.00767 0.01315 0.01439
Eigenvalues --- 0.01895 0.02056 0.02169 0.02353 0.02380
Eigenvalues --- 0.02632 0.02734 0.02875 0.03060 0.03091
Eigenvalues --- 0.03166 0.03545 0.03634 0.03973 0.04224
Eigenvalues --- 0.04294 0.04508 0.04672 0.05498 0.05606
Eigenvalues --- 0.05744 0.05774 0.05916 0.07770 0.08690
Eigenvalues --- 0.08900 0.09548 0.10018 0.11325 0.12484
Eigenvalues --- 0.12794 0.13100 0.14602 0.15766 0.15995
Eigenvalues --- 0.16001 0.16002 0.16011 0.16027 0.16130
Eigenvalues --- 0.16396 0.19591 0.21335 0.21791 0.22358
Eigenvalues --- 0.23153 0.23463 0.25141 0.26202 0.28016
Eigenvalues --- 0.29103 0.30044 0.30363 0.31943 0.32471
Eigenvalues --- 0.33684 0.34286 0.34345 0.34398 0.34550
Eigenvalues --- 0.34701 0.34729 0.35102 0.35212 0.35341
Eigenvalues --- 0.35568 0.35763 0.35846 0.35905 0.36419
Eigenvalues --- 0.36631 0.39567 0.40776 0.41882 0.42477
Eigenvalues --- 0.44864 0.45509 0.46485 0.49591 0.54878
Eigenvalues --- 0.58212 0.60633 1.18260
En-DIIS/RFO-DIIS IScMMF= 0 using points: 42 41 40 39 38
RFO step: Lambda=-8.37715819D-07.
DidBck=F Rises=F RFO-DIIS coefs: 2.59493 -1.31482 -0.89041 0.49039 0.11991
Iteration 1 RMS(Cart)= 0.00848796 RMS(Int)= 0.00004075
Iteration 2 RMS(Cart)= 0.00008762 RMS(Int)= 0.00001359

Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00001359

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56502	-0.00003	-0.00001	0.00001	0.00000	2.56502
R2	2.62130	0.00002	0.00001	0.00001	0.00002	2.62132
R3	2.03393	0.00000	0.00000	0.00000	0.00000	2.03393
R4	2.62520	-0.00003	-0.00007	0.00002	-0.00005	2.62514
R5	2.03077	-0.00001	0.00000	-0.00001	-0.00001	2.03075
R6	2.54367	-0.00002	0.00005	-0.00007	-0.00002	2.54365
R7	2.69876	0.00002	0.00014	-0.00001	0.00013	2.69889
R8	2.52053	0.00008	-0.00005	-0.00003	-0.00008	2.52045
R9	2.09299	0.00000	-0.00028	0.00000	-0.00028	2.09271
R10	2.78521	0.00007	0.00005	-0.00004	0.00001	2.78522
R11	2.89656	0.00000	0.00007	-0.00011	-0.00004	2.89652
R12	2.05984	0.00001	0.00009	-0.00004	0.00005	2.05989
R13	2.06130	0.00000	0.00002	0.00000	0.00001	2.06131
R14	2.06953	0.00000	0.00003	-0.00001	0.00003	2.06955
R15	2.07954	-0.00003	0.00010	-0.00006	0.00004	2.07958
R16	2.75462	0.00015	-0.00035	0.00022	-0.00013	2.75449
R17	4.24976	-0.00006	0.00214	-0.00073	0.00141	4.25117
R18	2.50649	0.00000	0.00000	0.00000	0.00000	2.50649
R19	2.05729	-0.00003	-0.00002	-0.00004	-0.00006	2.05723
R20	2.04352	0.00000	0.00001	-0.00001	0.00000	2.04352
R21	2.04721	-0.00001	-0.00002	-0.00001	-0.00003	2.04718
R22	1.91440	0.00003	-0.00002	0.00004	0.00002	1.91442
R23	1.92353	0.00010	-0.00009	0.00004	-0.00006	1.92347
R24	4.12515	0.00004	0.00385	0.00160	0.00546	4.13060
R25	2.76693	-0.00003	-0.00035	-0.00003	-0.00036	2.76657
R26	2.73589	-0.00002	-0.00006	-0.00010	-0.00017	2.73572
R27	2.05474	0.00004	0.00014	0.00002	0.00016	2.05490
R28	2.05188	-0.00001	0.00002	0.00001	0.00002	2.05190
R29	2.74695	0.00008	0.00005	0.00026	0.00031	2.74726
R30	2.05612	0.00000	-0.00005	0.00001	-0.00005	2.05608
R31	2.84192	0.00001	0.00016	-0.00002	0.00014	2.84206
R32	2.06756	0.00000	-0.00003	0.00003	0.00000	2.06756
R33	2.06784	0.00001	0.00001	-0.00001	0.00000	2.06784
R34	2.06534	0.00001	0.00000	-0.00001	-0.00001	2.06533
A1	1.87262	0.00003	-0.00008	0.00003	-0.00005	1.87257
A2	2.27896	0.00001	0.00013	0.00003	0.00016	2.27912
A3	2.13153	-0.00004	-0.00004	-0.00006	-0.00010	2.13143
A4	1.86464	-0.00001	0.00007	-0.00005	0.00002	1.86466
A5	2.27623	-0.00002	-0.00008	-0.00002	-0.00010	2.27613
A6	2.14225	0.00003	0.00000	0.00007	0.00008	2.14232
A7	1.89702	0.00004	-0.00002	0.00002	0.00000	1.89702

A8	2.25298	0.00000	-0.00027	0.00011	-0.00015	2.25282
A9	2.13316	-0.00004	0.00029	-0.00014	0.00015	2.13331
A10	1.89004	-0.00003	-0.00004	0.00003	-0.00001	1.89004
A11	2.14649	-0.00006	0.00028	0.00021	0.00049	2.14698
A12	2.24643	0.00009	-0.00021	-0.00022	-0.00044	2.24599
A13	1.90044	-0.00003	0.00007	-0.00003	0.00003	1.90048
A14	2.20578	-0.00019	-0.00011	0.00001	-0.00010	2.20568
A15	2.17641	0.00022	0.00003	0.00001	0.00005	2.17646
A16	1.95979	0.00009	0.00038	-0.00006	0.00031	1.96010
A17	1.87116	0.00004	-0.00005	0.00003	-0.00002	1.87114
A18	1.89095	-0.00008	-0.00015	0.00018	0.00002	1.89097
A19	1.90651	-0.00004	0.00011	-0.00027	-0.00016	1.90635
A20	1.93040	-0.00004	-0.00033	0.00003	-0.00030	1.93010
A21	1.90343	0.00003	0.00004	0.00010	0.00014	1.90357
A22	1.91631	-0.00002	-0.00008	0.00018	0.00009	1.91641
A23	1.89093	0.00004	0.00018	0.00004	0.00021	1.89114
A24	1.88108	0.00000	-0.00028	-0.00015	-0.00043	1.88065
A25	1.87574	0.00000	-0.00015	0.00007	-0.00008	1.87566
A26	1.90022	-0.00004	-0.00010	0.00011	0.00001	1.90022
A27	1.99894	0.00002	0.00044	-0.00024	0.00020	1.99914
A28	2.16109	0.00003	-0.00020	0.00017	-0.00003	2.16106
A29	1.94589	-0.00002	0.00007	-0.00007	-0.00001	1.94588
A30	2.17621	-0.00001	0.00014	-0.00010	0.00004	2.17625
A31	2.07392	0.00001	0.00006	0.00001	0.00008	2.07400
A32	2.16429	0.00000	-0.00006	0.00002	-0.00004	2.16425
A33	2.04497	-0.00001	0.00000	-0.00003	-0.00004	2.04494
A34	1.94162	-0.00016	0.00023	-0.00025	-0.00003	1.94159
A35	1.91609	0.00031	0.00049	-0.00008	0.00040	1.91649
A36	1.89180	-0.00010	0.00024	-0.00010	0.00014	1.89194
A37	2.08635	0.00004	-0.00043	0.00012	-0.00037	2.08598
A38	2.06802	0.00003	0.00096	-0.00005	0.00097	2.06899
A39	1.99364	0.00003	-0.00004	0.00015	0.00012	1.99376
A40	2.00062	0.00001	0.00033	0.00014	0.00046	2.00108
A41	2.03991	-0.00009	-0.00056	-0.00023	-0.00079	2.03912
A42	2.01678	-0.00006	0.00087	-0.00037	0.00052	2.01730
A43	2.13884	-0.00004	-0.00016	0.00004	-0.00015	2.13870
A44	1.96253	-0.00006	-0.00002	-0.00017	-0.00021	1.96233
A45	2.02897	0.00000	0.00037	-0.00008	0.00032	2.02929
A46	2.04203	0.00011	-0.00069	0.00038	-0.00031	2.04172
A47	2.58758	0.00006	0.01014	0.00383	0.01395	2.60153
A48	2.46437	-0.00001	-0.01030	-0.00386	-0.01410	2.45027
A49	1.93377	-0.00001	-0.00033	0.00016	-0.00017	1.93360
A50	1.91737	0.00000	-0.00001	-0.00006	-0.00008	1.91729
A51	1.94219	0.00002	0.00018	-0.00003	0.00015	1.94234

A52	1.87908	0.00001	0.00004	0.00003	0.00007	1.87915
A53	1.89443	-0.00001	0.00008	-0.00003	0.00005	1.89448
A54	1.89544	-0.00001	0.00004	-0.00006	-0.00003	1.89541
A55	3.49205	0.00017	-0.00064	-0.00059	-0.00124	3.49082
A56	2.52866	0.00023	-0.00121	0.00195	0.00080	2.52946
A57	2.98996	-0.00007	-0.00414	-0.00244	-0.00658	2.98339
A58	3.11185	0.00000	-0.00086	-0.00213	-0.00298	3.10886
D1	0.00312	0.00000	0.00002	0.00017	0.00018	0.00330
D2	-3.12557	0.00000	0.00018	0.00002	0.00020	-3.12537
D3	3.13219	0.00000	0.00009	0.00021	0.00030	3.13249
D4	0.00351	0.00001	0.00026	0.00006	0.00031	0.00382
D5	-0.00484	0.00001	0.00015	-0.00004	0.00011	-0.00473
D6	-3.11191	0.00001	0.00044	0.00025	0.00069	-3.11122
D7	-3.13521	0.00001	0.00008	-0.00008	0.00000	-3.13520
D8	0.04091	0.00000	0.00037	0.00021	0.00058	0.04149
D9	-0.00037	-0.00001	-0.00018	-0.00024	-0.00041	-0.00078
D10	-3.13330	0.00001	-0.00046	0.00005	-0.00041	-3.13371
D11	3.12954	-0.00001	-0.00032	-0.00010	-0.00043	3.12912
D12	-0.00339	0.00000	-0.00061	0.00018	-0.00042	-0.00381
D13	-0.00266	0.00002	0.00027	0.00021	0.00049	-0.00217
D14	-3.12307	0.00001	-0.00131	-0.00043	-0.00174	-3.12480
D15	3.13099	0.00000	0.00053	-0.00005	0.00048	3.13147
D16	0.01058	-0.00001	-0.00105	-0.00069	-0.00174	0.00884
D17	-0.05783	0.00001	0.00116	0.00193	0.00309	-0.05474
D18	3.08521	0.00000	0.00136	0.00178	0.00314	3.08834
D19	3.09346	0.00003	0.00085	0.00225	0.00309	3.09655
D20	-0.04669	0.00002	0.00105	0.00209	0.00314	-0.04355
D21	0.00462	-0.00002	-0.00026	-0.00011	-0.00037	0.00425
D22	3.11241	-0.00002	-0.00055	-0.00039	-0.00094	3.11147
D23	3.12344	-0.00002	0.00144	0.00059	0.00203	3.12548
D24	-0.05196	-0.00002	0.00116	0.00031	0.00147	-0.05049
D25	1.33577	-0.00003	-0.00059	0.00119	0.00060	1.33637
D26	-2.85339	0.00001	-0.00026	0.00084	0.00058	-2.85281
D27	-0.80140	0.00002	-0.00031	0.00106	0.00075	-0.80065
D28	-1.76609	-0.00003	-0.00025	0.00151	0.00126	-1.76482
D29	0.32794	0.00000	0.00008	0.00117	0.00125	0.32919
D30	2.37993	0.00002	0.00002	0.00139	0.00142	2.38135
D31	-1.10664	0.00006	0.00125	-0.00023	0.00102	-1.10562
D32	0.93711	0.00007	0.00113	-0.00002	0.00111	0.93821
D33	3.10912	0.00012	0.00159	-0.00038	0.00121	3.11033
D34	3.10318	-0.00002	0.00101	-0.00005	0.00095	3.10413
D35	-1.13626	-0.00001	0.00088	0.00016	0.00103	-1.13522
D36	1.03575	0.00004	0.00134	-0.00020	0.00114	1.03689
D37	1.00803	-0.00001	0.00109	-0.00002	0.00106	1.00910

D38	3.05178	0.00001	0.00096	0.00019	0.00114	3.05292
D39	-1.05939	0.00005	0.00142	-0.00017	0.00125	-1.05815
D40	2.93726	-0.00004	0.00013	0.00191	0.00205	2.93931
D41	-1.25197	-0.00007	0.00090	0.00157	0.00247	-1.24950
D42	0.85954	0.00000	0.00045	0.00172	0.00217	0.86171
D43	2.95349	-0.00002	0.00122	0.00138	0.00260	2.95609
D44	-1.24041	0.00003	0.00043	0.00170	0.00214	-1.23828
D45	0.85354	0.00000	0.00120	0.00136	0.00256	0.85610
D46	3.13855	-0.00001	0.00005	0.00002	0.00007	3.13862
D47	-0.00450	0.00000	0.00007	0.00018	0.00025	-0.00425
D48	-0.00468	0.00000	-0.00018	0.00019	0.00002	-0.00467
D49	3.13545	0.00001	-0.00015	0.00035	0.00020	3.13565
D50	2.20791	-0.00003	-0.00002	0.00075	0.00070	2.20861
D51	-1.40518	-0.00015	-0.00029	-0.00129	-0.00156	-1.40674
D52	-2.08691	0.00009	0.00049	0.00151	0.00197	-2.08494
D53	0.58317	-0.00003	0.00021	-0.00053	-0.00028	0.58289
D54	-2.71221	0.00000	-0.00025	0.00014	-0.00011	-2.71231
D55	-0.01681	0.00004	-0.00037	0.00035	-0.00002	-0.01683
D56	-0.02448	-0.00006	-0.00045	-0.00030	-0.00075	-0.02523
D57	2.67091	-0.00002	-0.00057	-0.00009	-0.00066	2.67026
D58	0.53787	-0.00005	-0.01094	-0.00435	-0.01534	0.52253
D59	-1.88347	0.00004	-0.01037	-0.00432	-0.01475	-1.89822
D60	1.80890	-0.00001	-0.00977	-0.00294	-0.01269	1.79620
D61	-0.61209	-0.00012	-0.00906	-0.00327	-0.01231	-0.62441
D62	2.55263	-0.00001	-0.00175	0.00028	-0.00147	2.55115
D63	-1.65654	0.00000	-0.00190	0.00037	-0.00154	-1.65808
D64	0.44317	-0.00001	-0.00175	0.00023	-0.00152	0.44165
D65	1.34656	0.00003	-0.00193	0.00041	-0.00152	1.34504
D66	-2.86261	0.00003	-0.00209	0.00051	-0.00158	-2.86419
D67	-0.76289	0.00003	-0.00193	0.00036	-0.00157	-0.76446
D68	-1.04118	-0.00001	-0.00150	0.00031	-0.00118	-1.04236
D69	1.03284	-0.00001	-0.00165	0.00041	-0.00125	1.03159
D70	3.13255	-0.00001	-0.00150	0.00027	-0.00123	3.13132

Item	Value	Threshold	Converged?
Maximum Force	0.000306	0.000450	YES
RMS Force	0.000058	0.000300	YES
Maximum Displacement	0.041010	0.001800	NO
RMS Displacement	0.008517	0.001200	NO

Predicted change in Energy=-2.057825D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-2.642092	2.100100	-0.187288
2	6	0	-3.531430	1.115667	0.099722
3	7	0	-2.820982	-0.078045	0.109686
4	6	0	-1.530391	0.185752	-0.167107
5	7	0	-1.402473	1.500211	-0.353554
6	6	0	-0.130597	2.186990	-0.641597
7	6	0	0.455677	2.870062	0.599003
8	1	0	-2.783499	3.161484	-0.296427
9	1	0	-4.589216	1.164111	0.282939
10	1	0	0.569378	1.432309	-1.000341
11	1	0	-0.305784	2.915857	-1.434002
12	1	0	-0.223123	3.656750	0.945021
13	1	0	0.531821	2.122355	1.402846
14	35	0	0.137712	-2.665918	-0.292916
15	1	0	-0.754678	-0.601687	-0.234761
16	6	0	-3.292690	-1.404471	0.350134
17	6	0	-4.545762	-1.695082	0.673613
18	1	0	-2.496332	-2.137846	0.235642
19	1	0	-4.816101	-2.729578	0.835254
20	1	0	-5.328600	-0.955317	0.789799
21	7	0	1.723931	3.477027	0.214598
22	1	0	2.066604	4.099752	0.936466
23	1	0	2.420498	2.751329	0.059072
24	6	0	3.326937	-0.422099	-1.128080
25	6	0	3.255777	-0.568024	0.326897
26	8	0	2.728656	0.621200	-0.322242
27	1	0	4.269198	-0.142004	-1.592987
28	1	0	2.625040	-0.980100	-1.740438
29	1	0	2.469106	-1.223092	0.695466
30	6	0	4.449147	-0.365566	1.219505
31	1	0	4.147762	0.065441	2.178914
32	1	0	4.928089	-1.328037	1.423618
33	1	0	5.183531	0.297835	0.755759

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357352	0.000000			
3	N	2.205564	1.389166	0.000000		
4	C	2.213824	2.222633	1.346043	0.000000	
5	N	1.387144	2.210382	2.172016	1.333764	0.000000
6	C	2.553734	3.641834	3.596246	2.487874	1.473874

7	C	3.287441	4.384541	4.434779	3.425917	2.497314
8	H	1.076310	2.213978	3.265100	3.231406	2.161094
9	H	2.210991	1.074629	2.167860	3.242860	3.267020
10	H	3.379429	4.257585	3.873999	2.580157	2.076329
11	H	2.770937	3.999723	4.203884	3.249331	2.091446
12	H	3.091390	4.256351	4.625511	3.872157	2.779896
13	H	3.550035	4.384240	4.213706	3.235414	2.685796
14	Br	5.518460	5.283669	3.951336	3.306119	4.442126
15	H	3.296094	3.282001	2.159273	1.107415	2.202663
16	C	3.604736	2.543777	1.428191	2.429413	3.536280
17	C	4.332265	3.042784	2.430574	3.651960	4.598395
18	H	4.261490	3.416906	2.089029	2.548403	3.844364
19	H	5.394228	4.120351	3.396700	4.505526	5.563922
20	H	4.184208	2.827543	2.742317	4.079718	4.769837
21	N	4.595606	5.762641	5.771116	4.644222	3.742326
22	H	5.237676	6.398663	6.482751	5.429147	4.522860
23	H	5.110245	6.172721	5.956596	4.716233	4.043595
24	C	6.547968	7.135083	6.280712	4.988645	5.163573
25	C	6.493700	6.996614	6.100350	4.870280	5.141975
26	O	5.572279	6.293745	5.610169	4.284059	4.223727
27	H	7.400605	8.080643	7.292040	5.981286	6.033317
28	H	6.296236	6.758738	5.822012	4.593711	4.929122
29	H	6.160131	6.467699	5.444200	4.327222	4.848293
30	C	7.638340	8.193752	7.359969	6.162914	6.340118
31	H	7.472675	8.024712	7.270880	6.144893	6.267142
32	H	8.464914	8.904372	7.958455	6.821577	7.157746
33	H	8.085658	8.777800	8.039336	6.777977	6.786142

		6	7	8	9	10
6	C	0.000000				
7	C	1.532773	0.000000			
8	H	2.847222	3.373276	0.000000		
9	H	4.666941	5.334896	2.754229	0.000000	
10	H	1.090049	2.153594	3.837621	5.322578	0.000000
11	H	1.090799	2.171412	2.737423	4.936020	1.776199
12	H	2.164742	1.095161	2.888253	5.070934	3.059515
13	H	2.150052	1.100466	3.867644	5.328926	2.500577
14	Br	4.872812	5.616378	6.518597	6.111022	4.181178
15	H	2.886471	3.770034	4.275672	4.253203	2.544872
16	C	4.886815	5.690679	4.639533	2.878039	4.978622
17	C	6.024446	6.772038	5.256689	2.886087	6.224737
18	H	5.007041	5.824563	5.333710	3.909644	4.865412
19	H	6.950372	7.694376	6.333781	3.939205	7.049404
20	H	6.240370	6.937419	4.960391	2.301210	6.609955
21	N	2.415893	1.457615	4.547268	6.723845	2.643850

22	H	3.313100	2.054533	5.091550	7.303769	3.620520
23	H	2.705087	2.041113	5.232226	7.190652	2.507751
24	C	4.358733	4.697368	7.132401	8.195884	3.325549
25	C	4.471646	4.442414	7.125351	8.034062	3.602726
26	O	3.275517	3.327537	6.069396	7.362897	2.404204
27	H	5.068289	5.331069	7.895229	9.148581	4.064278
28	H	4.339521	5.000286	6.963489	7.793406	3.254720
29	H	4.491643	4.562577	6.913626	7.462495	3.679114
30	C	5.563569	5.177075	8.188364	9.214612	4.817954
31	H	5.546225	4.898317	7.984684	9.007585	4.978034
32	H	6.496986	6.189223	9.087516	9.904092	5.700302
33	H	5.810461	5.384563	8.531187	9.822453	5.065700

		11	12	13	14	15
11	H	0.000000				
12	H	2.493091	0.000000			
13	H	3.062505	1.770286	0.000000		
14	Br	5.714454	6.452815	5.094948	0.000000	
15	H	3.743367	4.450699	3.428884	2.249621	0.000000
16	C	5.547070	5.949125	5.307881	3.711122	2.725448
17	C	6.609101	6.884837	6.394252	4.879717	4.048824
18	H	5.755530	6.264825	5.355501	2.737960	2.369477
19	H	7.573864	7.867190	7.243182	5.081052	4.708291
20	H	6.720116	6.881944	6.647739	5.829150	4.700589
21	N	2.674423	2.087304	2.160601	6.364703	4.793885
22	H	3.556536	2.332204	2.546207	7.141870	5.606687
23	H	3.112708	2.931454	2.401757	5.889107	4.627180
24	C	4.942893	5.791173	4.548901	3.987904	4.182087
25	C	5.284213	5.507590	3.976902	3.808892	4.049734
26	O	3.963494	4.419674	3.171038	4.185570	3.692793
27	H	5.505111	6.407259	5.298143	5.012933	5.224501
28	H	4.884886	6.068286	4.887435	3.335281	3.719241
29	H	5.418999	5.578820	3.930073	2.914454	3.412367
30	C	6.357531	6.171262	4.644223	5.115418	5.408367
31	H	6.404069	5.790046	4.231809	5.445252	5.504980
32	H	7.319156	7.184159	5.588631	5.261570	5.964196
33	H	6.463873	6.367891	5.038452	5.945068	6.087084

		16	17	18	19	20
16	C	0.000000				
17	C	1.326380	0.000000			
18	H	1.088638	2.141966	0.000000		
19	H	2.076543	1.081384	2.467997	0.000000	
20	H	2.130721	1.083322	3.118846	1.847355	0.000000
21	N	7.000992	8.140667	7.024092	9.037653	8.349534
22	H	7.704693	8.796169	7.760101	9.696475	8.959033

23	H	7.070778	8.287159	6.936168	9.111046	8.621003
24	C	6.853439	8.175938	6.222057	8.688395	8.881491
25	C	6.601713	7.890151	5.963173	8.371736	8.605568
26	O	6.388431	7.698964	5.934987	8.336118	8.285011
27	H	7.908963	9.233257	7.286952	9.753694	9.922543
28	H	6.290478	7.599950	5.610144	8.066315	8.346442
29	H	5.774985	7.030763	5.069891	7.440651	7.802873
30	C	7.859464	9.109006	7.235236	9.569797	9.804936
31	H	7.801629	8.996818	7.264625	9.485167	9.631875
32	H	8.290923	9.510577	7.562348	9.862034	10.283010
33	H	8.654981	9.931646	8.073621	10.448166	10.586616

		21	22	23	24	25
21	N	0.000000				
22	H	1.013067	0.000000			
23	H	1.017856	1.647211	0.000000		
24	C	4.424431	5.128150	3.507365	0.000000	
25	C	4.326847	4.855291	3.433298	1.464006	0.000000
26	O	3.074641	3.758056	2.185821	1.447683	1.453786
27	H	4.779449	5.407592	3.810298	1.087404	2.212345
28	H	4.949762	5.769104	4.147727	1.085821	2.200343
29	H	4.783058	5.343478	4.025343	2.168590	1.088030
30	C	4.816862	5.069092	3.895775	2.602634	1.503951
31	H	4.623031	4.706439	3.832906	3.442043	2.151019
32	H	5.900592	6.155185	4.979079	3.145722	2.139402
33	H	4.729582	4.919599	3.760234	2.741184	2.156355

		26	27	28	29	30
26	O	0.000000				
27	H	2.137882	0.000000			
28	H	2.141536	1.851324	0.000000		
29	H	2.122383	3.105817	2.452955	0.000000	
30	C	2.512127	2.827097	3.530762	2.220479	0.000000
31	H	2.928910	3.779553	4.332800	2.584342	1.094105
32	H	3.418341	3.307675	3.928911	2.566673	1.094256
33	H	2.700566	2.558529	3.796049	3.112066	1.092923

		31	32	33
31	H	0.000000		
32	H	1.766681	0.000000	
33	H	1.775442	1.776160	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.346761	2.471957	-0.264412
2	6	0	-3.331973	1.591889	0.047425
3	7	0	-2.745500	0.333729	0.100966
4	6	0	-1.433752	0.457172	-0.174552
5	7	0	-1.173233	1.745297	-0.402128
6	6	0	0.162572	2.290865	-0.702603
7	6	0	0.809539	2.951663	0.519760
8	1	0	-2.380021	3.538046	-0.408601
9	1	0	-4.380244	1.752457	0.221129
10	1	0	0.784408	1.458280	-1.031736
11	1	0	0.065034	3.007375	-1.519269
12	1	0	0.212048	3.813530	0.835302
13	1	0	0.806593	2.226756	1.347726
14	35	0	-0.061041	-2.550420	-0.196392
15	1	0	-0.741077	-0.406095	-0.211138
16	6	0	-3.349486	-0.929948	0.380344
17	6	0	-4.626801	-1.082303	0.703663
18	1	0	-2.630627	-1.743061	0.295364
19	1	0	-5.000696	-2.078519	0.896404
20	1	0	-5.331572	-0.264140	0.790231
21	7	0	2.134096	3.415081	0.125509
22	1	0	2.534780	4.023427	0.829548
23	1	0	2.754617	2.618299	-0.001471
24	6	0	3.341535	-0.667303	-1.079411
25	6	0	3.249979	-0.757711	0.378930
26	8	0	2.848104	0.456660	-0.311934
27	1	0	4.309153	-0.498759	-1.546054
28	1	0	2.589527	-1.171573	-1.678746
29	1	0	2.399766	-1.317924	0.762475
30	6	0	4.453954	-0.647273	1.273423
31	1	0	4.193555	-0.157017	2.216242
32	1	0	4.832601	-1.645855	1.511868
33	1	0	5.253382	-0.076622	0.794097

Rotational constants (GHZ): 0.4207628 0.2929034 0.1830007

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons
nuclear repulsion energy 1313.2079729428 Hartrees.
NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 482 RedAO= T EigKep= 3.65D-06 NBF= 482
NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 0.000337 -0.000082 0.000120 Ang= 0.04 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3205.64837590 A.U. after 9 cycles
NFock= 9 Conv=0.83D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Atomic Forces (Hartrees/Bohr)
Number Number X Y Z
---
1 6 -0.000019953 -0.000012127 -0.000020365
2 6 0.000003832 0.000001310 0.000035909
3 7 0.000007383 0.000020652 0.000007116
4 6 -0.000077496 -0.000063871 0.000054603
5 7 -0.000009201 0.000072688 -0.000058079

6	6	0.000004771	-0.000003580	0.000022368
7	6	-0.000187250	-0.000096352	0.000044966
8	1	0.000007452	0.000003475	-0.000011742
9	1	0.000004492	0.000014255	-0.000002284
10	1	0.000035258	0.000021433	-0.000003400
11	1	-0.000018035	0.000003478	0.000015010
12	1	0.000014154	-0.000002936	0.000003826
13	1	0.000027795	0.000027627	-0.000016669
14	35	-0.000060808	0.000048613	0.000015411
15	1	0.000064037	-0.000107854	-0.000040652
16	6	0.000012449	0.000009287	-0.000005393
17	6	0.000014329	-0.000009823	-0.000015504
18	1	-0.000002807	0.000010555	0.000007790
19	1	-0.000001793	0.000005548	0.000001039
20	1	-0.000006028	-0.000004931	-0.000009286
21	7	0.000096560	0.000121721	-0.000084905
22	1	0.000019743	-0.000015072	0.000035377
23	1	0.000036105	-0.000014942	0.000035896
24	6	0.000026849	0.000069328	0.000047687
25	6	0.000021822	-0.000115844	0.000291628
26	8	0.000020244	-0.000017942	-0.000107559
27	1	-0.000021500	-0.000007353	-0.000064412
28	1	0.000021200	-0.000015464	0.000024070
29	1	-0.000067352	0.000003804	-0.000122436
30	6	0.000000166	0.000046440	-0.000085346
31	1	0.000014338	0.000000220	0.000012323
32	1	0.000014654	-0.000004202	-0.000019559
33	1	0.000004589	0.000011856	0.000012572

Cartesian Forces: Max 0.000291628 RMS 0.000054347

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000224635 RMS 0.000050946
Search for a local minimum.
Step number 43 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 31 32 33 34 35
36 37 38 39 40

41 42 43

DE= -3.00D-06 DEPred=-2.06D-06 R= 1.46D+00

TightC=F SS= 1.41D+00 RLast= 3.72D-02 DXNew= 1.7446D+00 1.1147D-01

Trust test= 1.46D+00 RLast= 3.72D-02 DXMaxT set to 1.04D+00

ITU= 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0 0 -1

ITU= 1 -1 1 1 1 1 1 1 1 1 1 0 -1 -1 1 1 1 -1 1 0

ITU= 0 -1 0

Eigenvalues ---	0.00065	0.00102	0.00154	0.00243	0.00482
Eigenvalues ---	0.00663	0.00729	0.00757	0.01275	0.01431
Eigenvalues ---	0.01892	0.02030	0.02167	0.02365	0.02382
Eigenvalues ---	0.02631	0.02707	0.02878	0.03068	0.03096
Eigenvalues ---	0.03209	0.03526	0.03632	0.03980	0.04151
Eigenvalues ---	0.04301	0.04483	0.04717	0.05498	0.05560
Eigenvalues ---	0.05720	0.05746	0.05914	0.07722	0.08670
Eigenvalues ---	0.08955	0.09560	0.10227	0.11312	0.12206
Eigenvalues ---	0.12642	0.13101	0.14616	0.15791	0.15998
Eigenvalues ---	0.16001	0.16002	0.16012	0.16035	0.16156
Eigenvalues ---	0.16386	0.18861	0.21275	0.21722	0.22175
Eigenvalues ---	0.23167	0.23351	0.25225	0.26321	0.28479
Eigenvalues ---	0.29022	0.30103	0.30422	0.32031	0.32485
Eigenvalues ---	0.33705	0.34289	0.34340	0.34399	0.34550
Eigenvalues ---	0.34705	0.34730	0.35105	0.35226	0.35345
Eigenvalues ---	0.35568	0.35749	0.35874	0.35969	0.36421
Eigenvalues ---	0.36628	0.39683	0.41497	0.41875	0.42542
Eigenvalues ---	0.44754	0.45501	0.46515	0.49579	0.54914
Eigenvalues ---	0.58317	0.60653	1.07706		

En-DIIS/RFO-DIIS IScMMF= 0 using points: 43 42 41 40 39

RFO step: Lambda=-6.14267780D-07.

DidBck=F Rises=F RFO-DIIS coefs: 1.65903 -0.57939 -0.39030 0.00679 0.30388

Iteration 1 RMS(Cart)= 0.00814373 RMS(Int)= 0.00002320

Iteration 2 RMS(Cart)= 0.00004088 RMS(Int)= 0.00000418

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000418

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56502	-0.00002	-0.00001	-0.00002	-0.00003	2.56499
R2	2.62132	0.00001	0.00001	-0.00001	0.00000	2.62132
R3	2.03393	0.00000	0.00000	0.00001	0.00001	2.03394
R4	2.62514	-0.00001	-0.00002	0.00000	-0.00002	2.62512
R5	2.03075	0.00000	-0.00002	0.00000	-0.00001	2.03074
R6	2.54365	-0.00003	-0.00005	0.00000	-0.00005	2.54360
R7	2.69889	-0.00001	0.00007	-0.00002	0.00005	2.69894
R8	2.52045	0.00012	0.00003	0.00012	0.00015	2.52060
R9	2.09271	0.00005	-0.00004	0.00007	0.00003	2.09274

R10	2.78522	0.00006	0.00004	0.00002	0.00006	2.78528
R11	2.89652	0.00001	-0.00009	0.00004	-0.00005	2.89647
R12	2.05989	0.00001	0.00006	0.00002	0.00008	2.05998
R13	2.06131	-0.00001	0.00000	-0.00002	-0.00002	2.06129
R14	2.06955	-0.00001	0.00000	-0.00003	-0.00003	2.06952
R15	2.07958	-0.00003	-0.00006	-0.00004	-0.00010	2.07948
R16	2.75449	0.00020	0.00026	0.00021	0.00048	2.75497
R17	4.25117	-0.00007	0.00007	0.00010	0.00017	4.25133
R18	2.50649	-0.00001	0.00000	-0.00001	-0.00001	2.50649
R19	2.05723	-0.00001	-0.00009	0.00005	-0.00004	2.05719
R20	2.04352	0.00000	-0.00001	0.00000	0.00000	2.04352
R21	2.04718	0.00000	-0.00003	0.00001	-0.00001	2.04717
R22	1.91442	0.00002	0.00007	0.00000	0.00007	1.91449
R23	1.92347	0.00008	0.00005	0.00001	0.00006	1.92353
R24	4.13060	0.00002	0.00255	0.00124	0.00378	4.13439
R25	2.76657	0.00003	-0.00015	0.00008	-0.00007	2.76650
R26	2.73572	-0.00002	-0.00044	-0.00006	-0.00049	2.73523
R27	2.05490	0.00001	0.00016	-0.00004	0.00012	2.05502
R28	2.05190	-0.00002	0.00004	-0.00001	0.00002	2.05193
R29	2.74726	0.00004	0.00059	0.00010	0.00069	2.74794
R30	2.05608	0.00000	0.00002	0.00000	0.00002	2.05610
R31	2.84206	-0.00001	0.00001	-0.00010	-0.00008	2.84197
R32	2.06756	0.00001	-0.00003	0.00002	-0.00001	2.06755
R33	2.06784	0.00001	0.00001	0.00000	0.00002	2.06786
R34	2.06533	0.00001	0.00001	0.00000	0.00001	2.06533
A1	1.87257	0.00003	-0.00003	0.00005	0.00002	1.87259
A2	2.27912	-0.00001	0.00016	-0.00003	0.00013	2.27925
A3	2.13143	-0.00003	-0.00013	-0.00002	-0.00015	2.13128
A4	1.86466	-0.00001	0.00000	-0.00001	-0.00001	1.86464
A5	2.27613	-0.00001	-0.00009	0.00001	-0.00008	2.27605
A6	2.14232	0.00002	0.00010	0.00001	0.00010	2.14243
A7	1.89702	0.00003	0.00006	0.00002	0.00008	1.89710
A8	2.25282	0.00003	-0.00012	0.00005	-0.00007	2.25275
A9	2.13331	-0.00007	0.00006	-0.00007	-0.00001	2.13330
A10	1.89004	-0.00002	-0.00006	-0.00001	-0.00007	1.88996
A11	2.14698	-0.00010	0.00053	-0.00029	0.00024	2.14722
A12	2.24599	0.00012	-0.00044	0.00030	-0.00014	2.24585
A13	1.90048	-0.00005	0.00004	-0.00005	-0.00001	1.90047
A14	2.20568	-0.00014	-0.00029	-0.00015	-0.00044	2.20524
A15	2.17646	0.00018	0.00023	0.00019	0.00042	2.17688
A16	1.96010	0.00001	0.00035	-0.00012	0.00023	1.96034
A17	1.87114	0.00007	0.00017	0.00035	0.00052	1.87166
A18	1.89097	-0.00006	-0.00017	-0.00021	-0.00038	1.89060
A19	1.90635	-0.00003	-0.00012	0.00009	-0.00003	1.90632

A20	1.93010	0.00000	-0.00038	0.00001	-0.00037	1.92974
A21	1.90357	0.00000	0.00017	-0.00012	0.00005	1.90362
A22	1.91641	-0.00002	0.00016	-0.00003	0.00013	1.91653
A23	1.89114	0.00001	0.00038	-0.00004	0.00034	1.89148
A24	1.88065	0.00007	-0.00043	0.00015	-0.00027	1.88038
A25	1.87566	0.00001	0.00004	0.00004	0.00008	1.87574
A26	1.90022	-0.00006	-0.00006	-0.00005	-0.00011	1.90011
A27	1.99914	-0.00001	-0.00009	-0.00006	-0.00015	1.99899
A28	2.16106	0.00003	0.00004	-0.00001	0.00003	2.16109
A29	1.94588	-0.00002	-0.00002	-0.00002	-0.00004	1.94583
A30	2.17625	-0.00001	-0.00002	0.00003	0.00001	2.17626
A31	2.07400	0.00000	0.00009	-0.00006	0.00003	2.07403
A32	2.16425	0.00001	-0.00005	0.00008	0.00003	2.16428
A33	2.04494	-0.00001	-0.00004	-0.00001	-0.00006	2.04488
A34	1.94159	-0.00011	-0.00036	0.00001	-0.00035	1.94125
A35	1.91649	0.00022	0.00000	0.00001	0.00001	1.91651
A36	1.89194	-0.00008	-0.00021	-0.00012	-0.00033	1.89161
A37	2.08598	0.00008	-0.00004	0.00039	0.00037	2.08635
A38	2.06899	-0.00006	0.00103	-0.00052	0.00050	2.06948
A39	1.99376	0.00000	0.00031	-0.00001	0.00030	1.99406
A40	2.00108	0.00001	0.00054	-0.00013	0.00041	2.00148
A41	2.03912	-0.00003	-0.00124	0.00014	-0.00109	2.03803
A42	2.01730	-0.00009	0.00039	-0.00041	-0.00002	2.01728
A43	2.13870	-0.00003	-0.00046	0.00000	-0.00047	2.13823
A44	1.96233	-0.00002	-0.00058	0.00005	-0.00052	1.96180
A45	2.02929	-0.00005	0.00018	-0.00021	-0.00003	2.02926
A46	2.04172	0.00012	0.00031	0.00040	0.00072	2.04244
A47	2.60153	0.00002	0.00528	0.00300	0.00830	2.60982
A48	2.45027	0.00002	-0.00492	-0.00305	-0.00799	2.44227
A49	1.93360	0.00003	-0.00014	0.00019	0.00005	1.93364
A50	1.91729	-0.00001	-0.00002	-0.00002	-0.00004	1.91726
A51	1.94234	0.00001	0.00010	-0.00009	0.00000	1.94235
A52	1.87915	0.00000	0.00009	-0.00004	0.00005	1.87920
A53	1.89448	-0.00002	0.00003	-0.00002	0.00001	1.89448
A54	1.89541	-0.00001	-0.00005	-0.00002	-0.00007	1.89534
A55	3.49082	0.00013	-0.00120	-0.00091	-0.00211	3.48871
A56	2.52946	0.00020	0.00120	-0.00107	0.00012	2.52958
A57	2.98339	-0.00007	-0.00559	-0.00260	-0.00819	2.97519
A58	3.10886	0.00001	-0.00153	0.00066	-0.00086	3.10800
D1	0.00330	-0.00001	-0.00001	-0.00010	-0.00011	0.00319
D2	-3.12537	0.00000	-0.00002	-0.00027	-0.00029	-3.12566
D3	3.13249	-0.00001	0.00030	0.00001	0.00032	3.13281
D4	0.00382	0.00000	0.00029	-0.00016	0.00014	0.00396
D5	-0.00473	0.00001	0.00019	-0.00003	0.00016	-0.00457

D6	-3.11122	0.00000	0.00081	0.00035	0.00116	-3.11007
D7	-3.13520	0.00001	-0.00009	-0.00013	-0.00022	-3.13543
D8	0.04149	0.00000	0.00052	0.00025	0.00077	0.04226
D9	-0.00078	0.00001	-0.00018	0.00020	0.00002	-0.00076
D10	-3.13371	0.00001	0.00015	0.00007	0.00022	-3.13349
D11	3.12912	0.00000	-0.00017	0.00035	0.00018	3.12930
D12	-0.00381	0.00001	0.00016	0.00023	0.00039	-0.00343
D13	-0.00217	0.00000	0.00030	-0.00022	0.00008	-0.00209
D14	-3.12480	0.00000	-0.00123	-0.00041	-0.00164	-3.12645
D15	3.13147	-0.00001	0.00000	-0.00010	-0.00011	3.13137
D16	0.00884	0.00000	-0.00153	-0.00030	-0.00183	0.00701
D17	-0.05474	0.00002	0.00430	0.00216	0.00646	-0.04828
D18	3.08834	0.00001	0.00398	0.00221	0.00619	3.09454
D19	3.09655	0.00002	0.00467	0.00202	0.00669	3.10324
D20	-0.04355	0.00002	0.00435	0.00207	0.00642	-0.03713
D21	0.00425	0.00000	-0.00031	0.00015	-0.00015	0.00410
D22	3.11147	-0.00001	-0.00092	-0.00023	-0.00115	3.11032
D23	3.12548	-0.00001	0.00136	0.00035	0.00171	3.12718
D24	-0.05049	-0.00002	0.00075	-0.00003	0.00071	-0.04978
D25	1.33637	-0.00001	0.00119	0.00234	0.00353	1.33989
D26	-2.85281	0.00001	0.00136	0.00261	0.00397	-2.84884
D27	-0.80065	0.00002	0.00156	0.00255	0.00410	-0.79655
D28	-1.76482	-0.00001	0.00190	0.00279	0.00468	-1.76014
D29	0.32919	0.00001	0.00207	0.00306	0.00512	0.33431
D30	2.38135	0.00002	0.00227	0.00299	0.00526	2.38660
D31	-1.10562	0.00006	0.00158	0.00125	0.00283	-1.10279
D32	0.93821	0.00006	0.00194	0.00126	0.00319	0.94141
D33	3.11033	0.00010	0.00180	0.00125	0.00305	3.11338
D34	3.10413	-0.00001	0.00122	0.00083	0.00206	3.10619
D35	-1.13522	-0.00001	0.00158	0.00084	0.00242	-1.13280
D36	1.03689	0.00002	0.00145	0.00083	0.00228	1.03917
D37	1.00910	-0.00001	0.00133	0.00091	0.00224	1.01134
D38	3.05292	0.00000	0.00169	0.00092	0.00261	3.05553
D39	-1.05815	0.00003	0.00156	0.00091	0.00247	-1.05568
D40	2.93931	-0.00002	0.00153	-0.00011	0.00142	2.94073
D41	-1.24950	-0.00005	0.00104	-0.00024	0.00079	-1.24870
D42	0.86171	0.00000	0.00161	-0.00013	0.00148	0.86319
D43	2.95609	-0.00003	0.00112	-0.00026	0.00086	2.95695
D44	-1.23828	0.00003	0.00165	-0.00010	0.00155	-1.23672
D45	0.85610	0.00001	0.00116	-0.00023	0.00093	0.85703
D46	3.13862	0.00000	0.00006	0.00029	0.00035	3.13896
D47	-0.00425	0.00001	0.00036	0.00029	0.00064	-0.00361
D48	-0.00467	0.00000	0.00042	0.00024	0.00065	-0.00402
D49	3.13565	0.00001	0.00072	0.00023	0.00095	3.13660

D50	2.20861	-0.00004	0.00172	-0.00139	0.00033	2.20894
D51	-1.40674	-0.00009	0.00123	-0.00067	0.00055	-1.40619
D52	-2.08494	0.00005	0.00202	-0.00207	-0.00005	-2.08499
D53	0.58289	0.00000	0.00153	-0.00136	0.00016	0.58306
D54	-2.71231	-0.00002	-0.00042	0.00007	-0.00036	-2.71267
D55	-0.01683	0.00003	0.00027	0.00012	0.00039	-0.01645
D56	-0.02523	-0.00004	-0.00132	0.00014	-0.00118	-0.02641
D57	2.67026	0.00001	-0.00064	0.00020	-0.00044	2.66982
D58	0.52253	-0.00003	-0.00521	-0.00382	-0.00902	0.51351
D59	-1.89822	0.00000	-0.00421	-0.00389	-0.00809	-1.90631
D60	1.79620	0.00005	-0.00552	-0.00211	-0.00763	1.78858
D61	-0.62441	-0.00007	-0.00555	-0.00257	-0.00812	-0.63253
D62	2.55115	-0.00001	-0.00022	0.00054	0.00032	2.55147
D63	-1.65808	0.00000	-0.00021	0.00060	0.00039	-1.65769
D64	0.44165	-0.00001	-0.00022	0.00050	0.00028	0.44193
D65	1.34504	0.00004	0.00015	0.00073	0.00087	1.34592
D66	-2.86419	0.00005	0.00016	0.00078	0.00094	-2.86325
D67	-0.76446	0.00004	0.00015	0.00069	0.00083	-0.76363
D68	-1.04236	-0.00001	0.00049	0.00040	0.00089	-1.04147
D69	1.03159	-0.00001	0.00050	0.00046	0.00096	1.03256
D70	3.13132	-0.00001	0.00049	0.00037	0.00085	3.13218

Item	Value	Threshold	Converged?
Maximum Force	0.000225	0.000450	YES
RMS Force	0.000051	0.000300	YES
Maximum Displacement	0.053075	0.001800	NO
RMS Displacement	0.008153	0.001200	NO

Predicted change in Energy=-1.004469D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.642568	2.099997	-0.190370
2	6	0	-3.533090	1.116618	0.096494
3	7	0	-2.823383	-0.077486	0.110008
4	6	0	-1.532061	0.184959	-0.164514
5	7	0	-1.402935	1.499109	-0.352872
6	6	0	-0.130095	2.185359	-0.638062
7	6	0	0.455882	2.865059	0.604498
8	1	0	-2.782918	3.161328	-0.301422
9	1	0	-4.591192	1.166131	0.277552
10	1	0	0.569797	1.431294	-0.998395

11	1	0	-0.304335	2.916544	-1.428522
12	1	0	-0.223666	3.649743	0.953537
13	1	0	0.533855	2.114997	1.405896
14	35	0	0.136602	-2.667389	-0.264830
15	1	0	-0.756258	-0.602780	-0.227727
16	6	0	-3.296529	-1.403232	0.351551
17	6	0	-4.552103	-1.693217	0.665737
18	1	0	-2.498992	-2.136661	0.246153
19	1	0	-4.823270	-2.727182	0.829355
20	1	0	-5.336347	-0.953472	0.772095
21	7	0	1.723196	3.475156	0.220994
22	1	0	2.065972	4.094932	0.945402
23	1	0	2.420477	2.750898	0.061801
24	6	0	3.328287	-0.425857	-1.131737
25	6	0	3.259428	-0.565414	0.323936
26	8	0	2.731139	0.621012	-0.330172
27	1	0	4.269752	-0.148040	-1.599763
28	1	0	2.625983	-0.986735	-1.741016
29	1	0	2.472945	-1.218396	0.696615
30	6	0	4.454529	-0.358768	1.213188
31	1	0	4.155019	0.076189	2.171392
32	1	0	4.934251	-1.320217	1.420308
33	1	0	5.187740	0.302889	0.745106

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357334	0.000000			
3	N	2.205528	1.389155	0.000000		
4	C	2.213881	2.222664	1.346014	0.000000	
5	N	1.387143	2.210383	2.172000	1.333845	0.000000
6	C	2.553476	3.641725	3.596370	2.488244	1.473904
7	C	3.289001	4.384862	4.433585	3.424359	2.497514
8	H	1.076315	2.214031	3.265092	3.231433	2.161012
9	H	2.210926	1.074622	2.167903	3.242900	3.267001
10	H	3.379254	4.258108	3.875390	2.581960	2.076768
11	H	2.768953	3.998783	4.204390	3.250629	2.091188
12	H	3.092139	4.254825	4.621938	3.868678	2.778958
13	H	3.554990	4.387635	4.213948	3.234076	2.687701
14	Br	5.518814	5.283551	3.950901	3.306114	4.442705
15	H	3.296144	3.282110	2.159399	1.107429	2.202677
16	C	3.604714	2.543750	1.428220	2.429407	3.536311
17	C	4.332172	3.042630	2.430615	3.652056	4.598453
18	H	4.261507	3.416956	2.089011	2.548239	3.844346

19	H	5.394160	4.120249	3.396748	4.505596	5.563981
20	H	4.184072	2.827268	2.742389	4.079933	4.769952
21	N	4.595670	5.762530	5.771046	4.644429	3.742563
22	H	5.238329	6.398476	6.481725	5.428227	4.522956
23	H	5.110938	6.173900	5.958201	4.717820	4.044429
24	C	6.551124	7.139068	6.285407	4.993156	5.166874
25	C	6.496344	7.001376	6.106098	4.874424	5.143729
26	O	5.575273	6.298273	5.615548	4.288643	4.226362
27	H	7.404069	8.084615	7.296634	5.985973	6.037153
28	H	6.300004	6.762746	5.826545	4.598648	4.933411
29	H	6.161733	6.471854	5.449484	4.330245	4.848577
30	C	7.640961	8.199136	7.366419	6.167087	6.341461
31	H	7.475354	8.030861	7.278119	6.149079	6.267971
32	H	8.467605	8.909912	7.965059	6.825717	7.159098
33	H	8.088167	8.782696	8.045256	6.782112	6.787746

		6	7	8	9	10
6	C	0.000000				
7	C	1.532748	0.000000			
8	H	2.846632	3.376135	0.000000		
9	H	4.666751	5.335373	2.754247	0.000000	
10	H	1.090092	2.153584	3.836598	5.322984	0.000000
11	H	1.090788	2.171117	2.733797	4.934752	1.776255
12	H	2.164802	1.095145	2.891927	5.069573	3.059598
13	H	2.150243	1.100414	3.874367	5.332880	2.499871
14	Br	4.874381	5.609426	6.519116	6.110818	4.186285
15	H	2.886897	3.766668	4.275662	4.253360	2.547510
16	C	4.887087	5.688838	4.639545	2.878064	4.980499
17	C	6.024732	6.772115	5.256616	2.885842	6.226216
18	H	5.007331	5.820386	5.333773	3.909824	4.867923
19	H	6.950702	7.693710	6.333738	3.939065	7.051153
20	H	6.240662	6.939682	4.960244	2.300553	6.610921
21	N	2.415832	1.457868	4.547139	6.723562	2.644733
22	H	3.313086	2.054554	5.092929	7.303542	3.621029
23	H	2.704637	2.041368	5.232179	7.191769	2.508065
24	C	4.361487	4.700569	7.134714	8.199919	3.328072
25	C	4.470017	4.439226	7.126683	8.039442	3.601322
26	O	3.275460	3.329587	6.071149	7.367700	2.403015
27	H	5.072305	5.336960	7.897960	9.152469	4.067630
28	H	4.344497	5.004707	6.966711	7.797247	3.259794
29	H	4.488064	4.555396	6.913910	7.467504	3.676396
30	C	5.560439	5.172305	8.189368	9.220943	4.815243
31	H	5.541104	4.890457	7.985478	9.015032	4.973699
32	H	6.494117	6.183678	9.088636	9.910695	5.698193
33	H	5.808289	5.382840	8.532132	9.828088	5.063447

		11	12	13	14	15
11	H	0.000000				
12	H	2.493651	0.000000			
13	H	3.062509	1.770285	0.000000		
14	Br	5.720919	6.443630	5.081374	0.000000	
15	H	3.745902	4.445559	3.423365	2.249709	0.000000
16	C	5.548184	5.944530	5.306734	3.710041	2.725667
17	C	6.609035	6.882254	6.396663	4.878414	4.049169
18	H	5.758119	6.257793	5.349744	2.736628	2.369488
19	H	7.574327	7.863647	7.244162	5.079483	4.708619
20	H	6.718697	6.882007	6.654058	5.828027	4.701047
21	N	2.672795	2.087432	2.160684	6.362717	4.793601
22	H	3.555625	2.332531	2.545501	7.135553	5.604437
23	H	3.110162	2.931656	2.402145	5.889025	4.628459
24	C	4.945268	5.794416	4.550206	3.995353	4.187129
25	C	5.281624	5.504170	3.972907	3.810117	4.053575
26	O	3.961054	4.421763	3.173953	4.189209	3.697310
27	H	5.508474	6.413525	5.302099	5.021165	5.229728
28	H	4.890808	6.072729	4.888844	3.346752	3.725188
29	H	5.415461	5.571040	3.921053	2.912466	3.414842
30	C	6.352408	6.166124	4.639864	5.114563	5.411846
31	H	6.396315	5.781552	4.225583	5.441514	5.507942
32	H	7.314969	7.177916	5.582508	5.260418	5.967632
33	H	6.459005	6.366175	5.037760	5.946135	6.090793

		16	17	18	19	20
16	C	0.000000				
17	C	1.326375	0.000000			
18	H	1.088619	2.141952	0.000000		
19	H	2.076554	1.081382	2.468017	0.000000	
20	H	2.130728	1.083316	3.118836	1.847315	0.000000
21	N	7.000954	8.141822	7.022820	9.038546	8.351863
22	H	7.703174	8.796579	7.756326	9.696203	8.961627
23	H	7.072829	8.290463	6.937103	9.114295	8.625265
24	C	6.858833	8.181544	6.227569	8.694243	8.887005
25	C	6.609332	7.899923	5.969445	8.382046	8.616194
26	O	6.394927	7.706692	5.940638	8.344100	8.293270
27	H	7.914022	9.238246	7.292319	9.758875	9.927315
28	H	6.295114	7.603716	5.615741	8.070151	8.349584
29	H	5.782738	7.041144	5.076050	7.451766	7.814149
30	C	7.868432	9.121396	7.242065	9.583019	9.818833
31	H	7.811919	9.011757	7.271803	9.501033	9.649055
32	H	8.300294	9.523625	7.569566	9.876133	10.297566
33	H	8.663057	9.942600	8.079989	10.459864	10.598849

		21	22	23	24	25

21	N	0.000000				
22	H	1.013106	0.000000			
23	H	1.017886	1.647073	0.000000		
24	C	4.429910	5.132785	3.512895	0.000000	
25	C	4.323981	4.850709	3.430813	1.463967	0.000000
26	O	3.076666	3.760007	2.187823	1.447421	1.454150
27	H	4.788284	5.416394	3.818961	1.087468	2.212594
28	H	4.957114	5.775274	4.154790	1.085834	2.200634
29	H	4.776795	5.334695	4.020079	2.168547	1.088040
30	C	4.810780	5.060865	3.890126	2.602228	1.503907
31	H	4.612027	4.692277	3.822706	3.441831	2.151008
32	H	5.894475	6.146251	4.973789	3.145144	2.139344
33	H	4.726631	4.915805	3.757313	2.740653	2.156322

		26	27	28	29	30
26	O	0.000000				
27	H	2.137904	0.000000			
28	H	2.141585	1.850767	0.000000		
29	H	2.122351	3.106047	2.453392	0.000000	
30	C	2.512370	2.826879	3.530615	2.220919	0.000000
31	H	2.929521	3.779558	4.332978	2.584626	1.094098
32	H	3.418516	3.307021	3.928522	2.567514	1.094265
33	H	2.700429	2.558213	3.795594	3.112358	1.092927

		31	32	33
31	H	0.000000		
32	H	1.766714	0.000000	
33	H	1.775443	1.776127	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.346526	2.473177	-0.264478
2	6	0	-3.332917	1.593183	0.043743
3	7	0	-2.747352	0.334563	0.096117
4	6	0	-1.434988	0.457581	-0.176500
5	7	0	-1.173153	1.746053	-0.401054
6	6	0	0.163621	2.292097	-0.696462
7	6	0	0.809892	2.944927	0.530511

8	1	0	-2.378623	3.539593	-0.406526
9	1	0	-4.381385	1.754218	0.215770
10	1	0	0.785398	1.461287	-1.030301
11	1	0	0.067388	3.013977	-1.508526
12	1	0	0.211490	3.803812	0.852341
13	1	0	0.808398	2.214286	1.353355
14	35	0	-0.062163	-2.550023	-0.184125
15	1	0	-0.742346	-0.405782	-0.211851
16	6	0	-3.352843	-0.929257	0.371706
17	6	0	-4.632589	-1.082118	0.685004
18	1	0	-2.632921	-1.742017	0.292806
19	1	0	-5.007368	-2.078356	0.875884
20	1	0	-5.338654	-0.264388	0.764780
21	7	0	2.133903	3.412954	0.138948
22	1	0	2.534372	4.015717	0.847951
23	1	0	2.755236	2.617858	0.005301
24	6	0	3.343015	-0.667313	-1.091329
25	6	0	3.254246	-0.757125	0.367182
26	8	0	2.851118	0.457086	-0.324000
27	1	0	4.309682	-0.499361	-1.560300
28	1	0	2.590308	-1.171968	-1.689485
29	1	0	2.404328	-1.316539	0.752571
30	6	0	4.460308	-0.646297	1.258736
31	1	0	4.202136	-0.155895	2.202083
32	1	0	4.839711	-1.644787	1.496407
33	1	0	5.258507	-0.075645	0.777359

Rotational constants (GHZ): 0.4213572 0.2925557 0.1828560

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1313.0441780097 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 3.64D-06 NBF= 482

NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"

B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 -0.000099 -0.000032 0.000090 Ang= -0.02 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3205.64837802 A.U. after 9 cycles
NFock= 9 Conv=0.83D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000004678	-0.000014000	-0.000002250
2	6	0.000000788	0.000016132	0.000011788
3	7	-0.000027267	-0.000033104	-0.000005922
4	6	-0.000017412	0.000038105	0.000048169
5	7	-0.000000446	0.000055562	-0.000027599
6	6	-0.000017945	-0.000026230	-0.000006400
7	6	-0.000085192	-0.000047734	0.000007358
8	1	-0.000001798	0.000001966	-0.000008450
9	1	0.000003174	0.000005454	0.000007212
10	1	0.000007108	0.000028323	-0.000000183
11	1	-0.000000999	-0.000001244	0.000002914
12	1	0.000005008	-0.000005507	-0.000007995
13	1	0.000010371	0.000008994	-0.000014062
14	35	-0.000029755	0.000053019	0.000013377
15	1	0.000033388	-0.000122304	-0.000020507
16	6	0.000015110	0.000024605	-0.000004374
17	6	0.000007650	-0.000002913	-0.000013260

18	1	0.000006533	-0.000003540	0.000003841
19	1	0.000002945	0.000002296	0.000002168
20	1	-0.000008340	-0.000002312	-0.000006251
21	7	0.000056775	0.000072244	-0.000012962
22	1	0.000014652	-0.000015005	0.000015894
23	1	0.000011991	-0.000005500	0.000012916
24	6	0.000062047	0.000028768	-0.000096828
25	6	-0.000040631	-0.000030981	0.000187382
26	8	0.000057285	-0.000043742	-0.000019284
27	1	-0.000024639	0.000003051	-0.000004497
28	1	-0.000022468	-0.000008852	0.000057899
29	1	-0.000028552	-0.000022704	-0.000087522
30	6	-0.000015665	0.000043004	-0.000046633
31	1	0.000019842	-0.000004806	0.000019926
32	1	0.000006377	-0.000000987	-0.000012238
33	1	-0.000004610	0.000009943	0.000006371

Cartesian Forces: Max 0.000187382 RMS 0.000036273

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000093502 RMS 0.000025315
Search for a local minimum.
Step number 44 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 31 32 33 34 35
36 37 38 39 40
41 42 43 44
DE= -2.12D-06 DEPred=-1.00D-06 R= 2.11D+00
TightC=F SS= 1.41D+00 RLast= 2.96D-02 DXNew= 1.7446D+00 8.8738D-02
Trust test= 2.11D+00 RLast= 2.96D-02 DXMaxT set to 1.04D+00
ITU= 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0 0
ITU= -1 1 -1 1 1 1 1 1 1 1 1 1 0 -1 -1 1 1 1 -1 1
ITU= 0 0 -1 0
Eigenvalues --- 0.00064 0.00100 0.00129 0.00240 0.00452
Eigenvalues --- 0.00585 0.00705 0.00759 0.01266 0.01420
Eigenvalues --- 0.01885 0.02000 0.02173 0.02366 0.02382
Eigenvalues --- 0.02583 0.02695 0.02895 0.03066 0.03098
Eigenvalues --- 0.03226 0.03519 0.03648 0.03981 0.04057

Eigenvalues --- 0.04278 0.04462 0.04717 0.05489 0.05552
Eigenvalues --- 0.05724 0.05748 0.05909 0.07933 0.08668
Eigenvalues --- 0.08944 0.09569 0.10669 0.11478 0.11673
Eigenvalues --- 0.12697 0.13109 0.13714 0.15769 0.15971
Eigenvalues --- 0.16001 0.16002 0.16013 0.16028 0.16169
Eigenvalues --- 0.16209 0.19165 0.21472 0.21700 0.22127
Eigenvalues --- 0.23171 0.23450 0.25833 0.26573 0.28954
Eigenvalues --- 0.29191 0.30335 0.30628 0.32130 0.32686
Eigenvalues --- 0.33696 0.34290 0.34336 0.34408 0.34550
Eigenvalues --- 0.34715 0.34767 0.35131 0.35227 0.35339
Eigenvalues --- 0.35557 0.35702 0.35889 0.36162 0.36423
Eigenvalues --- 0.36626 0.39418 0.41496 0.41902 0.42508
Eigenvalues --- 0.44697 0.45473 0.46520 0.49578 0.54904
Eigenvalues --- 0.58328 0.60646 1.01552
En-DIIS/RFO-DIIS IScMMF= 0 using points: 44 43 42 41 40
RFO step: Lambda=-2.63972698D-07.
DidBck=F Rises=F RFO-DIIS coefs: 1.97065 -0.95064 -0.83282 0.89632 -0.08352
Iteration 1 RMS(Cart)= 0.00944589 RMS(Int)= 0.00003520
Iteration 2 RMS(Cart)= 0.00005094 RMS(Int)= 0.00000812
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000812

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56499	0.00000	-0.00002	-0.00001	-0.00003	2.56496
R2	2.62132	0.00000	0.00000	0.00000	0.00000	2.62132
R3	2.03394	0.00000	0.00001	0.00001	0.00002	2.03396
R4	2.62512	0.00001	0.00000	0.00002	0.00002	2.62514
R5	2.03074	0.00000	-0.00001	0.00000	-0.00001	2.03073
R6	2.54360	-0.00001	-0.00006	0.00004	-0.00002	2.54358
R7	2.69894	-0.00002	0.00000	-0.00004	-0.00003	2.69891
R8	2.52060	0.00004	0.00014	-0.00002	0.00012	2.52072
R9	2.09274	0.00005	0.00015	0.00011	0.00026	2.09300
R10	2.78528	0.00001	0.00002	-0.00006	-0.00003	2.78524
R11	2.89647	0.00000	-0.00008	0.00003	-0.00005	2.89643
R12	2.05998	-0.00002	0.00003	-0.00003	0.00001	2.05998
R13	2.06129	0.00000	-0.00003	0.00000	-0.00002	2.06127
R14	2.06952	-0.00001	-0.00004	-0.00001	-0.00005	2.06948
R15	2.07948	-0.00002	-0.00013	0.00002	-0.00011	2.07937
R16	2.75497	0.00009	0.00057	-0.00011	0.00046	2.75543
R17	4.25133	-0.00006	-0.00095	-0.00046	-0.00140	4.24993
R18	2.50649	-0.00001	-0.00001	0.00001	-0.00001	2.50648
R19	2.05719	0.00001	-0.00003	0.00002	-0.00001	2.05718
R20	2.04352	0.00000	-0.00001	0.00001	0.00000	2.04351
R21	2.04717	0.00000	-0.00001	0.00000	0.00000	2.04717

R22	1.91449	0.00001	0.00008	-0.00001	0.00007	1.91457
R23	1.92353	0.00003	0.00008	-0.00004	0.00006	1.92358
R24	4.13439	0.00002	0.00203	0.00042	0.00245	4.13683
R25	2.76650	0.00005	0.00009	0.00018	0.00026	2.76676
R26	2.73523	-0.00001	-0.00047	-0.00016	-0.00062	2.73461
R27	2.05502	-0.00002	0.00007	-0.00004	0.00003	2.05504
R28	2.05193	-0.00001	0.00001	0.00002	0.00003	2.05196
R29	2.74794	-0.00002	0.00055	-0.00007	0.00048	2.74843
R30	2.05610	0.00000	0.00002	0.00004	0.00006	2.05616
R31	2.84197	-0.00001	-0.00012	-0.00001	-0.00012	2.84185
R32	2.06755	0.00001	0.00000	-0.00001	-0.00001	2.06753
R33	2.06786	0.00000	0.00002	0.00000	0.00002	2.06788
R34	2.06533	0.00000	0.00001	0.00001	0.00001	2.06535
A1	1.87259	0.00001	0.00005	0.00000	0.00005	1.87264
A2	2.27925	-0.00001	0.00008	-0.00003	0.00005	2.27930
A3	2.13128	-0.00001	-0.00013	0.00003	-0.00010	2.13119
A4	1.86464	0.00000	-0.00004	0.00001	-0.00003	1.86461
A5	2.27605	0.00000	-0.00007	0.00002	-0.00004	2.27600
A6	2.14243	0.00000	0.00011	-0.00003	0.00008	2.14251
A7	1.89710	0.00000	0.00008	-0.00002	0.00006	1.89716
A8	2.25275	0.00005	0.00006	0.00003	0.00008	2.25283
A9	2.13330	-0.00005	-0.00014	-0.00001	-0.00014	2.13316
A10	1.88996	0.00001	-0.00005	0.00000	-0.00005	1.88992
A11	2.14722	-0.00006	0.00011	-0.00024	-0.00013	2.14708
A12	2.24585	0.00006	-0.00004	0.00025	0.00021	2.24606
A13	1.90047	-0.00002	-0.00004	0.00001	-0.00002	1.90044
A14	2.20524	-0.00001	-0.00032	-0.00003	-0.00035	2.20489
A15	2.17688	0.00004	0.00033	0.00000	0.00033	2.17720
A16	1.96034	-0.00004	0.00013	-0.00024	-0.00011	1.96023
A17	1.87166	0.00004	0.00044	0.00013	0.00057	1.87223
A18	1.89060	0.00000	-0.00027	0.00008	-0.00019	1.89041
A19	1.90632	-0.00001	-0.00010	0.00008	-0.00002	1.90630
A20	1.92974	0.00002	-0.00022	0.00004	-0.00018	1.92955
A21	1.90362	-0.00001	0.00004	-0.00008	-0.00004	1.90358
A22	1.91653	-0.00002	0.00014	-0.00014	0.00000	1.91654
A23	1.89148	-0.00002	0.00023	-0.00011	0.00012	1.89160
A24	1.88038	0.00007	-0.00017	0.00024	0.00006	1.88044
A25	1.87574	0.00001	0.00014	-0.00002	0.00013	1.87587
A26	1.90011	-0.00002	-0.00005	-0.00002	-0.00007	1.90004
A27	1.99899	-0.00002	-0.00027	0.00003	-0.00024	1.99875
A28	2.16109	0.00002	0.00011	0.00000	0.00011	2.16120
A29	1.94583	-0.00001	-0.00007	0.00004	-0.00003	1.94580
A30	2.17626	-0.00001	-0.00004	-0.00004	-0.00008	2.17618
A31	2.07403	-0.00001	0.00001	-0.00004	-0.00003	2.07399

A32	2.16428	0.00001	0.00005	0.00003	0.00008	2.16436
A33	2.04488	0.00000	-0.00005	0.00001	-0.00005	2.04483
A34	1.94125	-0.00003	-0.00045	0.00002	-0.00043	1.94081
A35	1.91651	0.00006	-0.00020	0.00007	-0.00014	1.91637
A36	1.89161	-0.00003	-0.00042	0.00001	-0.00041	1.89120
A37	2.08635	0.00006	0.00049	0.00003	0.00056	2.08691
A38	2.06948	-0.00008	0.00010	0.00002	0.00008	2.06957
A39	1.99406	-0.00001	0.00035	0.00003	0.00037	1.99443
A40	2.00148	0.00001	0.00028	-0.00015	0.00013	2.00162
A41	2.03803	0.00002	-0.00082	0.00003	-0.00079	2.03724
A42	2.01728	-0.00006	-0.00042	0.00029	-0.00014	2.01714
A43	2.13823	-0.00001	-0.00044	-0.00015	-0.00059	2.13764
A44	1.96180	0.00001	-0.00049	0.00021	-0.00027	1.96154
A45	2.02926	-0.00005	-0.00016	-0.00009	-0.00026	2.02900
A46	2.04244	0.00008	0.00103	-0.00013	0.00091	2.04334
A47	2.60982	-0.00001	0.00411	0.00190	0.00604	2.61587
A48	2.44227	0.00001	-0.00352	-0.00147	-0.00503	2.43724
A49	1.93364	0.00004	0.00020	0.00002	0.00022	1.93386
A50	1.91726	-0.00001	-0.00005	0.00001	-0.00003	1.91722
A51	1.94235	-0.00001	-0.00007	-0.00004	-0.00010	1.94224
A52	1.87920	-0.00001	0.00005	-0.00010	-0.00005	1.87915
A53	1.89448	-0.00002	-0.00005	0.00006	0.00001	1.89449
A54	1.89534	0.00000	-0.00009	0.00005	-0.00004	1.89530
A55	3.48871	0.00001	-0.00190	-0.00159	-0.00349	3.48522
A56	2.52958	0.00009	0.00103	0.00105	0.00205	2.53163
A57	2.97519	-0.00004	-0.00573	-0.00329	-0.00902	2.96617
A58	3.10800	-0.00001	0.00006	-0.00163	-0.00158	3.10643
D1	0.00319	0.00000	-0.00009	0.00004	-0.00005	0.00314
D2	-3.12566	0.00000	-0.00027	-0.00037	-0.00065	-3.12631
D3	3.13281	-0.00001	0.00028	0.00014	0.00042	3.13323
D4	0.00396	0.00000	0.00010	-0.00028	-0.00017	0.00378
D5	-0.00457	0.00000	0.00013	-0.00016	-0.00003	-0.00460
D6	-3.11007	0.00000	0.00103	0.00028	0.00131	-3.10875
D7	-3.13543	0.00000	-0.00021	-0.00025	-0.00046	-3.13588
D8	0.04226	0.00000	0.00069	0.00019	0.00089	0.04315
D9	-0.00076	0.00001	0.00003	0.00009	0.00011	-0.00065
D10	-3.13349	0.00001	0.00044	-0.00022	0.00022	-3.13327
D11	3.12930	0.00001	0.00019	0.00047	0.00065	3.12995
D12	-0.00343	0.00000	0.00060	0.00016	0.00076	-0.00267
D13	-0.00209	-0.00001	0.00005	-0.00019	-0.00014	-0.00222
D14	-3.12645	-0.00001	-0.00095	-0.00084	-0.00179	-3.12824
D15	3.13137	-0.00001	-0.00033	0.00010	-0.00023	3.13114
D16	0.00701	0.00000	-0.00132	-0.00056	-0.00189	0.00512
D17	-0.04828	0.00002	0.00522	0.00263	0.00785	-0.04043

D18	3.09454	0.00001	0.00490	0.00249	0.00739	3.10193
D19	3.10324	0.00001	0.00568	0.00228	0.00796	3.11121
D20	-0.03713	0.00001	0.00536	0.00215	0.00751	-0.02962
D21	0.00410	0.00001	-0.00011	0.00021	0.00010	0.00421
D22	3.11032	0.00000	-0.00101	-0.00022	-0.00123	3.10909
D23	3.12718	0.00000	0.00096	0.00091	0.00188	3.12906
D24	-0.04978	0.00000	0.00006	0.00048	0.00054	-0.04924
D25	1.33989	0.00002	0.00351	0.00100	0.00451	1.34440
D26	-2.84884	0.00000	0.00374	0.00104	0.00478	-2.84406
D27	-0.79655	0.00001	0.00389	0.00105	0.00494	-0.79161
D28	-1.76014	0.00002	0.00455	0.00151	0.00607	-1.75408
D29	0.33431	0.00001	0.00479	0.00155	0.00634	0.34065
D30	2.38660	0.00002	0.00494	0.00156	0.00650	2.39310
D31	-1.10279	0.00002	0.00189	0.00049	0.00238	-1.10041
D32	0.94141	0.00001	0.00227	0.00033	0.00260	0.94401
D33	3.11338	0.00002	0.00197	0.00045	0.00243	3.11581
D34	3.10619	0.00000	0.00133	0.00043	0.00176	3.10795
D35	-1.13280	0.00000	0.00172	0.00027	0.00198	-1.13082
D36	1.03917	0.00000	0.00142	0.00039	0.00181	1.04098
D37	1.01134	0.00000	0.00148	0.00045	0.00194	1.01328
D38	3.05553	0.00000	0.00186	0.00029	0.00216	3.05769
D39	-1.05568	0.00000	0.00156	0.00042	0.00198	-1.05370
D40	2.94073	0.00001	0.00139	0.00114	0.00253	2.94326
D41	-1.24870	0.00000	0.00044	0.00121	0.00165	-1.24705
D42	0.86319	0.00000	0.00135	0.00118	0.00253	0.86572
D43	2.95695	-0.00001	0.00040	0.00125	0.00165	2.95860
D44	-1.23672	0.00002	0.00138	0.00120	0.00258	-1.23415
D45	0.85703	0.00001	0.00043	0.00127	0.00170	0.85873
D46	3.13896	0.00000	0.00028	0.00008	0.00036	3.13932
D47	-0.00361	0.00000	0.00054	0.00022	0.00076	-0.00284
D48	-0.00402	0.00000	0.00064	0.00023	0.00087	-0.00314
D49	3.13660	0.00001	0.00090	0.00038	0.00128	3.13788
D50	2.20894	-0.00003	-0.00158	0.00109	-0.00048	2.20846
D51	-1.40619	-0.00002	-0.00073	0.00196	0.00121	-1.40498
D52	-2.08499	0.00000	-0.00218	0.00188	-0.00029	-2.08528
D53	0.58306	0.00001	-0.00133	0.00275	0.00140	0.58446
D54	-2.71267	-0.00001	-0.00016	0.00008	-0.00008	-2.71276
D55	-0.01645	0.00001	0.00051	0.00009	0.00060	-0.01585
D56	-0.02641	0.00000	-0.00093	0.00029	-0.00064	-0.02705
D57	2.66982	0.00003	-0.00026	0.00030	0.00003	2.66985
D58	0.51351	0.00000	-0.00386	-0.00088	-0.00471	0.50881
D59	-1.90631	-0.00003	-0.00328	-0.00078	-0.00403	-1.91034
D60	1.78858	0.00005	-0.00381	-0.00247	-0.00628	1.78230
D61	-0.63253	-0.00002	-0.00471	-0.00241	-0.00712	-0.63965

D62	2.55147	0.00000	0.00107	0.00058	0.00165	2.55312
D63	-1.65769	0.00000	0.00122	0.00048	0.00170	-1.65599
D64	0.44193	-0.00001	0.00104	0.00052	0.00156	0.44349
D65	1.34592	0.00003	0.00167	0.00077	0.00245	1.34836
D66	-2.86325	0.00004	0.00183	0.00067	0.00250	-2.86075
D67	-0.76363	0.00003	0.00164	0.00072	0.00236	-0.76127
D68	-1.04147	-0.00001	0.00140	0.00069	0.00208	-1.03939
D69	1.03256	0.00000	0.00155	0.00058	0.00213	1.03469
D70	3.13218	-0.00001	0.00136	0.00063	0.00199	3.13417

Item	Value	Threshold	Converged?
Maximum Force	0.000094	0.000450	YES
RMS Force	0.000025	0.000300	YES
Maximum Displacement	0.073142	0.001800	NO
RMS Displacement	0.009453	0.001200	NO

Predicted change in Energy=-7.542515D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.643879	2.099875	-0.196032
2	6	0	-3.535584	1.117805	0.091567
3	7	0	-2.826307	-0.076480	0.111240
4	6	0	-1.534064	0.184557	-0.160232
5	7	0	-1.403949	1.498066	-0.352782
6	6	0	-0.130054	2.183543	-0.635018
7	6	0	0.454689	2.860513	0.609581
8	1	0	-2.783405	3.160927	-0.310798
9	1	0	-4.594105	1.168416	0.269812
10	1	0	0.569961	1.429881	-0.995963
11	1	0	-0.302761	2.916475	-1.424181
12	1	0	-0.225766	3.643587	0.960386
13	1	0	0.533301	2.108487	1.408992
14	35	0	0.136913	-2.666890	-0.226125
15	1	0	-0.758076	-0.603699	-0.216787
16	6	0	-3.300520	-1.401298	0.355658
17	6	0	-4.558948	-1.690982	0.658487
18	1	0	-2.501228	-2.134457	0.262426
19	1	0	-4.830487	-2.724279	0.825672
20	1	0	-5.345320	-0.951725	0.751705
21	7	0	1.721770	3.473053	0.228273
22	1	0	2.064400	4.089332	0.955781

23	1	0	2.419377	2.749759	0.065967
24	6	0	3.332799	-0.425726	-1.137535
25	6	0	3.264391	-0.564175	0.318404
26	8	0	2.735290	0.621397	-0.337162
27	1	0	4.273798	-0.148031	-1.606601
28	1	0	2.630847	-0.987659	-1.746277
29	1	0	2.478081	-1.217069	0.691694
30	6	0	4.459962	-0.355599	1.206460
31	1	0	4.160845	0.078439	2.165197
32	1	0	4.941730	-1.316232	1.412674
33	1	0	5.191414	0.307558	0.737733

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357317	0.000000			
3	N	2.205497	1.389165	0.000000		
4	C	2.213914	2.222710	1.346005	0.000000	
5	N	1.387145	2.210410	2.172008	1.333909	0.000000
6	C	2.553238	3.641614	3.596441	2.488496	1.473887
7	C	3.290701	4.384934	4.431615	3.421768	2.497386
8	H	1.076323	2.214050	3.265083	3.231456	2.160965
9	H	2.210884	1.074617	2.167953	3.242957	3.267016
10	H	3.378987	4.258593	3.876811	2.583835	2.077174
11	H	2.766951	3.997980	4.205185	3.252238	2.091027
12	H	3.093157	4.253153	4.617658	3.864236	2.777730
13	H	3.559586	4.390089	4.212506	3.230785	2.688754
14	Br	5.518673	5.283188	3.950279	3.305639	4.442652
15	H	3.296361	3.282257	2.159431	1.107566	2.202967
16	C	3.604685	2.543793	1.428202	2.429289	3.536267
17	C	4.332239	3.042690	2.430667	3.652105	4.598556
18	H	4.261466	3.417059	2.088971	2.547914	3.844181
19	H	5.394218	4.120351	3.396761	4.505522	5.564001
20	H	4.184286	2.827346	2.742567	4.080250	4.770302
21	N	4.596145	5.762434	5.770432	4.643878	3.742769
22	H	5.239514	6.398176	6.479680	5.426020	4.522879
23	H	5.111512	6.174583	5.958765	4.718169	4.044738
24	C	6.556353	7.146178	6.294124	5.001391	5.172387
25	C	6.501497	7.008579	6.113703	4.880047	5.147497
26	O	5.580437	6.305084	5.623118	4.295290	4.231086
27	H	7.409254	8.091512	7.305312	5.994486	6.043054
28	H	6.305463	6.770193	5.836193	4.608265	4.939659
29	H	6.166413	6.478885	5.456592	4.334471	4.851087
30	C	7.645973	8.206258	7.373408	6.171545	6.344507

31	H	7.481034	8.038360	7.284438	6.152306	6.270764
32	H	8.473440	8.918223	7.973275	6.830981	7.162733
33	H	8.091733	8.788317	8.051325	6.786275	6.790092

		6	7	8	9	10
6	C	0.000000				
7	C	1.532723	0.000000			
8	H	2.846168	3.379734	0.000000		
9	H	4.666579	5.335632	2.754241	0.000000	
10	H	1.090096	2.153547	3.835498	5.323358	0.000000
11	H	1.090777	2.170956	2.730014	4.933656	1.776225
12	H	2.164764	1.095121	2.896617	5.068111	3.059572
13	H	2.150268	1.100355	3.881475	5.335894	2.499132
14	Br	4.874953	5.599247	6.519116	6.110487	4.190909
15	H	2.887568	3.762240	4.275887	4.253503	2.550735
16	C	4.887165	5.685870	4.639555	2.878222	4.982277
17	C	6.024965	6.771637	5.256719	2.885907	6.227577
18	H	5.007294	5.814438	5.333788	3.910135	4.870344
19	H	6.950856	7.692183	6.333858	3.939280	7.052676
20	H	6.241146	6.942152	4.960466	2.300335	6.611879
21	N	2.416063	1.458113	4.548036	6.723345	2.645746
22	H	3.313352	2.054512	5.095819	7.303287	3.621509
23	H	2.703993	2.041514	5.232586	7.192436	2.508009
24	C	4.364878	4.704816	7.138314	8.207175	3.331154
25	C	4.470037	4.439335	7.130787	8.047372	3.600524
26	O	3.277075	3.333332	6.075023	7.374801	2.403396
27	H	5.076822	5.343069	7.901420	9.159349	4.071988
28	H	4.349022	5.009407	6.970330	7.804692	3.264157
29	H	4.486279	4.552750	6.917737	7.475583	3.673616
30	C	5.559365	5.171252	8.193559	9.229089	4.813597
31	H	5.539358	4.888299	7.990926	9.023840	4.971295
32	H	6.493417	6.182531	9.093571	9.920270	5.696932
33	H	5.807047	5.382431	8.534570	9.834451	5.061930

		11	12	13	14	15
11	H	0.000000				
12	H	2.494150	0.000000			
13	H	3.062469	1.770300	0.000000		
14	Br	5.727356	6.431288	5.063097	0.000000	
15	H	3.749232	4.439429	3.415665	2.248966	0.000000
16	C	5.549554	5.938912	5.303422	3.708927	2.725414
17	C	6.609183	6.879334	6.397674	4.877094	4.049064
18	H	5.761059	6.249053	5.340931	2.735316	2.368848
19	H	7.574974	7.859473	7.243349	5.077856	4.708302
20	H	6.717503	6.882606	6.659963	5.826905	4.701266
21	N	2.671912	2.087575	2.160694	6.357448	4.792455

22	H	3.555737	2.333146	2.544290	7.124510	5.600520
23	H	3.107792	2.931842	2.402547	5.885154	4.628373
24	C	4.946692	5.798618	4.554583	4.008387	4.196988
25	C	5.279782	5.504417	3.973835	3.807761	4.058107
26	O	3.959640	4.425508	3.179505	4.192460	3.703911
27	H	5.510840	6.419647	5.308201	5.036287	5.240131
28	H	4.894084	6.077393	4.893010	3.369033	3.737856
29	H	5.412596	5.568569	3.918675	2.902661	3.416763
30	C	6.349037	6.165233	4.640195	5.107164	5.414343
31	H	6.392328	5.779637	4.225165	5.426535	5.507717
32	H	7.312198	7.176865	5.582380	5.253209	5.970815
33	H	6.454942	6.365886	5.039043	5.943429	6.094090

		16	17	18	19	20
16	C	0.000000				
17	C	1.326372	0.000000			
18	H	1.088615	2.141903	0.000000		
19	H	2.076532	1.081381	2.467911	0.000000	
20	H	2.130769	1.083315	3.118831	1.847288	0.000000
21	N	6.999923	8.142467	7.019903	9.038577	8.354424
22	H	7.699970	8.795974	7.749918	9.694415	8.964254
23	H	7.073360	8.292664	6.935885	9.116071	8.629121
24	C	6.868936	8.191840	6.238230	8.704984	8.896946
25	C	6.618174	7.911384	5.975891	8.393474	8.629315
26	O	6.403304	7.716497	5.947718	8.353844	8.304011
27	H	7.924105	9.248174	7.303432	9.769391	9.936547
28	H	6.306373	7.613850	5.629229	8.080982	8.358256
29	H	5.791295	7.053048	5.081278	7.463564	7.828130
30	C	7.876703	9.133689	7.246634	9.595212	9.833907
31	H	7.818953	9.024180	7.273284	9.512812	9.665732
32	H	8.310187	9.537931	7.575631	9.890570	10.314705
33	H	8.670590	9.953392	8.084930	10.470829	10.611727

		21	22	23	24	25
21	N	0.000000				
22	H	1.013145	0.000000			
23	H	1.017916	1.646886	0.000000		
24	C	4.434109	5.135811	3.516598	0.000000	
25	C	4.322848	4.847820	3.429276	1.464106	0.000000
26	O	3.078780	3.761432	2.189118	1.447094	1.454406
27	H	4.794983	5.422406	3.825382	1.087482	2.213080
28	H	4.962179	5.779084	4.158995	1.085850	2.200824
29	H	4.773260	5.329049	4.016305	2.168604	1.088071
30	C	4.807611	5.055588	3.886896	2.601871	1.503841
31	H	4.606969	4.684552	3.817778	3.442076	2.151099
32	H	5.891366	6.140676	4.970731	3.144078	2.139271

33	H	4.724229	4.911983	3.754971	2.740217	2.156194
		26	27	28	29	30
26	O	0.000000				
27	H	2.137873	0.000000			
28	H	2.141395	1.850344	0.000000		
29	H	2.122418	3.106381	2.453501	0.000000	
30	C	2.512327	2.826846	3.530414	2.221479	0.000000
31	H	2.930667	3.780279	4.333254	2.584811	1.094091
32	H	3.418290	3.305579	3.927736	2.568893	1.094276
33	H	2.699341	2.558414	3.795313	3.112681	1.092934
		31	32	33		
31	H	0.000000				
32	H	1.766686	0.000000			
33	H	1.775450	1.776114	0.000000		

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.350195	2.471818	-0.264854
2	6	0	-3.336828	1.590446	0.038543
3	7	0	-2.750464	0.332143	0.089816
4	6	0	-1.437380	0.456691	-0.178566
5	7	0	-1.175858	1.745904	-0.399584
6	6	0	0.161406	2.294246	-0.688358
7	6	0	0.805117	2.937923	0.544750
8	1	0	-2.382532	3.538579	-0.404305
9	1	0	-4.385810	1.750457	0.208348
10	1	0	0.784304	1.466435	-1.027528
11	1	0	0.066379	3.022430	-1.494900
12	1	0	0.204664	3.792807	0.873259
13	1	0	0.804565	2.200364	1.361321
14	35	0	-0.059237	-2.547953	-0.169133
15	1	0	-0.743741	-0.406119	-0.212134
16	6	0	-3.355728	-0.932809	0.360582
17	6	0	-4.638171	-1.088506	0.661186
18	1	0	-2.633230	-1.743977	0.289273
19	1	0	-5.012307	-2.085454	0.849601

20	1	0	-5.347203	-0.272560	0.732433
21	7	0	2.128772	3.412115	0.158519
22	1	0	2.527893	4.007692	0.874377
23	1	0	2.751395	2.619315	0.017236
24	6	0	3.348636	-0.658235	-1.108566
25	6	0	3.260066	-0.755699	0.349606
26	8	0	2.855022	0.461363	-0.335957
27	1	0	4.314806	-0.486622	-1.577270
28	1	0	2.596875	-1.161187	-1.709370
29	1	0	2.410781	-1.318168	0.732021
30	6	0	4.466404	-0.647066	1.240945
31	1	0	4.207733	-0.163457	2.187649
32	1	0	4.848877	-1.645969	1.471916
33	1	0	5.262569	-0.071108	0.762512

Rotational constants (GHZ): 0.4222383 0.2920996 0.1827110

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1312.8918944969 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 3.63D-06 NBF= 482

NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000436 0.000045 -0.000508 Ang= -0.08 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0

NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3205.64837887 A.U. after 10 cycles

NFock= 10 Conv=0.63D-08 -V/T= 2.0018

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000013785	-0.000005685	0.000006186
2	6	0.000001572	0.000010055	0.000000812
3	7	-0.000032227	-0.000036688	-0.000007605
4	6	0.000019133	0.000059722	0.000010410
5	7	-0.000004471	0.000026768	-0.000004346
6	6	-0.000010685	-0.000018758	-0.000003072
7	6	0.000024811	0.000005705	-0.000016006
8	1	-0.000004873	-0.000000803	-0.000006968
9	1	0.000000510	0.000000328	0.000008494
10	1	-0.000002084	0.000008660	-0.000009299
11	1	0.000001620	-0.000005429	-0.000004200
12	1	-0.000004218	-0.000002223	-0.000008347
13	1	-0.000010317	-0.000009504	0.000001198
14	35	-0.000008435	0.000022354	0.000004006
15	1	0.000005836	-0.000072006	0.000000907
16	6	0.000007543	0.000017830	-0.000006134
17	6	-0.000003420	0.000002696	-0.000011043
18	1	0.000007765	-0.000005692	0.000005590
19	1	0.000003459	0.000001049	0.000005116
20	1	-0.000004726	0.000000916	-0.000002814
21	7	-0.000005102	0.000008878	0.000029417
22	1	0.000007531	-0.000006751	-0.000003435
23	1	0.000007684	0.000003777	-0.000008124
24	6	0.000047371	-0.000023168	-0.000092572
25	6	-0.000046346	0.000033775	0.000031452
26	8	0.000029908	-0.000024481	0.000040299
27	1	-0.000014689	0.000005347	0.000027682
28	1	-0.000027338	0.000000802	0.000045986
29	1	-0.000001184	-0.000019520	-0.000036538

30	6	-0.000003085	0.000018555	-0.000011139
31	1	0.000008807	-0.000004720	0.000012850
32	1	-0.000000048	0.000001326	-0.000002226
33	1	-0.000004088	0.000006884	0.000003465

Cartesian Forces: Max 0.000092572 RMS 0.000020738

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000047551 RMS 0.000012387
Search for a local minimum.
Step number 45 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 31 32 33 34 35
36 37 38 39 40
41 42 43 44 45
DE= -8.55D-07 DEPred=-7.54D-07 R= 1.13D+00
Trust test= 1.13D+00 RLast= 2.93D-02 DXMaxT set to 1.04D+00
ITU= 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 0
ITU= 0 -1 1 -1 1 1 1 1 1 1 1 1 1 0 -1 -1 1 1 1 -1
ITU= 1 0 0 -1 0

Eigenvalues ---	0.00065	0.00103	0.00119	0.00239	0.00386
Eigenvalues ---	0.00532	0.00707	0.00762	0.01275	0.01419
Eigenvalues ---	0.01892	0.02044	0.02174	0.02352	0.02383
Eigenvalues ---	0.02547	0.02683	0.02891	0.03065	0.03103
Eigenvalues ---	0.03226	0.03519	0.03628	0.03980	0.04087
Eigenvalues ---	0.04263	0.04465	0.04680	0.05490	0.05599
Eigenvalues ---	0.05741	0.05750	0.05906	0.07921	0.08693
Eigenvalues ---	0.08889	0.09568	0.10230	0.11101	0.12019
Eigenvalues ---	0.12668	0.13060	0.13237	0.15737	0.15940
Eigenvalues ---	0.16002	0.16002	0.16013	0.16015	0.16130
Eigenvalues ---	0.16217	0.19181	0.21422	0.21791	0.22141
Eigenvalues ---	0.23168	0.23452	0.26010	0.26444	0.28298
Eigenvalues ---	0.29135	0.30273	0.30504	0.32029	0.32546
Eigenvalues ---	0.33666	0.34286	0.34337	0.34401	0.34550
Eigenvalues ---	0.34720	0.34771	0.35126	0.35177	0.35335
Eigenvalues ---	0.35557	0.35690	0.35890	0.35989	0.36419
Eigenvalues ---	0.36628	0.39248	0.41203	0.41939	0.42509
Eigenvalues ---	0.44769	0.45487	0.46484	0.49557	0.54935

Eigenvalues --- 0.58273 0.60635 1.04765

En-DIIS/RFO-DIIS IScMMF= 0 using points: 45 44 43 42 41

RFO step: Lambda=-6.25948570D-08.

DidBck=F Rises=F RFO-DIIS coefs: 1.26029 -0.14199 -0.30657 0.11854 0.06974

Iteration 1 RMS(Cart)= 0.00258223 RMS(Int)= 0.00000774

Iteration 2 RMS(Cart)= 0.00000297 RMS(Int)= 0.00000746

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000746

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56496	0.00001	-0.00001	0.00000	-0.00001	2.56495
R2	2.62132	0.00000	0.00000	-0.00001	-0.00001	2.62131
R3	2.03396	0.00000	0.00001	0.00000	0.00000	2.03396
R4	2.62514	0.00000	0.00001	-0.00001	0.00000	2.62514
R5	2.03073	0.00000	0.00000	0.00000	0.00000	2.03073
R6	2.54358	0.00001	-0.00001	0.00004	0.00004	2.54362
R7	2.69891	-0.00002	-0.00003	-0.00001	-0.00004	2.69887
R8	2.52072	0.00001	0.00007	-0.00001	0.00006	2.52078
R9	2.09300	0.00003	0.00014	0.00007	0.00020	2.09320
R10	2.78524	-0.00001	-0.00001	-0.00001	-0.00002	2.78522
R11	2.89643	0.00001	-0.00001	0.00002	0.00001	2.89644
R12	2.05998	0.00000	0.00000	-0.00001	-0.00001	2.05997
R13	2.06127	0.00000	-0.00001	0.00001	-0.00001	2.06126
R14	2.06948	0.00000	-0.00002	0.00001	-0.00001	2.06947
R15	2.07937	0.00001	-0.00005	0.00004	-0.00002	2.07935
R16	2.75543	0.00000	0.00022	-0.00009	0.00012	2.75556
R17	4.24993	-0.00002	-0.00072	-0.00028	-0.00100	4.24893
R18	2.50648	0.00000	0.00000	0.00001	0.00000	2.50648
R19	2.05718	0.00001	0.00000	0.00001	0.00001	2.05720
R20	2.04351	0.00000	0.00000	0.00000	0.00000	2.04352
R21	2.04717	0.00000	0.00000	0.00000	0.00000	2.04717
R22	1.91457	0.00000	0.00003	-0.00001	0.00002	1.91458
R23	1.92358	-0.00001	0.00004	-0.00002	0.00003	1.92361
R24	4.13683	0.00000	-0.00011	0.00049	0.00038	4.13721
R25	2.76676	0.00001	0.00014	-0.00014	-0.00001	2.76675
R26	2.73461	0.00001	-0.00019	0.00016	-0.00003	2.73458
R27	2.05504	-0.00002	-0.00001	-0.00004	-0.00005	2.05499
R28	2.05196	-0.00001	0.00001	-0.00002	-0.00001	2.05195
R29	2.74843	-0.00005	0.00015	-0.00014	0.00001	2.74844
R30	2.05616	0.00000	0.00003	-0.00002	0.00000	2.05616
R31	2.84185	0.00000	-0.00007	0.00005	-0.00002	2.84182
R32	2.06753	0.00001	0.00000	0.00001	0.00001	2.06754
R33	2.06788	0.00000	0.00001	0.00000	0.00001	2.06789
R34	2.06535	0.00000	0.00001	0.00000	0.00001	2.06535

A1	1.87264	0.00001	0.00003	0.00001	0.00004	1.87268
A2	2.27930	-0.00001	0.00000	-0.00002	-0.00002	2.27928
A3	2.13119	0.00000	-0.00002	0.00001	-0.00002	2.13117
A4	1.86461	0.00000	-0.00002	0.00000	-0.00002	1.86460
A5	2.27600	0.00000	0.00000	0.00000	0.00000	2.27600
A6	2.14251	0.00000	0.00002	0.00000	0.00002	2.14253
A7	1.89716	-0.00001	0.00002	-0.00001	0.00002	1.89717
A8	2.25283	0.00002	0.00005	0.00000	0.00005	2.25289
A9	2.13316	-0.00001	-0.00008	0.00001	-0.00007	2.13309
A10	1.88992	0.00001	-0.00002	0.00000	-0.00002	1.88990
A11	2.14708	-0.00004	-0.00011	-0.00014	-0.00024	2.14684
A12	2.24606	0.00003	0.00013	0.00013	0.00026	2.24632
A13	1.90044	-0.00001	-0.00002	0.00000	-0.00002	1.90042
A14	2.20489	0.00001	-0.00012	0.00002	-0.00010	2.20479
A15	2.17720	0.00000	0.00012	-0.00002	0.00010	2.17731
A16	1.96023	-0.00004	-0.00007	-0.00007	-0.00014	1.96009
A17	1.87223	0.00001	0.00021	-0.00004	0.00017	1.87239
A18	1.89041	0.00001	-0.00009	-0.00001	-0.00010	1.89030
A19	1.90630	0.00001	0.00001	0.00006	0.00008	1.90638
A20	1.92955	0.00002	-0.00003	0.00005	0.00003	1.92958
A21	1.90358	-0.00001	-0.00003	0.00000	-0.00003	1.90355
A22	1.91654	-0.00001	0.00000	-0.00012	-0.00012	1.91642
A23	1.89160	-0.00002	0.00003	-0.00009	-0.00007	1.89153
A24	1.88044	0.00004	0.00007	0.00011	0.00018	1.88062
A25	1.87587	0.00001	0.00006	-0.00002	0.00005	1.87592
A26	1.90004	-0.00001	-0.00003	-0.00001	-0.00004	1.90000
A27	1.99875	0.00000	-0.00013	0.00011	-0.00002	1.99873
A28	2.16120	0.00001	0.00005	-0.00001	0.00004	2.16124
A29	1.94580	0.00000	-0.00001	0.00001	-0.00001	1.94580
A30	2.17618	0.00000	-0.00003	0.00000	-0.00003	2.17615
A31	2.07399	-0.00001	-0.00002	-0.00001	-0.00003	2.07396
A32	2.16436	0.00001	0.00003	0.00001	0.00004	2.16440
A33	2.04483	0.00000	-0.00001	0.00000	-0.00001	2.04482
A34	1.94081	0.00001	-0.00016	0.00008	-0.00008	1.94074
A35	1.91637	0.00000	-0.00013	0.00007	-0.00006	1.91631
A36	1.89120	0.00000	-0.00018	0.00000	-0.00019	1.89101
A37	2.08691	0.00001	0.00027	-0.00010	0.00020	2.08711
A38	2.06957	-0.00004	-0.00013	-0.00021	-0.00038	2.06919
A39	1.99443	-0.00001	0.00012	-0.00004	0.00007	1.99449
A40	2.00162	0.00000	-0.00001	-0.00012	-0.00013	2.00149
A41	2.03724	0.00003	-0.00018	0.00033	0.00015	2.03740
A42	2.01714	-0.00003	-0.00017	-0.00034	-0.00052	2.01661
A43	2.13764	0.00000	-0.00018	0.00009	-0.00008	2.13756
A44	1.96154	0.00001	-0.00010	0.00007	-0.00001	1.96152

A45	2.02900	-0.00003	-0.00015	-0.00005	-0.00021	2.02879
A46	2.04334	0.00003	0.00042	0.00013	0.00055	2.04389
A47	2.61587	-0.00001	-0.00051	0.00046	-0.00004	2.61583
A48	2.43724	0.00000	0.00087	-0.00150	-0.00066	2.43658
A49	1.93386	0.00002	0.00011	0.00005	0.00016	1.93402
A50	1.91722	0.00000	0.00000	0.00003	0.00004	1.91726
A51	1.94224	0.00000	-0.00006	-0.00004	-0.00011	1.94214
A52	1.87915	-0.00001	-0.00002	-0.00001	-0.00003	1.87912
A53	1.89449	-0.00001	-0.00001	-0.00003	-0.00004	1.89446
A54	1.89530	0.00000	-0.00002	-0.00001	-0.00002	1.89528
A55	3.48522	-0.00001	-0.00091	-0.00002	-0.00094	3.48428
A56	2.53163	0.00001	0.00048	-0.00103	-0.00059	2.53104
A57	2.96617	-0.00001	-0.00190	0.00047	-0.00142	2.96475
A58	3.10643	0.00000	0.00013	0.00087	0.00099	3.10741
D1	0.00314	0.00000	-0.00006	-0.00001	-0.00007	0.00307
D2	-3.12631	0.00000	-0.00024	-0.00003	-0.00027	-3.12658
D3	3.13323	0.00000	0.00009	-0.00009	0.00000	3.13323
D4	0.00378	0.00000	-0.00009	-0.00011	-0.00020	0.00358
D5	-0.00460	0.00000	-0.00001	-0.00002	-0.00003	-0.00463
D6	-3.10875	0.00000	0.00034	0.00014	0.00048	-3.10827
D7	-3.13588	0.00000	-0.00015	0.00006	-0.00009	-3.13597
D8	0.04315	0.00000	0.00021	0.00021	0.00042	0.04357
D9	-0.00065	0.00000	0.00011	0.00003	0.00015	-0.00050
D10	-3.13327	0.00000	0.00019	-0.00003	0.00016	-3.13311
D11	3.12995	0.00001	0.00028	0.00005	0.00033	3.13028
D12	-0.00267	0.00000	0.00035	-0.00001	0.00034	-0.00233
D13	-0.00222	-0.00001	-0.00012	-0.00004	-0.00017	-0.00239
D14	-3.12824	0.00000	-0.00028	0.00010	-0.00018	-3.12841
D15	3.13114	0.00000	-0.00019	0.00001	-0.00018	3.13096
D16	0.00512	0.00000	-0.00034	0.00016	-0.00019	0.00494
D17	-0.04043	0.00001	0.00217	-0.00013	0.00204	-0.03840
D18	3.10193	0.00001	0.00200	-0.00004	0.00196	3.10389
D19	3.11121	0.00000	0.00225	-0.00020	0.00205	3.11325
D20	-0.02962	0.00001	0.00208	-0.00011	0.00198	-0.02764
D21	0.00421	0.00001	0.00008	0.00004	0.00012	0.00433
D22	3.10909	0.00000	-0.00027	-0.00011	-0.00039	3.10871
D23	3.12906	0.00000	0.00024	-0.00012	0.00012	3.12919
D24	-0.04924	0.00000	-0.00011	-0.00027	-0.00038	-0.04962
D25	1.34440	0.00001	0.00150	0.00011	0.00161	1.34601
D26	-2.84406	0.00000	0.00161	0.00012	0.00173	-2.84233
D27	-0.79161	0.00000	0.00164	0.00010	0.00173	-0.78987
D28	-1.75408	0.00001	0.00191	0.00029	0.00220	-1.75188
D29	0.34065	0.00001	0.00202	0.00030	0.00232	0.34297
D30	2.39310	0.00001	0.00205	0.00027	0.00232	2.39543

D31	-1.10041	0.00001	0.00070	-0.00006	0.00064	-1.09977
D32	0.94401	-0.00001	0.00080	-0.00020	0.00059	0.94460
D33	3.11581	0.00000	0.00069	-0.00005	0.00064	3.11645
D34	3.10795	0.00001	0.00047	-0.00001	0.00047	3.10842
D35	-1.13082	-0.00001	0.00057	-0.00015	0.00042	-1.13040
D36	1.04098	0.00000	0.00047	0.00000	0.00047	1.04145
D37	1.01328	0.00000	0.00052	-0.00008	0.00043	1.01371
D38	3.05769	-0.00001	0.00061	-0.00022	0.00039	3.05808
D39	-1.05370	0.00000	0.00051	-0.00008	0.00044	-1.05326
D40	2.94326	0.00000	0.00044	0.00009	0.00053	2.94378
D41	-1.24705	0.00001	0.00002	0.00019	0.00020	-1.24684
D42	0.86572	0.00000	0.00042	0.00017	0.00059	0.86631
D43	2.95860	0.00000	-0.00001	0.00027	0.00026	2.95886
D44	-1.23415	0.00000	0.00044	0.00012	0.00057	-1.23358
D45	0.85873	0.00000	0.00002	0.00022	0.00024	0.85897
D46	3.13932	0.00001	0.00012	0.00013	0.00025	3.13957
D47	-0.00284	0.00000	0.00022	0.00003	0.00025	-0.00260
D48	-0.00314	0.00000	0.00031	0.00002	0.00033	-0.00282
D49	3.13788	0.00000	0.00041	-0.00008	0.00033	3.13821
D50	2.20846	-0.00002	-0.00033	-0.00068	-0.00098	2.20748
D51	-1.40498	0.00000	0.00061	-0.00345	-0.00286	-1.40784
D52	-2.08528	-0.00001	-0.00059	-0.00120	-0.00177	-2.08706
D53	0.58446	0.00001	0.00035	-0.00398	-0.00365	0.58081
D54	-2.71276	0.00000	-0.00003	0.00027	0.00023	-2.71252
D55	-0.01585	0.00000	0.00022	0.00001	0.00023	-0.01562
D56	-0.02705	0.00002	-0.00016	0.00038	0.00022	-0.02683
D57	2.66985	0.00002	0.00009	0.00012	0.00021	2.67007
D58	0.50881	0.00001	0.00112	-0.00294	-0.00179	0.50702
D59	-1.91034	-0.00003	0.00128	-0.00327	-0.00196	-1.91230
D60	1.78230	0.00003	0.00025	0.00106	0.00130	1.78359
D61	-0.63965	0.00001	-0.00014	0.00082	0.00067	-0.63898
D62	2.55312	0.00001	0.00083	0.00055	0.00138	2.55450
D63	-1.65599	0.00001	0.00087	0.00059	0.00146	-1.65453
D64	0.44349	0.00000	0.00081	0.00058	0.00139	0.44488
D65	1.34836	0.00001	0.00112	0.00040	0.00152	1.34988
D66	-2.86075	0.00001	0.00116	0.00044	0.00160	-2.85914
D67	-0.76127	0.00001	0.00110	0.00043	0.00153	-0.75974
D68	-1.03939	0.00000	0.00094	0.00017	0.00111	-1.03827
D69	1.03469	0.00000	0.00098	0.00022	0.00120	1.03588
D70	3.13417	0.00000	0.00092	0.00020	0.00112	3.13529

Item	Value	Threshold	Converged?
Maximum Force	0.000048	0.000450	YES
RMS Force	0.000012	0.000300	YES
Maximum Displacement	0.013829	0.001800	NO

RMS Displacement 0.002583 0.001200 NO

Predicted change in Energy=-1.874583D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.644100	2.099981	-0.197798
2	6	0	-3.536075	1.118257	0.090122
3	7	0	-2.826914	-0.076074	0.111255
4	6	0	-1.534431	0.184621	-0.159492
5	7	0	-1.404104	1.497970	-0.353199
6	6	0	-0.129977	2.183306	-0.634673
7	6	0	0.454693	2.858874	0.610727
8	1	0	-2.783473	3.160946	-0.313571
9	1	0	-4.594670	1.169157	0.267850
10	1	0	0.569926	1.429915	-0.996383
11	1	0	-0.302513	2.917079	-1.423086
12	1	0	-0.226002	3.641319	0.962453
13	1	0	0.533465	2.105844	1.409165
14	35	0	0.136734	-2.666497	-0.218807
15	1	0	-0.758562	-0.604002	-0.214648
16	6	0	-3.301341	-1.400665	0.356356
17	6	0	-4.560455	-1.690362	0.656318
18	1	0	-2.501580	-2.133710	0.266206
19	1	0	-4.831981	-2.723499	0.824508
20	1	0	-5.347407	-0.951308	0.746207
21	7	0	1.721689	3.472306	0.230325
22	1	0	2.064270	4.087321	0.958937
23	1	0	2.419431	2.749365	0.066940
24	6	0	3.331610	-0.426282	-1.137557
25	6	0	3.265693	-0.564107	0.318554
26	8	0	2.734712	0.620800	-0.336703
27	1	0	4.271524	-0.148172	-1.608485
28	1	0	2.628891	-0.989144	-1.744540
29	1	0	2.480421	-1.217652	0.692893
30	6	0	4.462572	-0.353997	1.204462
31	1	0	4.164683	0.078944	2.164082
32	1	0	4.946470	-1.313894	1.409134
33	1	0	5.191913	0.310729	0.734664

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357313	0.000000			
3	N	2.205482	1.389166	0.000000		
4	C	2.213919	2.222738	1.346024	0.000000	
5	N	1.387140	2.210433	2.172032	1.333939	0.000000
6	C	2.553159	3.641588	3.596482	2.488580	1.473877
7	C	3.291224	4.384861	4.430840	3.420743	2.497267
8	H	1.076325	2.214036	3.265067	3.231464	2.160953
9	H	2.210879	1.074617	2.167967	3.242992	3.267037
10	H	3.378860	4.258740	3.877292	2.584466	2.077285
11	H	2.766227	3.997685	4.205446	3.252787	2.090941
12	H	3.093396	4.252456	4.616090	3.862578	2.777194
13	H	3.560799	4.390485	4.211590	3.229239	2.688794
14	Br	5.518405	5.282928	3.949993	3.305327	4.442413
15	H	3.296523	3.282322	2.159398	1.107673	2.203226
16	C	3.604660	2.543806	1.428179	2.429239	3.536249
17	C	4.332277	3.042741	2.430675	3.652113	4.598601
18	H	4.261426	3.417085	2.088951	2.547794	3.844114
19	H	5.394246	4.120411	3.396746	4.505470	5.564003
20	H	4.184421	2.827450	2.742642	4.080370	4.770461
21	N	4.596377	5.762403	5.770179	4.643614	3.742871
22	H	5.239877	6.397972	6.478897	5.425182	4.522838
23	H	5.111862	6.174877	5.958961	4.718284	4.044988
24	C	6.555476	7.145480	6.293616	5.000816	5.171552
25	C	6.503048	7.010461	6.115636	4.881629	5.148826
26	O	5.580223	6.304951	5.622987	4.295024	4.230779
27	H	7.407435	8.089976	7.304145	5.993283	6.041381
28	H	6.303931	6.768599	5.834680	4.606881	4.938281
29	H	6.169338	6.482131	5.459790	4.337276	4.853704
30	C	7.648080	8.208997	7.376242	6.173696	6.346178
31	H	7.484825	8.042584	7.288386	6.155491	6.273893
32	H	8.476646	8.922372	7.977605	6.834340	7.165346
33	H	8.091601	8.788931	8.052319	6.786687	6.789729

		6	7	8	9	10
6	C	0.000000				
7	C	1.532728	0.000000			
8	H	2.846037	3.381020	0.000000		
9	H	4.666534	5.335614	2.754217	0.000000	
10	H	1.090090	2.153604	3.835099	5.323470	0.000000
11	H	1.090774	2.170978	2.728673	4.933266	1.776199
12	H	2.164678	1.095115	2.898215	5.067476	3.059550
13	H	2.150217	1.100346	3.883702	5.336456	2.498975
14	Br	4.874903	5.596334	6.518872	6.110259	4.192001

15	H	2.888015	3.760950	4.276083	4.253542	2.552021
16	C	4.887181	5.684731	4.639535	2.878284	4.982850
17	C	6.025040	6.771214	5.256761	2.885987	6.228030
18	H	5.007266	5.812413	5.333759	3.910237	4.871110
19	H	6.950884	7.691392	6.333901	3.939410	7.053162
20	H	6.241332	6.942637	4.960597	2.300393	6.612237
21	N	2.416280	1.458178	4.548544	6.723265	2.646268
22	H	3.313546	2.054524	5.096868	7.303066	3.621899
23	H	2.704101	2.041542	5.233011	7.192708	2.508440
24	C	4.364106	4.703764	7.137324	8.206492	3.330510
25	C	4.470737	4.438905	7.132181	8.049352	3.601713
26	O	3.276683	3.332430	6.074804	7.374688	2.403361
27	H	5.075166	5.341856	7.899370	9.157805	4.070240
28	H	4.348287	5.008160	6.968831	7.803065	3.263575
29	H	4.488109	4.552844	6.920525	7.478932	3.676038
30	C	5.559841	5.170895	8.195390	9.232056	4.814432
31	H	5.541252	4.889269	7.994647	9.028318	4.973524
32	H	6.494449	6.182678	9.096369	9.924788	5.698170
33	H	5.805526	5.380488	8.534009	9.835244	5.060816

		11	12	13	14	15
11	H	0.000000				
12	H	2.494228	0.000000			
13	H	3.062452	1.770318	0.000000		
14	Br	5.728835	6.427713	5.057958	0.000000	
15	H	3.750509	4.437560	3.413118	2.248435	0.000000
16	C	5.549982	5.936890	5.301863	3.708572	2.725150
17	C	6.609274	6.878082	6.397342	4.876707	4.048845
18	H	5.761951	6.246117	5.337760	2.734923	2.368404
19	H	7.575215	7.857797	7.242403	5.077390	4.707956
20	H	6.717233	6.882425	6.661108	5.826571	4.701209
21	N	2.671973	2.087601	2.160731	6.355998	4.792279
22	H	3.556004	2.333298	2.544075	7.121555	5.599482
23	H	3.107617	2.931867	2.402614	5.884209	4.628607
24	C	4.946356	5.797587	4.552699	4.008728	4.196767
25	C	5.280536	5.503830	3.972800	3.807779	4.059621
26	O	3.959528	4.424610	3.177877	4.191624	3.703782
27	H	5.509261	6.418544	5.306589	5.036830	5.239497
28	H	4.894389	6.076135	4.890360	3.369306	3.736810
29	H	5.414618	5.568391	3.917819	2.902278	3.419241
30	C	6.349014	6.164726	4.640108	5.107467	5.416328
31	H	6.393640	5.780359	4.226579	5.425863	5.510274
32	H	7.312621	7.176917	5.582940	5.254834	5.973944
33	H	6.452725	6.363845	5.037710	5.943721	6.094758

		16	17	18	19	20

16	C	0.000000				
17	C	1.326375	0.000000			
18	H	1.088623	2.141894	0.000000		
19	H	2.076515	1.081382	2.467857	0.000000	
20	H	2.130796	1.083316	3.118847	1.847283	0.000000
21	N	6.999469	8.142478	7.018882	9.038343	8.355036
22	H	7.698758	8.795464	7.747780	9.693484	8.964709
23	H	7.073454	8.293211	6.935451	9.116421	8.630189
24	C	6.868569	8.191494	6.237946	8.704661	8.896604
25	C	6.620210	7.913982	5.977276	8.395909	8.632398
26	O	6.403170	7.716672	5.947233	8.353897	8.304509
27	H	7.923233	9.247245	7.302861	9.768601	9.935464
28	H	6.304821	7.611999	5.628043	8.079147	8.356231
29	H	5.794439	7.056821	5.083459	7.467002	7.832539
30	C	7.879920	9.137907	7.248939	9.599355	9.838824
31	H	7.822956	9.029498	7.275771	9.517779	9.672211
32	H	8.315182	9.544112	7.579699	9.896811	10.321572
33	H	8.672217	9.955862	8.086073	10.473445	10.614619

		21	22	23	24	25
21	N	0.000000				
22	H	1.013154	0.000000			
23	H	1.017931	1.646792	0.000000		
24	C	4.434178	5.135567	3.516762	0.000000	
25	C	4.322541	4.846575	3.429076	1.464104	0.000000
26	O	3.078770	3.760977	2.189319	1.447078	1.454409
27	H	4.794867	5.422456	3.825313	1.087455	2.213183
28	H	4.962625	5.779108	4.159541	1.085844	2.200575
29	H	4.773400	5.327917	4.016560	2.168257	1.088073
30	C	4.806452	5.053458	3.885774	2.601798	1.503828
31	H	4.606793	4.683075	3.817729	3.442396	2.151203
32	H	5.890375	6.138638	4.969656	3.143447	2.139289
33	H	4.721481	4.908675	3.752260	2.740278	2.156110

		26	27	28	29	30
26	O	0.000000				
27	H	2.137882	0.000000			
28	H	2.141290	1.850402	0.000000		
29	H	2.122413	3.106152	2.452620	0.000000	
30	C	2.512155	2.826931	3.530214	2.221829	0.000000
31	H	2.931272	3.780908	4.333221	2.585014	1.094096
32	H	3.418020	3.304616	3.927123	2.569759	1.094281
33	H	2.698482	2.558917	3.795419	3.112857	1.092937

		31	32	33
31	H	0.000000		
32	H	1.766674	0.000000	

33 H 1.775433 1.776106 0.000000

Stoichiometry C10H18BrN3O

Framework group C1[X(C10H18BrN3O)]

Deg. of freedom 93

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.350820	2.471581	-0.265207
2	6	0	-3.337459	1.590049	0.037685
3	7	0	-2.750955	0.331808	0.088934
4	6	0	-1.437738	0.456574	-0.178786
5	7	0	-1.176316	1.745879	-0.399571
6	6	0	0.161003	2.294668	-0.687185
7	6	0	0.804562	2.935744	0.547363
8	1	0	-2.383250	3.538365	-0.404476
9	1	0	-4.386489	1.749940	0.207310
10	1	0	0.783936	1.467625	-1.028140
11	1	0	0.065950	3.024561	-1.492174
12	1	0	0.203681	3.789559	0.877843
13	1	0	0.804356	2.196246	1.362167
14	35	0	-0.058785	-2.547343	-0.166324
15	1	0	-0.744089	-0.406378	-0.212012
16	6	0	-3.356109	-0.933304	0.359073
17	6	0	-4.639143	-1.089604	0.656838
18	1	0	-2.632993	-1.744111	0.289834
19	1	0	-5.013021	-2.086658	0.845212
20	1	0	-5.348915	-0.274101	0.725772
21	7	0	2.128058	3.411551	0.162331
22	1	0	2.526993	4.005189	0.879913
23	1	0	2.750997	2.619349	0.018988
24	6	0	3.347483	-0.656890	-1.111532
25	6	0	3.261705	-0.755608	0.346719
26	8	0	2.854364	0.461660	-0.337122
27	1	0	4.312513	-0.484081	-1.582077
28	1	0	2.594867	-1.160142	-1.711000
29	1	0	2.413559	-1.319402	0.729718
30	6	0	4.469626	-0.646364	1.235816
31	1	0	4.212116	-0.165049	2.184009
32	1	0	4.854541	-1.644957	1.464078

```
      33        1        0        5.263657     -0.067966      0.756775
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.4225000           0.2920279           0.1827001
 Standard basis: 6-311++G(d,p) (5D, 7F)
 There are     499 symmetry adapted cartesian basis functions of A      symmetry.
 There are     482 symmetry adapted basis functions of A      symmetry.
   482 basis functions,      760 primitive gaussians,      499 cartesian basis functions
    71 alpha electrons              71 beta electrons
         nuclear repulsion energy           1312.9285256524 Hartrees.
 NAtoms=       33 NActive=       33 NUniq=       33 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      482 RedAO= T EigKep=    3.63D-06    NBF=      482
 NBsUse=      482 1.00D-06 EigRej= -1.00D+00 NBFU=      482
 Initial                guess                from                the                checkpoint                file:
"/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"
 B after Tr=          0.000000        0.000000        0.000000
              Rot=        1.000000      -0.000074      -0.000057      -0.000086 Ang=    -0.01 deg.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3205.64837896         A.U. after        9 cycles
                  NFock=    9    Conv=0.25D-08         -V/T= 2.0018
 Calling FoFJK, ICntrl=              2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 ---------------------------------------------------------------------
 Center         Atomic                             Forces (Hartrees/Bohr)
 Number          Number                       X                       Y                       Z
 ---------------------------------------------------------------------
        1              6                 0.000008156       0.000002781       0.000009801
        2              6                -0.000000593       0.000004528      -0.000006868
        3              7                -0.000014501      -0.000017893      -0.000004419
        4              6                 0.000018855       0.000034484      -0.000015043
        5              7                -0.000004443      -0.000005522       0.000007678
        6              6                -0.000003265      -0.000008207      -0.000009415
        7              6                 0.000045776       0.000020699      -0.000015531
        8              1                -0.000002766      -0.000000140      -0.000003273
        9              1                 0.000000202      -0.000000535       0.000004433
       10              1                -0.000007438       0.000001903      -0.000000157
```

11	1	0.000004108	-0.000001577	-0.000003773
12	1	-0.000004710	0.000000063	-0.000004524
13	1	-0.000006650	-0.000006846	0.000001903
14	35	0.000003144	0.000007188	0.000002024
15	1	0.000000172	-0.000020278	0.000007257
16	6	0.000004539	0.000010320	0.000006072
17	6	-0.000003572	0.000001406	-0.000005407
18	1	0.000000866	-0.000002899	0.000001487
19	1	0.000000883	0.000000888	0.000000543
20	1	-0.000001813	0.000002178	-0.000002998
21	7	-0.000015918	-0.000019806	0.000024468
22	1	-0.000002671	-0.000001302	-0.000005652
23	1	-0.000007406	0.000003625	-0.000003947
24	6	0.000039688	-0.000017818	-0.000086751
25	6	-0.000038147	0.000049138	-0.000011156
26	8	0.000008186	-0.000035490	0.000035829
27	1	-0.000000702	0.000006584	0.000022194
28	1	-0.000018331	0.000004875	0.000017584
29	1	0.000005119	0.000000094	0.000022825
30	6	-0.000000886	-0.000010398	0.000010150
31	1	-0.000000085	-0.000004154	0.000003546
32	1	-0.000000057	0.000001219	0.000002899
33	1	-0.000005739	0.000000893	-0.000001778

Cartesian Forces: Max 0.000086751 RMS 0.000016227

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000045320 RMS 0.000010809
Search for a local minimum.
Step number 46 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 31 32 33 34 35
36 37 38 39 40
41 42 43 44 45
46
DE= -8.11D-08 DEPred=-1.87D-07 R= 4.33D-01
Trust test= 4.33D-01 RLast= 1.02D-02 DXMaxT set to 1.04D+00
ITU= 0 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1

ITU= 0 0 -1 1 -1 1 1 1 1 1 1 1 1 1 0 -1 -1 1 1 1

ITU= -1 1 0 0 -1 0

Eigenvalues --- 0.00062 0.00090 0.00148 0.00235 0.00358

Eigenvalues --- 0.00521 0.00697 0.00765 0.01265 0.01416

Eigenvalues --- 0.01892 0.02051 0.02169 0.02349 0.02380

Eigenvalues --- 0.02530 0.02675 0.02841 0.03062 0.03103

Eigenvalues --- 0.03234 0.03499 0.03616 0.03969 0.04078

Eigenvalues --- 0.04291 0.04467 0.04669 0.05495 0.05599

Eigenvalues --- 0.05735 0.05744 0.05901 0.07719 0.08683

Eigenvalues --- 0.08885 0.09563 0.09827 0.11011 0.12320

Eigenvalues --- 0.12435 0.13058 0.13345 0.15726 0.15929

Eigenvalues --- 0.16001 0.16002 0.16004 0.16015 0.16125

Eigenvalues --- 0.16275 0.18608 0.21382 0.21727 0.22140

Eigenvalues --- 0.23170 0.23386 0.25562 0.26078 0.27475

Eigenvalues --- 0.29133 0.30090 0.30383 0.31866 0.32455

Eigenvalues --- 0.33666 0.34288 0.34337 0.34401 0.34550

Eigenvalues --- 0.34724 0.34745 0.35086 0.35184 0.35328

Eigenvalues --- 0.35556 0.35710 0.35879 0.35969 0.36419

Eigenvalues --- 0.36627 0.39659 0.41156 0.41904 0.42508

Eigenvalues --- 0.44699 0.45484 0.46483 0.49556 0.54930

Eigenvalues --- 0.58290 0.60637 1.08911

En-DIIS/RFO-DIIS IScMMF= 0 using points: 46 45 44 43 42

RFO step: Lambda=-3.04256018D-08.

DidBck=F Rises=F RFO-DIIS coefs: 0.84890 0.42398 -0.47573 0.16308 0.03976

Iteration 1 RMS(Cart)= 0.00151351 RMS(Int)= 0.00000321

Iteration 2 RMS(Cart)= 0.00000124 RMS(Int)= 0.00000310

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000310

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56495	0.00000	0.00000	0.00000	0.00000	2.56495
R2	2.62131	0.00000	0.00000	0.00000	0.00000	2.62132
R3	2.03396	0.00000	0.00000	0.00000	0.00000	2.03396
R4	2.62514	0.00000	0.00001	-0.00001	0.00000	2.62515
R5	2.03073	0.00000	0.00000	0.00000	0.00000	2.03073
R6	2.54362	0.00001	0.00000	0.00003	0.00003	2.54365
R7	2.69887	-0.00001	-0.00002	-0.00001	-0.00002	2.69884
R8	2.52078	-0.00002	0.00000	0.00000	0.00000	2.52078
R9	2.09320	0.00001	0.00005	0.00002	0.00007	2.09326
R10	2.78522	-0.00001	-0.00002	0.00000	-0.00001	2.78521
R11	2.89644	0.00000	0.00000	0.00003	0.00003	2.89646
R12	2.05997	-0.00001	-0.00001	0.00000	-0.00001	2.05996
R13	2.06126	0.00000	0.00000	0.00000	0.00000	2.06126
R14	2.06947	0.00000	-0.00001	0.00001	0.00000	2.06947

R15	2.07935	0.00001	-0.00001	0.00003	0.00002	2.07937
R16	2.75556	-0.00004	0.00002	-0.00009	-0.00007	2.75548
R17	4.24893	-0.00001	-0.00032	0.00007	-0.00025	4.24868
R18	2.50648	0.00000	0.00000	0.00000	0.00000	2.50649
R19	2.05720	0.00000	0.00001	0.00001	0.00001	2.05721
R20	2.04352	0.00000	0.00000	0.00000	0.00000	2.04352
R21	2.04717	0.00000	0.00000	0.00000	0.00000	2.04717
R22	1.91458	-0.00001	0.00000	-0.00001	-0.00001	1.91457
R23	1.92361	-0.00002	0.00000	-0.00003	-0.00002	1.92359
R24	4.13721	0.00000	-0.00037	0.00001	-0.00036	4.13685
R25	2.76675	0.00004	0.00010	0.00004	0.00014	2.76689
R26	2.73458	0.00001	-0.00006	0.00002	-0.00003	2.73455
R27	2.05499	-0.00001	-0.00002	-0.00002	-0.00003	2.05496
R28	2.05195	0.00000	0.00000	-0.00001	0.00000	2.05195
R29	2.74844	-0.00005	-0.00002	-0.00010	-0.00012	2.74832
R30	2.05616	0.00000	0.00001	0.00001	0.00002	2.05618
R31	2.84182	0.00000	-0.00002	0.00002	0.00000	2.84182
R32	2.06754	0.00000	0.00000	0.00000	0.00000	2.06754
R33	2.06789	0.00000	0.00000	0.00000	0.00000	2.06789
R34	2.06535	0.00000	0.00000	0.00000	0.00000	2.06535
A1	1.87268	0.00000	0.00001	0.00000	0.00001	1.87268
A2	2.27928	0.00000	-0.00001	-0.00001	-0.00003	2.27926
A3	2.13117	0.00001	0.00001	0.00001	0.00002	2.13119
A4	1.86460	0.00000	0.00000	0.00000	0.00000	1.86460
A5	2.27600	0.00000	0.00001	0.00001	0.00002	2.27601
A6	2.14253	0.00000	0.00000	-0.00001	-0.00001	2.14251
A7	1.89717	-0.00001	0.00000	0.00000	-0.00001	1.89717
A8	2.25289	0.00000	0.00004	-0.00003	0.00001	2.25290
A9	2.13309	0.00000	-0.00003	0.00003	0.00000	2.13309
A10	1.88990	0.00000	0.00000	-0.00001	0.00000	1.88989
A11	2.14684	0.00000	-0.00007	-0.00009	-0.00016	2.14668
A12	2.24632	-0.00001	0.00006	0.00010	0.00016	2.24649
A13	1.90042	0.00001	0.00000	0.00000	0.00000	1.90042
A14	2.20479	0.00003	0.00001	-0.00003	-0.00002	2.20477
A15	2.17731	-0.00004	-0.00001	0.00003	0.00001	2.17732
A16	1.96009	-0.00002	-0.00007	-0.00006	-0.00013	1.95996
A17	1.87239	-0.00001	0.00002	0.00004	0.00007	1.87246
A18	1.89030	0.00001	0.00004	-0.00003	0.00001	1.89032
A19	1.90638	0.00001	-0.00001	0.00008	0.00008	1.90645
A20	1.92958	0.00001	0.00003	-0.00001	0.00003	1.92961
A21	1.90355	0.00000	-0.00002	-0.00003	-0.00005	1.90351
A22	1.91642	0.00000	-0.00001	-0.00009	-0.00010	1.91632
A23	1.89153	-0.00001	-0.00003	-0.00004	-0.00008	1.89146
A24	1.88062	0.00001	0.00006	0.00009	0.00015	1.88077

A25	1.87592	0.00000	0.00001	-0.00004	-0.00002	1.87589
A26	1.90000	0.00001	0.00001	-0.00001	0.00000	1.90000
A27	1.99873	0.00000	-0.00004	0.00009	0.00005	1.99878
A28	2.16124	0.00000	0.00002	-0.00002	0.00000	2.16124
A29	1.94580	0.00000	0.00000	0.00001	0.00001	1.94581
A30	2.17615	0.00000	-0.00002	0.00001	-0.00001	2.17614
A31	2.07396	0.00000	-0.00001	-0.00001	-0.00002	2.07394
A32	2.16440	0.00000	0.00001	0.00001	0.00002	2.16442
A33	2.04482	0.00000	0.00000	0.00000	0.00001	2.04483
A34	1.94074	0.00002	-0.00003	0.00006	0.00003	1.94076
A35	1.91631	-0.00004	-0.00005	0.00009	0.00004	1.91636
A36	1.89101	0.00002	-0.00002	0.00003	0.00001	1.89102
A37	2.08711	-0.00001	0.00006	-0.00006	0.00002	2.08713
A38	2.06919	-0.00001	-0.00006	0.00004	-0.00003	2.06915
A39	1.99449	0.00001	0.00002	-0.00002	0.00000	1.99449
A40	2.00149	-0.00001	-0.00005	-0.00006	-0.00010	2.00138
A41	2.03740	0.00002	0.00002	0.00007	0.00008	2.03748
A42	2.01661	0.00002	0.00003	0.00015	0.00017	2.01678
A43	2.13756	-0.00001	-0.00005	-0.00007	-0.00011	2.13745
A44	1.96152	0.00000	0.00004	0.00006	0.00010	1.96163
A45	2.02879	0.00000	-0.00004	0.00001	-0.00004	2.02875
A46	2.04389	-0.00001	0.00003	-0.00010	-0.00007	2.04383
A47	2.61583	-0.00002	-0.00058	0.00037	-0.00020	2.61563
A48	2.43658	-0.00001	0.00091	-0.00035	0.00055	2.43712
A49	1.93402	0.00000	0.00003	-0.00002	0.00001	1.93403
A50	1.91726	0.00000	0.00000	0.00002	0.00001	1.91727
A51	1.94214	-0.00001	-0.00002	-0.00001	-0.00003	1.94211
A52	1.87912	0.00000	-0.00002	-0.00002	-0.00004	1.87908
A53	1.89446	0.00000	0.00001	0.00002	0.00002	1.89448
A54	1.89528	0.00000	0.00001	0.00002	0.00003	1.89531
A55	3.48428	-0.00003	-0.00033	-0.00036	-0.00069	3.48359
A56	2.53104	-0.00004	0.00059	-0.00028	0.00030	2.53134
A57	2.96475	0.00000	-0.00032	-0.00093	-0.00125	2.96349
A58	3.10741	-0.00001	-0.00029	0.00008	-0.00020	3.10721
D1	0.00307	0.00000	0.00001	0.00000	0.00002	0.00308
D2	-3.12658	0.00000	-0.00008	-0.00014	-0.00022	-3.12680
D3	3.13323	0.00000	0.00004	-0.00002	0.00002	3.13325
D4	0.00358	0.00000	-0.00006	-0.00016	-0.00022	0.00336
D5	-0.00463	0.00000	-0.00004	-0.00002	-0.00006	-0.00469
D6	-3.10827	0.00000	0.00002	0.00008	0.00011	-3.10816
D7	-3.13597	0.00000	-0.00007	0.00000	-0.00007	-3.13604
D8	0.04357	0.00000	0.00000	0.00010	0.00010	0.04367
D9	-0.00050	0.00000	0.00002	0.00001	0.00003	-0.00046
D10	-3.13311	0.00000	0.00001	-0.00012	-0.00011	-3.13322

D11	3.13028	0.00000	0.00011	0.00014	0.00025	3.13053
D12	-0.00233	0.00000	0.00009	0.00001	0.00010	-0.00222
D13	-0.00239	0.00000	-0.00005	-0.00003	-0.00007	-0.00246
D14	-3.12841	0.00000	-0.00006	-0.00028	-0.00034	-3.12875
D15	3.13096	0.00000	-0.00003	0.00010	0.00006	3.13102
D16	0.00494	0.00000	-0.00005	-0.00016	-0.00021	0.00473
D17	-0.03840	0.00001	0.00040	0.00099	0.00139	-0.03700
D18	3.10389	0.00001	0.00034	0.00098	0.00132	3.10521
D19	3.11325	0.00000	0.00038	0.00085	0.00123	3.11448
D20	-0.02764	0.00000	0.00032	0.00083	0.00115	-0.02649
D21	0.00433	0.00000	0.00006	0.00003	0.00008	0.00441
D22	3.10871	0.00000	-0.00001	-0.00007	-0.00008	3.10862
D23	3.12919	0.00001	0.00007	0.00030	0.00037	3.12955
D24	-0.04962	0.00001	0.00000	0.00020	0.00020	-0.04942
D25	1.34601	0.00001	0.00025	0.00002	0.00027	1.34628
D26	-2.84233	0.00000	0.00022	0.00011	0.00033	-2.84200
D27	-0.78987	0.00000	0.00022	0.00009	0.00031	-0.78956
D28	-1.75188	0.00001	0.00032	0.00014	0.00046	-1.75142
D29	0.34297	0.00000	0.00029	0.00023	0.00052	0.34349
D30	2.39543	0.00000	0.00030	0.00021	0.00051	2.39593
D31	-1.09977	-0.00001	-0.00006	0.00037	0.00030	-1.09946
D32	0.94460	-0.00001	-0.00007	0.00025	0.00018	0.94478
D33	3.11645	-0.00002	-0.00010	0.00038	0.00028	3.11673
D34	3.10842	0.00001	-0.00005	0.00030	0.00025	3.10867
D35	-1.13040	0.00000	-0.00005	0.00018	0.00012	-1.13028
D36	1.04145	0.00000	-0.00009	0.00031	0.00023	1.04167
D37	1.01371	0.00000	-0.00004	0.00028	0.00025	1.01396
D38	3.05808	0.00000	-0.00004	0.00016	0.00012	3.05820
D39	-1.05326	-0.00001	-0.00008	0.00030	0.00022	-1.05304
D40	2.94378	0.00001	0.00024	-0.00005	0.00019	2.94398
D41	-1.24684	0.00001	0.00016	0.00009	0.00025	-1.24659
D42	0.86631	0.00000	0.00021	0.00002	0.00023	0.86654
D43	2.95886	0.00001	0.00013	0.00016	0.00029	2.95915
D44	-1.23358	0.00000	0.00022	0.00002	0.00023	-1.23335
D45	0.85897	0.00000	0.00014	0.00016	0.00029	0.85927
D46	3.13957	0.00000	-0.00001	0.00010	0.00009	3.13966
D47	-0.00260	0.00000	0.00003	0.00010	0.00013	-0.00247
D48	-0.00282	0.00000	0.00005	0.00012	0.00018	-0.00264
D49	3.13821	0.00000	0.00010	0.00011	0.00021	3.13842
D50	2.20748	0.00001	-0.00008	0.00028	0.00021	2.20769
D51	-1.40784	0.00002	0.00071	0.00066	0.00137	-1.40647
D52	-2.08706	-0.00001	0.00012	0.00029	0.00042	-2.08664
D53	0.58081	0.00000	0.00091	0.00067	0.00158	0.58239
D54	-2.71252	-0.00001	0.00002	-0.00003	-0.00001	-2.71253

D55	-0.01562	-0.00001	0.00005	-0.00008	-0.00003	-0.01565
D56	-0.02683	0.00002	0.00006	0.00012	0.00018	-0.02666
D57	2.67007	0.00001	0.00009	0.00007	0.00016	2.67022
D58	0.50702	0.00002	0.00143	-0.00023	0.00121	0.50823
D59	-1.91230	-0.00001	0.00143	-0.00024	0.00120	-1.91110
D60	1.78359	-0.00001	0.00014	-0.00055	-0.00042	1.78318
D61	-0.63898	0.00001	0.00009	-0.00047	-0.00039	-0.63937
D62	2.55450	0.00000	0.00024	0.00021	0.00044	2.55494
D63	-1.65453	0.00000	0.00023	0.00018	0.00041	-1.65412
D64	0.44488	0.00000	0.00022	0.00021	0.00043	0.44531
D65	1.34988	0.00000	0.00032	0.00020	0.00052	1.35040
D66	-2.85914	0.00000	0.00031	0.00017	0.00048	-2.85866
D67	-0.75974	0.00000	0.00031	0.00020	0.00051	-0.75923
D68	-1.03827	0.00000	0.00026	0.00021	0.00048	-1.03779
D69	1.03588	0.00000	0.00026	0.00019	0.00044	1.03633
D70	3.13529	0.00000	0.00025	0.00022	0.00047	3.13576

Item	Value	Threshold	Converged?
Maximum Force	0.000045	0.000450	YES
RMS Force	0.000011	0.000300	YES
Maximum Displacement	0.010304	0.001800	NO
RMS Displacement	0.001514	0.001200	NO

Predicted change in Energy=-5.420873D-08

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.644127	2.099866	-0.198346
2	6	0	-3.536189	1.118317	0.089889
3	7	0	-2.827082	-0.076035	0.111706
4	6	0	-1.534521	0.184493	-0.158909
5	7	0	-1.404128	1.497737	-0.353276
6	6	0	-0.129932	2.182931	-0.634744
7	6	0	0.454549	2.858557	0.610730
8	1	0	-2.783460	3.160782	-0.314622
9	1	0	-4.594780	1.169354	0.267609
10	1	0	0.569967	1.429500	-0.996365
11	1	0	-0.302348	2.916650	-1.423234
12	1	0	-0.226388	3.640829	0.962378
13	1	0	0.533275	2.105470	1.409132
14	35	0	0.137039	-2.666452	-0.213355
15	1	0	-0.758709	-0.604293	-0.213209

16	6	0	-3.301568	-1.400468	0.357471
17	6	0	-4.561033	-1.690126	0.656004
18	1	0	-2.501556	-2.133461	0.269067
19	1	0	-4.832537	-2.723149	0.824928
20	1	0	-5.348294	-0.951169	0.743981
21	7	0	1.721454	3.472282	0.230644
22	1	0	2.063879	4.087151	0.959444
23	1	0	2.419337	2.749535	0.067067
24	6	0	3.333170	-0.424784	-1.138807
25	6	0	3.265883	-0.564067	0.317175
26	8	0	2.735629	0.621472	-0.337387
27	1	0	4.273511	-0.146239	-1.608587
28	1	0	2.630875	-0.986896	-1.746974
29	1	0	2.480282	-1.217927	0.690304
30	6	0	4.462037	-0.354883	1.204279
31	1	0	4.163330	0.076721	2.164246
32	1	0	4.945966	-1.314946	1.408084
33	1	0	5.191584	0.310615	0.735891

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357311	0.000000			
3	N	2.205482	1.389167	0.000000		
4	C	2.213918	2.222746	1.346039	0.000000	
5	N	1.387140	2.210438	2.172041	1.333938	0.000000
6	C	2.553139	3.641577	3.596489	2.488582	1.473870
7	C	3.291202	4.384713	4.430571	3.420433	2.497163
8	H	1.076325	2.214022	3.265064	3.231468	2.160964
9	H	2.210886	1.074618	2.167961	3.243001	3.267046
10	H	3.378850	4.258791	3.877422	2.584617	2.077324
11	H	2.766119	3.997658	4.205530	3.252914	2.090943
12	H	3.093106	4.251951	4.615445	3.861962	2.776844
13	H	3.560884	4.390377	4.211208	3.228727	2.688671
14	Br	5.518414	5.282900	3.949929	3.305294	4.442437
15	H	3.296589	3.282324	2.159350	1.107708	2.203342
16	C	3.604649	2.543801	1.428166	2.429240	3.536245
17	C	4.332260	3.042719	2.430665	3.652130	4.598604
18	H	4.261438	3.417108	2.088954	2.547790	3.844120
19	H	5.394229	4.120396	3.396726	4.505467	5.563994
20	H	4.184413	2.827425	2.742652	4.080417	4.770488
21	N	4.596287	5.762271	5.770085	4.643563	3.742867
22	H	5.239761	6.397724	6.478602	5.424936	4.522762
23	H	5.111867	6.174924	5.959090	4.718421	4.045068

24	C	6.556402	7.146954	6.295563	5.002583	5.172538
25	C	6.503116	7.010724	6.115931	4.881688	5.148742
26	O	5.580928	6.305959	5.624229	4.296159	4.231511
27	H	7.408608	8.091683	7.306350	5.995347	6.042686
28	H	6.304918	6.770426	5.837264	4.609189	4.939336
29	H	6.169037	6.482010	5.459561	4.336656	4.853096
30	C	7.647922	8.208763	7.375820	6.173161	6.345870
31	H	7.484412	8.041795	7.287120	6.154199	6.273261
32	H	8.476501	8.922184	7.977203	6.833777	7.165004
33	H	8.091513	8.788841	8.052211	6.786535	6.789622

		6	7	8	9	10
6	C	0.000000				
7	C	1.532741	0.000000			
8	H	2.846029	3.381171	0.000000		
9	H	4.666525	5.335435	2.754208	0.000000	
10	H	1.090085	2.153667	3.835046	5.323525	0.000000
11	H	1.090774	2.171009	2.728468	4.933251	1.776166
12	H	2.164618	1.095117	2.898238	5.066926	3.059547
13	H	2.150179	1.100356	3.884036	5.336322	2.498939
14	Br	4.874972	5.595146	6.518913	6.110225	4.192536
15	H	2.888195	3.760612	4.276177	4.253522	2.552456
16	C	4.887178	5.684352	4.639520	2.878273	4.983009
17	C	6.025052	6.771162	5.256728	2.885934	6.228126
18	H	5.007266	5.811673	5.333776	3.910265	4.871372
19	H	6.950882	7.691204	6.333872	3.939380	7.053273
20	H	6.241376	6.942965	4.960560	2.300289	6.612277
21	N	2.416392	1.458139	4.548471	6.723069	2.646588
22	H	3.313653	2.054504	5.096871	7.302734	3.622164
23	H	2.704136	2.041530	5.232963	7.192707	2.508695
24	C	4.364325	4.704006	7.137838	8.208025	3.330758
25	C	4.470313	4.438933	7.132195	8.049672	3.601063
26	O	3.276890	3.332687	6.075274	7.375710	2.403591
27	H	5.075796	5.342157	7.900099	9.159557	4.071118
28	H	4.348207	5.008260	6.969209	7.805001	3.263391
29	H	4.487182	4.552763	6.920256	7.478923	3.674647
30	C	5.559557	5.170923	8.195375	9.231824	4.814048
31	H	5.540989	4.889486	7.994630	9.027490	4.973101
32	H	6.494076	6.182777	9.096366	9.924630	5.697608
33	H	5.805406	5.380258	8.533953	9.835123	5.060826

		11	12	13	14	15
11	H	0.000000				
12	H	2.494263	0.000000			
13	H	3.062446	1.770312	0.000000		
14	Br	5.729563	6.426214	5.055760	0.000000	

15	H	3.750929	4.436939	3.412335	2.248303	0.000000
16	C	5.550111	5.936103	5.301284	3.708447	2.725014
17	C	6.609237	6.877651	6.397321	4.876564	4.048731
18	H	5.762293	6.244957	5.336523	2.734775	2.368219
19	H	7.575235	7.857208	7.242154	5.077197	4.707797
20	H	6.717024	6.882446	6.661705	5.826454	4.701151
21	N	2.672043	2.087566	2.160736	6.355436	4.792356
22	H	3.556158	2.333353	2.544018	7.120346	5.599265
23	H	3.107490	2.931868	2.402746	5.883914	4.628898
24	C	4.946016	5.797814	4.553416	4.012081	4.199099
25	C	5.279837	5.503943	3.973153	3.806724	4.059589
26	O	3.959319	4.424867	3.178513	4.192673	3.705175
27	H	5.509458	6.418788	5.307183	5.040689	5.242150
28	H	4.893493	6.076214	4.891181	3.375221	3.740067
29	H	5.413391	5.568447	3.918229	2.899243	3.418179
30	C	6.348710	6.164865	4.640094	5.104767	5.415502
31	H	6.393551	5.780742	4.226502	5.421163	5.508407
32	H	7.312152	7.177159	5.583108	5.251801	5.973018
33	H	6.452637	6.363651	5.037321	5.942426	6.094574

		16	17	18	19	20
16	C	0.000000				
17	C	1.326376	0.000000			
18	H	1.088629	2.141894	0.000000		
19	H	2.076504	1.081382	2.467830	0.000000	
20	H	2.130809	1.083318	3.118858	1.847288	0.000000
21	N	6.999323	8.142544	7.018521	9.038326	8.355344
22	H	7.698335	8.795366	7.746989	9.693237	8.965010
23	H	7.073586	8.293551	6.935391	9.116705	8.630731
24	C	6.870995	8.193954	6.240651	8.707326	8.898865
25	C	6.620619	7.914759	5.977346	8.396657	8.633427
26	O	6.404594	7.718263	5.948576	8.355514	8.306165
27	H	7.925926	9.249925	7.305900	9.771518	9.937888
28	H	6.308218	7.615272	5.632129	8.082807	8.359023
29	H	5.794298	7.057213	5.082751	7.467338	7.833303
30	C	7.879333	9.137793	7.247730	9.599047	9.839208
31	H	7.821204	9.028347	7.273055	9.516232	9.671851
32	H	8.314621	9.544077	7.578451	9.896577	10.322072
33	H	8.672061	9.956047	8.085533	10.473522	10.615140

		21	22	23	24	25
21	N	0.000000				
22	H	1.013148	0.000000			
23	H	1.017921	1.646786	0.000000		
24	C	4.433977	5.135301	3.516465	0.000000	
25	C	4.322599	4.846767	3.429162	1.464176	0.000000

26	O	3.078689	3.760845	2.189126	1.447060	1.454346
27	H	4.794733	5.422071	3.825086	1.087437	2.213245
28	H	4.962085	5.778593	4.158895	1.085843	2.200620
29	H	4.773382	5.328198	4.016578	2.168443	1.088085
30	C	4.806865	5.053986	3.886294	2.601784	1.503827
31	H	4.607756	4.684314	3.818849	3.442504	2.151208
32	H	5.890790	6.139248	4.970130	3.143272	2.139295
33	H	4.721570	4.908640	3.752467	2.740257	2.156088

		26	27	28	29	30
26	O	0.000000				
27	H	2.137852	0.000000			
28	H	2.141204	1.850434	0.000000		
29	H	2.122438	3.106298	2.452830	0.000000	
30	C	2.512068	2.826888	3.530225	2.221794	0.000000
31	H	2.931425	3.781022	4.333283	2.584816	1.094095
32	H	3.417891	3.304297	3.927042	2.569868	1.094279
33	H	2.698198	2.558936	3.795442	3.112825	1.092938

		31	32	33
31	H	0.000000		
32	H	1.766646	0.000000	
33	H	1.775447	1.776125	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.351202	2.471386	-0.264925
2	6	0	-3.337857	1.589633	0.037264
3	7	0	-2.751273	0.331410	0.088061
4	6	0	-1.437970	0.456419	-0.179198
5	7	0	-1.176605	1.745843	-0.399344
6	6	0	0.160750	2.294919	-0.686205
7	6	0	0.803861	2.934944	0.549137
8	1	0	-2.383697	3.538237	-0.403662
9	1	0	-4.386914	1.749374	0.206871
10	1	0	0.783823	1.468244	-1.027781
11	1	0	0.065850	3.025518	-1.490573
12	1	0	0.202572	3.788217	0.880281

13	1	0	0.803563	2.194599	1.363184
14	35	0	-0.058283	-2.547115	-0.164585
15	1	0	-0.744292	-0.406559	-0.212300
16	6	0	-3.356369	-0.933858	0.357533
17	6	0	-4.639769	-1.090553	0.653516
18	1	0	-2.632900	-1.744450	0.289362
19	1	0	-5.013531	-2.087708	0.841591
20	1	0	-5.349954	-0.275305	0.721223
21	7	0	2.127298	3.411586	0.165083
22	1	0	2.525882	4.004446	0.883497
23	1	0	2.750512	2.619772	0.020870
24	6	0	3.349338	-0.654166	-1.114145
25	6	0	3.261837	-0.755632	0.343888
26	8	0	2.855244	0.462826	-0.338142
27	1	0	4.314882	-0.480372	-1.583230
28	1	0	2.597373	-1.156240	-1.715415
29	1	0	2.413345	-1.320205	0.725000
30	6	0	4.468789	-0.647939	1.234486
31	1	0	4.210128	-0.168821	2.183477
32	1	0	4.853803	-1.646896	1.460972
33	1	0	5.263103	-0.068206	0.757528

Rotational constants (GHZ): 0.4225782 0.2919931 0.1826904

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1312.9135586379 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 3.63D-06 NBF= 482

NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000121 0.000046 -0.000070 Ang= -0.02 deg.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3205.64837892 A.U. after 8 cycles

NFock= 8 Conv=0.89D-08 -V/T= 2.0018

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000002419	0.000003471	0.000004120
2	6	-0.000000733	-0.000000874	-0.000003011
3	7	-0.000002051	-0.000000610	0.000000769
4	6	0.000002233	0.000007168	-0.000019033
5	7	-0.000001214	-0.000012114	0.000005940
6	6	0.000001957	0.000002134	-0.000004069
7	6	0.000026766	0.000013917	-0.000007489
8	1	0.000000132	0.000000204	-0.000002681
9	1	0.000000459	0.000001492	0.000000565
10	1	-0.000003323	-0.000002395	0.000003073
11	1	0.000001806	0.000000286	-0.000001804
12	1	-0.000002776	0.000000641	-0.000001487
13	1	-0.000002670	-0.000002654	0.000001241
14	35	0.000000798	0.000002473	0.000000084
15	1	0.000002404	0.000001107	0.000004893
16	6	0.000002443	0.000004550	0.000005181
17	6	-0.000002835	-0.000000574	-0.000003598
18	1	-0.000002477	0.000000738	0.000001576
19	1	-0.000000954	0.000001405	0.000000036
20	1	-0.000000246	0.000001093	-0.000002742
21	7	-0.000011173	-0.000014838	0.000008012
22	1	-0.000003346	0.000000511	-0.000002480
23	1	-0.000001193	-0.000002575	-0.000002556
24	6	0.000011103	-0.000019887	-0.000024049
25	6	-0.000009982	0.000029623	-0.000016147
26	8	-0.000010038	-0.000008421	0.000019886
27	1	0.000001937	0.000001166	0.000010356
28	1	-0.000003170	0.000001587	0.000004100
29	1	0.000002143	0.000001547	0.000009962
30	6	0.000005231	-0.000009568	0.000007724
31	1	-0.000002357	-0.000000902	0.000000473
32	1	0.000000069	0.000000088	0.000001861
33	1	-0.000001362	0.000000213	0.000001296

Cartesian Forces: Max 0.000029623 RMS 0.000007541

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000025430 RMS 0.000004429
Search for a local minimum.
Step number 47 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 31 32 33 34 35
36 37 38 39 40
41 42 43 44 45
46 47
DE= 3.01D-08 DEPred=-5.42D-08 R=-5.56D-01
Trust test=-5.56D-01 RLast= 4.67D-03 DXMaxT set to 5.19D-01
ITU= -1 0 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
ITU= 1 0 0 -1 1 -1 1 1 1 1 1 1 1 1 0 -1 -1 1 1
ITU= 1 -1 1 0 0 -1 0
Eigenvalues --- 0.00066 0.00109 0.00140 0.00254 0.00313
Eigenvalues --- 0.00537 0.00697 0.00765 0.01257 0.01432
Eigenvalues --- 0.01873 0.02045 0.02166 0.02338 0.02376
Eigenvalues --- 0.02544 0.02680 0.02730 0.03058 0.03098
Eigenvalues --- 0.03241 0.03522 0.03607 0.03968 0.04067
Eigenvalues --- 0.04290 0.04472 0.04734 0.05498 0.05564
Eigenvalues --- 0.05686 0.05743 0.05904 0.07821 0.08553
Eigenvalues --- 0.08884 0.09550 0.09861 0.10804 0.11535
Eigenvalues --- 0.12468 0.13106 0.13377 0.15748 0.15929
Eigenvalues --- 0.15992 0.16001 0.16005 0.16015 0.16133
Eigenvalues --- 0.16245 0.18425 0.21464 0.21690 0.22147
Eigenvalues --- 0.23187 0.23418 0.25078 0.26111 0.27462
Eigenvalues --- 0.28942 0.29728 0.30604 0.31846 0.32595
Eigenvalues --- 0.33662 0.34290 0.34335 0.34404 0.34550
Eigenvalues --- 0.34720 0.34730 0.35090 0.35205 0.35337
Eigenvalues --- 0.35542 0.35679 0.35883 0.36009 0.36419
Eigenvalues --- 0.36625 0.39463 0.41324 0.41878 0.42535
Eigenvalues --- 0.44665 0.45473 0.46482 0.49549 0.54904
Eigenvalues --- 0.58381 0.60645 1.05328
En-DIIS/RFO-DIIS IScMMF= 0 using points: 47 46 45 44 43
RFO step: Lambda=-6.29098378D-09.
DidBck=F Rises=F RFO-DIIS coefs: 1.05300 0.03756 -0.10887 -0.02734

0.04565

Iteration 1 RMS(Cart)= 0.00050150 RMS(Int)= 0.00000049

Iteration 2 RMS(Cart)= 0.00000014 RMS(Int)= 0.00000049

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56495	0.00000	0.00000	0.00000	0.00000	2.56495
R2	2.62132	0.00000	0.00000	0.00000	0.00000	2.62132
R3	2.03396	0.00000	0.00000	0.00000	0.00000	2.03396
R4	2.62515	0.00000	0.00000	0.00000	0.00000	2.62515
R5	2.03073	0.00000	0.00000	0.00000	0.00000	2.03073
R6	2.54365	0.00000	0.00001	0.00001	0.00001	2.54366
R7	2.69884	0.00000	-0.00001	-0.00001	-0.00001	2.69883
R8	2.52078	-0.00001	0.00000	-0.00002	-0.00002	2.52076
R9	2.09326	0.00000	0.00002	0.00001	0.00003	2.09329
R10	2.78521	0.00000	0.00000	0.00000	0.00000	2.78521
R11	2.89646	0.00000	0.00001	0.00000	0.00001	2.89647
R12	2.05996	0.00000	-0.00001	-0.00001	-0.00001	2.05995
R13	2.06126	0.00000	0.00000	0.00000	0.00000	2.06127
R14	2.06947	0.00000	0.00000	0.00001	0.00001	2.06948
R15	2.07937	0.00000	0.00001	0.00001	0.00002	2.07939
R16	2.75548	-0.00003	-0.00002	-0.00006	-0.00008	2.75540
R17	4.24868	0.00000	-0.00009	-0.00015	-0.00023	4.24844
R18	2.50649	0.00000	0.00000	0.00000	0.00000	2.50649
R19	2.05721	0.00000	0.00000	-0.00001	0.00000	2.05721
R20	2.04352	0.00000	0.00000	0.00000	0.00000	2.04352
R21	2.04717	0.00000	0.00000	0.00000	0.00000	2.04717
R22	1.91457	0.00000	0.00000	0.00000	-0.00001	1.91457
R23	1.92359	0.00000	0.00000	-0.00001	-0.00001	1.92358
R24	4.13685	0.00000	-0.00020	-0.00009	-0.00029	4.13656
R25	2.76689	0.00001	0.00001	0.00000	0.00001	2.76690
R26	2.73455	0.00001	0.00003	0.00005	0.00008	2.73463
R27	2.05496	0.00000	-0.00001	0.00000	-0.00002	2.05494
R28	2.05195	0.00000	0.00000	-0.00001	-0.00001	2.05194
R29	2.74832	-0.00002	-0.00005	-0.00007	-0.00012	2.74820
R30	2.05618	0.00000	0.00000	0.00000	0.00000	2.05618
R31	2.84182	0.00000	0.00000	0.00002	0.00002	2.84185
R32	2.06754	0.00000	0.00000	0.00000	0.00000	2.06754
R33	2.06789	0.00000	0.00000	0.00000	0.00000	2.06789
R34	2.06535	0.00000	0.00000	0.00000	0.00000	2.06535
A1	1.87268	0.00000	0.00000	-0.00001	-0.00001	1.87268
A2	2.27926	0.00000	-0.00001	0.00000	-0.00001	2.27925
A3	2.13119	0.00000	0.00001	0.00001	0.00001	2.13120
A4	1.86460	0.00000	0.00000	0.00000	0.00000	1.86460
A5	2.27601	0.00000	0.00001	0.00000	0.00000	2.27602

A6	2.14251	0.00000	0.00000	0.00000	0.00000	2.14251
A7	1.89717	0.00000	0.00000	0.00000	0.00000	1.89716
A8	2.25290	0.00000	0.00001	0.00000	0.00001	2.25290
A9	2.13309	0.00000	0.00000	0.00000	0.00000	2.13308
A10	1.88989	0.00000	0.00000	0.00000	0.00000	1.88989
A11	2.14668	0.00001	-0.00004	0.00002	-0.00002	2.14667
A12	2.24649	-0.00001	0.00003	-0.00002	0.00002	2.24651
A13	1.90042	0.00000	0.00000	0.00001	0.00001	1.90043
A14	2.20477	0.00001	0.00002	0.00001	0.00002	2.20479
A15	2.17732	-0.00001	-0.00001	-0.00002	-0.00003	2.17729
A16	1.95996	0.00000	-0.00003	-0.00001	-0.00004	1.95992
A17	1.87246	-0.00001	-0.00002	-0.00004	-0.00005	1.87241
A18	1.89032	0.00000	0.00001	0.00002	0.00004	1.89035
A19	1.90645	0.00000	0.00001	-0.00001	0.00001	1.90646
A20	1.92961	0.00000	0.00002	0.00001	0.00003	1.92964
A21	1.90351	0.00000	-0.00001	0.00002	0.00001	1.90352
A22	1.91632	0.00000	-0.00002	-0.00002	-0.00004	1.91628
A23	1.89146	0.00000	-0.00003	-0.00002	-0.00004	1.89142
A24	1.88077	0.00000	0.00004	0.00000	0.00003	1.88081
A25	1.87589	0.00000	0.00000	-0.00001	-0.00001	1.87588
A26	1.90000	0.00000	0.00000	0.00001	0.00002	1.90002
A27	1.99878	0.00000	0.00001	0.00002	0.00003	1.99881
A28	2.16124	0.00000	0.00000	0.00001	0.00001	2.16125
A29	1.94581	0.00000	0.00000	0.00000	0.00001	1.94582
A30	2.17614	0.00000	0.00000	-0.00002	-0.00002	2.17612
A31	2.07394	0.00000	0.00000	0.00000	0.00000	2.07394
A32	2.16442	0.00000	0.00000	0.00000	0.00000	2.16442
A33	2.04483	0.00000	0.00000	0.00000	0.00000	2.04483
A34	1.94076	0.00001	0.00002	0.00001	0.00003	1.94079
A35	1.91636	-0.00001	0.00000	0.00001	0.00001	1.91637
A36	1.89102	0.00000	0.00001	0.00002	0.00003	1.89105
A37	2.08713	-0.00001	-0.00001	-0.00005	-0.00006	2.08707
A38	2.06915	0.00000	-0.00006	0.00000	-0.00006	2.06909
A39	1.99449	0.00000	-0.00001	-0.00003	-0.00004	1.99445
A40	2.00138	0.00000	-0.00004	-0.00003	-0.00007	2.00132
A41	2.03748	0.00001	0.00008	0.00008	0.00016	2.03764
A42	2.01678	0.00001	-0.00003	0.00002	-0.00002	2.01676
A43	2.13745	0.00000	0.00002	-0.00001	0.00001	2.13745
A44	1.96163	0.00000	0.00003	0.00000	0.00004	1.96166
A45	2.02875	0.00000	-0.00001	0.00004	0.00003	2.02877
A46	2.04383	-0.00001	0.00000	-0.00003	-0.00004	2.04379
A47	2.61563	0.00000	-0.00050	0.00036	-0.00014	2.61548
A48	2.43712	0.00000	0.00043	-0.00033	0.00009	2.43722
A49	1.93403	0.00000	0.00001	-0.00001	0.00000	1.93403

A50	1.91727	0.00000	0.00001	0.00001	0.00002	1.91729
A51	1.94211	0.00000	-0.00001	-0.00001	-0.00002	1.94208
A52	1.87908	0.00000	-0.00001	0.00001	0.00000	1.87908
A53	1.89448	0.00000	0.00000	0.00000	-0.00001	1.89447
A54	1.89531	0.00000	0.00000	0.00000	0.00000	1.89531
A55	3.48359	-0.00001	0.00004	-0.00018	-0.00015	3.48345
A56	2.53134	-0.00001	-0.00008	0.00013	0.00005	2.53139
A57	2.96349	0.00001	0.00034	-0.00028	0.00007	2.96356
A58	3.10721	0.00000	0.00015	0.00010	0.00025	3.10746
D1	0.00308	0.00000	0.00000	0.00002	0.00002	0.00310
D2	-3.12680	0.00000	-0.00001	-0.00005	-0.00006	-3.12686
D3	3.13325	0.00000	-0.00002	0.00000	-0.00002	3.13322
D4	0.00336	0.00000	-0.00003	-0.00007	-0.00010	0.00326
D5	-0.00469	0.00000	-0.00001	0.00000	-0.00001	-0.00470
D6	-3.10816	0.00000	-0.00003	0.00003	0.00000	-3.10816
D7	-3.13604	0.00000	0.00001	0.00002	0.00003	-3.13601
D8	0.04367	0.00000	-0.00001	0.00005	0.00004	0.04371
D9	-0.00046	0.00000	0.00001	-0.00003	-0.00002	-0.00048
D10	-3.13322	0.00000	-0.00001	-0.00005	-0.00005	-3.13327
D11	3.13053	0.00000	0.00002	0.00003	0.00005	3.13058
D12	-0.00222	0.00000	0.00000	0.00001	0.00001	-0.00221
D13	-0.00246	0.00000	-0.00002	0.00003	0.00001	-0.00245
D14	-3.12875	0.00000	0.00007	-0.00009	-0.00002	-3.12877
D15	3.13102	0.00000	0.00000	0.00005	0.00004	3.13106
D16	0.00473	0.00000	0.00009	-0.00008	0.00001	0.00474
D17	-0.03700	0.00000	-0.00018	0.00039	0.00021	-0.03679
D18	3.10521	0.00000	-0.00017	0.00032	0.00015	3.10536
D19	3.11448	0.00000	-0.00020	0.00037	0.00017	3.11466
D20	-0.02649	0.00000	-0.00019	0.00030	0.00011	-0.02638
D21	0.00441	0.00000	0.00002	-0.00002	0.00000	0.00441
D22	3.10862	0.00000	0.00004	-0.00005	-0.00001	3.10861
D23	3.12955	0.00000	-0.00008	0.00011	0.00003	3.12959
D24	-0.04942	0.00000	-0.00007	0.00009	0.00002	-0.04939
D25	1.34628	0.00000	-0.00008	-0.00025	-0.00033	1.34594
D26	-2.84200	0.00000	-0.00009	-0.00029	-0.00038	-2.84238
D27	-0.78956	0.00000	-0.00010	-0.00027	-0.00037	-0.78993
D28	-1.75142	0.00000	-0.00010	-0.00022	-0.00032	-1.75174
D29	0.34349	0.00000	-0.00011	-0.00026	-0.00037	0.34312
D30	2.39593	0.00000	-0.00012	-0.00024	-0.00036	2.39557
D31	-1.09946	0.00000	-0.00010	-0.00010	-0.00020	-1.09966
D32	0.94478	-0.00001	-0.00013	-0.00013	-0.00026	0.94452
D33	3.11673	-0.00001	-0.00011	-0.00011	-0.00022	3.11650
D34	3.10867	0.00000	-0.00007	-0.00005	-0.00012	3.10855
D35	-1.13028	0.00000	-0.00010	-0.00008	-0.00018	-1.13045

D36	1.04167	0.00000	-0.00008	-0.00006	-0.00014	1.04153
D37	1.01396	0.00000	-0.00009	-0.00007	-0.00016	1.01380
D38	3.05820	0.00000	-0.00012	-0.00010	-0.00022	3.05798
D39	-1.05304	0.00000	-0.00010	-0.00008	-0.00018	-1.05322
D40	2.94398	0.00000	-0.00005	0.00012	0.00007	2.94404
D41	-1.24659	0.00000	-0.00003	0.00016	0.00013	-1.24646
D42	0.86654	0.00000	-0.00005	0.00013	0.00008	0.86662
D43	2.95915	0.00000	-0.00003	0.00017	0.00014	2.95930
D44	-1.23335	0.00000	-0.00005	0.00011	0.00006	-1.23329
D45	0.85927	0.00000	-0.00004	0.00016	0.00012	0.85939
D46	3.13966	0.00000	0.00000	-0.00003	-0.00002	3.13963
D47	-0.00247	0.00000	-0.00001	0.00001	0.00000	-0.00247
D48	-0.00264	0.00000	-0.00001	0.00006	0.00005	-0.00259
D49	3.13842	0.00000	-0.00003	0.00010	0.00007	3.13849
D50	2.20769	0.00000	-0.00008	-0.00047	-0.00055	2.20714
D51	-1.40647	0.00000	-0.00023	-0.00048	-0.00071	-1.40718
D52	-2.08664	0.00000	-0.00013	-0.00041	-0.00054	-2.08718
D53	0.58239	0.00000	-0.00028	-0.00042	-0.00070	0.58169
D54	-2.71253	0.00000	0.00004	-0.00002	0.00002	-2.71251
D55	-0.01565	-0.00001	-0.00001	-0.00011	-0.00012	-0.01577
D56	-0.02666	0.00001	0.00010	0.00006	0.00016	-0.02650
D57	2.67022	0.00000	0.00005	-0.00003	0.00002	2.67024
D58	0.50823	0.00001	0.00040	-0.00028	0.00013	0.50835
D59	-1.91110	0.00000	0.00033	-0.00033	0.00000	-1.91111
D60	1.78318	-0.00001	0.00056	-0.00037	0.00019	1.78337
D61	-0.63937	0.00000	0.00054	-0.00037	0.00017	-0.63920
D62	2.55494	0.00000	0.00010	0.00017	0.00027	2.55521
D63	-1.65412	0.00000	0.00010	0.00018	0.00029	-1.65383
D64	0.44531	0.00000	0.00011	0.00018	0.00029	0.44560
D65	1.35040	0.00000	0.00008	0.00010	0.00018	1.35058
D66	-2.85866	0.00000	0.00008	0.00012	0.00020	-2.85846
D67	-0.75923	0.00000	0.00008	0.00012	0.00021	-0.75903
D68	-1.03779	0.00000	0.00005	0.00009	0.00013	-1.03766
D69	1.03633	0.00000	0.00005	0.00010	0.00015	1.03648
D70	3.13576	0.00000	0.00005	0.00011	0.00016	3.13591

Item	Value	Threshold	Converged?
Maximum Force	0.000025	0.000450	YES
RMS Force	0.000004	0.000300	YES
Maximum Displacement	0.002339	0.001800	NO
RMS Displacement	0.000501	0.001200	YES

Predicted change in Energy=-1.482386D-08

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.644108	2.099961	-0.197992
2	6	0	-3.536140	1.118369	0.090198
3	7	0	-2.827058	-0.076007	0.111609
4	6	0	-1.534543	0.184553	-0.159225
5	7	0	-1.404162	1.497827	-0.353321
6	6	0	-0.129986	2.183010	-0.634891
7	6	0	0.454512	2.858696	0.610546
8	1	0	-2.783450	3.160903	-0.314022
9	1	0	-4.594684	1.169400	0.268196
10	1	0	0.569870	1.429519	-0.996451
11	1	0	-0.302400	2.916665	-1.423444
12	1	0	-0.226360	3.641106	0.962025
13	1	0	0.532995	2.105666	1.409037
14	35	0	0.137195	-2.666196	-0.214592
15	1	0	-0.758757	-0.604260	-0.213838
16	6	0	-3.301510	-1.400472	0.357226
17	6	0	-4.560953	-1.690205	0.655782
18	1	0	-2.501509	-2.133452	0.268631
19	1	0	-4.832421	-2.723261	0.824564
20	1	0	-5.348230	-0.951282	0.743892
21	7	0	1.721518	3.472160	0.230540
22	1	0	2.064017	4.087011	0.959316
23	1	0	2.419274	2.749288	0.066997
24	6	0	3.332593	-0.425193	-1.138331
25	6	0	3.265917	-0.564086	0.317719
26	8	0	2.735340	0.621233	-0.336838
27	1	0	4.272731	-0.146680	-1.608514
28	1	0	2.629994	-0.987464	-1.745991
29	1	0	2.480541	-1.217942	0.691328
30	6	0	4.462454	-0.354684	1.204277
31	1	0	4.164125	0.076929	2.164359
32	1	0	4.946639	-1.314654	1.407910
33	1	0	5.191669	0.310914	0.735512

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357312	0.000000			
3	N	2.205484	1.389168	0.000000		
4	C	2.213917	2.222750	1.346046	0.000000	

5	N	1.387140	2.210435	2.172037	1.333927	0.000000
6	C	2.553153	3.641579	3.596474	2.488548	1.473867
7	C	3.291028	4.384610	4.430590	3.420516	2.497134
8	H	1.076325	2.214019	3.265065	3.231469	2.160972
9	H	2.210887	1.074618	2.167962	3.243005	3.267044
10	H	3.378859	4.258748	3.877309	2.584461	2.077279
11	H	2.766286	3.997756	4.205517	3.252824	2.090968
12	H	3.092940	4.251932	4.615601	3.862163	2.776869
13	H	3.560417	4.389983	4.211055	3.228752	2.688486
14	Br	5.518349	5.282917	3.949972	3.305229	4.442309
15	H	3.296606	3.282338	2.159360	1.107723	2.203354
16	C	3.604646	2.543799	1.428159	2.429238	3.536232
17	C	4.332272	3.042731	2.430668	3.652138	4.598604
18	H	4.261439	3.417109	2.088951	2.547790	3.844110
19	H	5.394238	4.120408	3.396725	4.505466	5.563987
20	H	4.184436	2.827444	2.742662	4.080436	4.770501
21	N	4.596223	5.762204	5.770025	4.643513	3.742828
22	H	5.239674	6.397653	6.478576	5.424938	4.522738
23	H	5.111721	6.174738	5.958883	4.718232	4.044934
24	C	6.556035	7.146422	6.294885	5.001944	5.172146
25	C	6.503192	7.010734	6.115967	4.881839	5.148924
26	O	5.580715	6.305629	5.623836	4.295828	4.231332
27	H	7.408079	8.091009	7.305534	5.994546	6.042105
28	H	6.304337	6.769589	5.836168	4.608125	4.938687
29	H	6.169392	6.482295	5.459918	4.337203	4.853618
30	C	7.648194	8.209053	7.376217	6.173644	6.346266
31	H	7.485012	8.042438	7.287922	6.155114	6.274032
32	H	8.476908	8.922639	7.977782	6.834416	7.165519
33	H	8.091448	8.788803	8.052263	6.786637	6.789647

		6	7	8	9	10
6	C	0.000000				
7	C	1.532744	0.000000			
8	H	2.846068	3.380910	0.000000		
9	H	4.666531	5.335290	2.754203	0.000000	
10	H	1.090079	2.153669	3.835121	5.323497	0.000000
11	H	1.090776	2.171035	2.728751	4.933385	1.776170
12	H	2.164596	1.095121	2.897861	5.066852	3.059530
13	H	2.150156	1.100364	3.883460	5.335843	2.498981
14	Br	4.874714	5.595174	6.518829	6.110283	4.192063
15	H	2.888167	3.760810	4.276197	4.253535	2.552252
16	C	4.887147	5.684398	4.639515	2.878275	4.982858
17	C	6.025040	6.771221	5.256737	2.885949	6.227993
18	H	5.007227	5.811756	5.333776	3.910270	4.871198
19	H	6.950857	7.691275	6.333881	3.939400	7.053115

20	H	6.241387	6.943021	4.960579	2.300306	6.612180
21	N	2.416391	1.458097	4.548424	6.722986	2.646541
22	H	3.313664	2.054484	5.096764	7.302631	3.622121
23	H	2.704079	2.041496	5.232871	7.192506	2.508587
24	C	4.364130	4.703812	7.137615	8.207483	3.330574
25	C	4.470588	4.439052	7.132284	8.049626	3.601413
26	O	3.276900	3.332559	6.075153	7.375352	2.403680
27	H	5.075363	5.341845	7.899715	9.158884	4.070652
28	H	4.347866	5.007888	6.968850	7.804166	3.263087
29	H	4.487782	4.553053	6.920593	7.479121	3.675366
30	C	5.559940	5.171259	8.195590	9.232055	4.814436
31	H	5.541729	4.890173	7.995127	9.028049	4.973820
32	H	6.494522	6.183190	9.096699	9.925035	5.698030
33	H	5.805408	5.380284	8.533843	9.835044	5.060830

		11	12	13	14	15
11	H	0.000000				
12	H	2.494206	0.000000			
13	H	3.062443	1.770315	0.000000		
14	Br	5.729127	6.426404	5.056036	0.000000	
15	H	3.750776	4.437255	3.412630	2.248180	0.000000
16	C	5.550056	5.936315	5.301202	3.708601	2.725006
17	C	6.609214	6.877889	6.397214	4.876751	4.048729
18	H	5.762194	6.245208	5.336560	2.734974	2.368204
19	H	7.575183	7.857472	7.242089	5.077420	4.707780
20	H	6.717050	6.882671	6.661544	5.826621	4.701163
21	N	2.672169	2.087545	2.160728	6.355127	4.792330
22	H	3.556289	2.333381	2.544013	7.120148	5.599318
23	H	3.107562	2.931859	2.402783	5.883421	4.628718
24	C	4.945955	5.797623	4.553250	4.010730	4.198321
25	C	5.280167	5.504069	3.973338	3.806721	4.059824
26	O	3.959493	4.424743	3.178356	4.191956	3.704818
27	H	5.509097	6.418475	5.307005	5.039210	5.241219
28	H	4.893383	6.075836	4.890713	3.373036	3.738713
29	H	5.414055	5.568747	3.918471	2.899897	3.418915
30	C	6.349053	6.165225	4.640678	5.105306	5.416122
31	H	6.394238	5.781464	4.227456	5.422205	5.509501
32	H	7.312526	7.177624	5.583802	5.252612	5.973798
33	H	6.452582	6.363688	5.037659	5.942523	6.094782

		16	17	18	19	20
16	C	0.000000				
17	C	1.326378	0.000000			
18	H	1.088627	2.141883	0.000000		
19	H	2.076504	1.081382	2.467810	0.000000	
20	H	2.130809	1.083318	3.118849	1.847289	0.000000

21	N	6.999243	8.142499	7.018425	9.038265	8.355340
22	H	7.698302	8.795373	7.746950	9.693236	8.965055
23	H	7.073338	8.293331	6.935122	9.116457	8.630558
24	C	6.870166	8.193117	6.239747	8.706408	8.898102
25	C	6.620589	7.914690	5.977334	8.396548	8.633370
26	O	6.404106	7.717767	5.948065	8.354969	8.305714
27	H	7.924976	9.248971	7.304880	9.770488	9.937006
28	H	6.306888	7.613940	5.630659	8.081361	8.357805
29	H	5.794571	7.057402	5.083075	7.467473	7.833488
30	C	7.879740	9.138180	7.248188	9.599430	9.839584
31	H	7.822029	9.029149	7.273942	9.517035	9.672633
32	H	8.315242	9.544686	7.579135	9.897196	10.322659
33	H	8.672140	9.956127	8.085659	10.473611	10.615210

		21	22	23	24	25
21	N	0.000000				
22	H	1.013144	0.000000			
23	H	1.017916	1.646798	0.000000		
24	C	4.433817	5.135114	3.516291	0.000000	
25	C	4.322505	4.846536	3.429011	1.464179	0.000000
26	O	3.078561	3.760626	2.188972	1.447104	1.454283
27	H	4.794456	5.421836	3.824823	1.087429	2.213205
28	H	4.961880	5.778349	4.158684	1.085838	2.200579
29	H	4.773416	5.328023	4.016523	2.168432	1.088084
30	C	4.806831	5.053825	3.886210	2.601801	1.503840
31	H	4.607990	4.684372	3.819023	3.442577	2.151222
32	H	5.890772	6.139114	4.970035	3.143188	2.139321
33	H	4.721273	4.908279	3.752166	2.740311	2.156083

		26	27	28	29	30
26	O	0.000000				
27	H	2.137854	0.000000			
28	H	2.141195	1.850514	0.000000		
29	H	2.122408	3.106255	2.452750	0.000000	
30	C	2.512046	2.826845	3.530213	2.221781	0.000000
31	H	2.931498	3.781053	4.333281	2.584756	1.094096
32	H	3.417843	3.304108	3.926956	2.569919	1.094278
33	H	2.698107	2.558964	3.795500	3.112807	1.092938

		31	32	33
31	H	0.000000		
32	H	1.766648	0.000000	
33	H	1.775444	1.776128	0.000000

Stoichiometry C10H18BrN3O

Framework group C1[X(C10H18BrN3O)]

Deg. of freedom 93

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.351417	2.471198	-0.264707
2	6	0	-3.337957	1.589387	0.037692
3	7	0	-2.751298	0.331191	0.088321
4	6	0	-1.438061	0.456276	-0.179266
5	7	0	-1.176822	1.745710	-0.399438
6	6	0	0.160451	2.294818	-0.686605
7	6	0	0.803612	2.935219	0.548521
8	1	0	-2.384011	3.538049	-0.403428
9	1	0	-4.386972	1.749078	0.207608
10	1	0	0.783519	1.468063	-1.027975
11	1	0	0.065441	3.025169	-1.491186
12	1	0	0.202355	3.788645	0.879346
13	1	0	0.803186	2.195135	1.362817
14	35	0	-0.057937	-2.546987	-0.165007
15	1	0	-0.744345	-0.406684	-0.212535
16	6	0	-3.356245	-0.934104	0.357959
17	6	0	-4.639601	-1.090912	0.654080
18	1	0	-2.632726	-1.744644	0.289729
19	1	0	-5.013240	-2.088094	0.842255
20	1	0	-5.349866	-0.275734	0.721787
21	7	0	2.127062	3.411614	0.164369
22	1	0	2.525716	4.004635	0.882604
23	1	0	2.750190	2.619707	0.020325
24	6	0	3.348672	-0.654531	-1.113467
25	6	0	3.261917	-0.755358	0.344657
26	8	0	2.854842	0.462734	-0.337606
27	1	0	4.313971	-0.480784	-1.583053
28	1	0	2.596391	-1.156913	-1.714075
29	1	0	2.413714	-1.319921	0.726425
30	6	0	4.469320	-0.647208	1.234610
31	1	0	4.211056	-0.167930	2.183629
32	1	0	4.854691	-1.646022	1.461117
33	1	0	5.263240	-0.067392	0.757095

Rotational constants (GHZ): 0.4225985 0.2920003 0.1826974

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.
482 basis functions, 760 primitive gaussians, 499 cartesian basis functions
71 alpha electrons 71 beta electrons
nuclear repulsion energy 1312.9364638488 Hartrees.
NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 482 RedAO= T EigKep= 3.63D-06 NBF= 482
NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 0.000024 -0.000017 -0.000042 Ang= 0.01 deg.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3205.64837894 A.U. after 7 cycles
NFock= 7 Conv=0.75D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000000877	0.000002041	0.000000878
2	6	0.000000094	-0.000000899	0.000000218
3	7	0.000001995	0.000003952	0.000000341
4	6	-0.000003559	-0.000004814	-0.000014126
5	7	0.000000133	-0.000005354	0.000002356
6	6	0.000002447	0.000002874	-0.000001837
7	6	0.000005524	0.000004681	-0.000000887
8	1	0.000001109	0.000000242	-0.000001664
9	1	0.000000262	0.000001663	-0.000000606
10	1	0.000000789	-0.000002735	0.000001517
11	1	0.000000890	-0.000000061	-0.000001156
12	1	-0.000000138	0.000000653	0.000000377
13	1	-0.000000135	0.000000134	-0.000000084
14	35	-0.000000537	-0.000000788	0.000000206
15	1	0.000002127	0.000005981	0.000004162

16	6	0.000000309	0.000000840	0.000001596
17	6	-0.000001628	-0.000000057	-0.000003731
18	1	-0.000001745	0.000001877	0.000002176
19	1	-0.000001159	0.000001585	0.000000596
20	1	-0.000000226	0.000001199	-0.000002269
21	7	-0.000000504	-0.000005826	-0.000001501
22	1	-0.000002301	0.000001260	-0.000001118
23	1	0.000002404	-0.000004343	0.000000038
24	6	0.000002788	-0.000009784	-0.000006133
25	6	-0.000001097	0.000012105	-0.000006461
26	8	-0.000010613	-0.000001168	0.000007657
27	1	0.000002572	-0.000000059	0.000002744
28	1	0.000001656	-0.000000177	-0.000000697
29	1	0.000000610	0.000003705	0.000008675
30	6	0.000001836	-0.000007091	0.000006278
31	1	-0.000002258	-0.000000431	-0.000000277
32	1	-0.000000340	-0.000000493	0.000001450
33	1	-0.000000425	-0.000000710	0.000001280

Cartesian Forces: Max 0.000014126 RMS 0.000003582

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000007395 RMS 0.000002248
Search for a local minimum.
Step number 48 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 31 32 33 34 35
36 37 38 39 40
41 42 43 44 45
46 47 48
DE= -1.56D-08 DEPred=-1.48D-08 R= 1.05D+00
Trust test= 1.05D+00 RLast= 1.95D-03 DXMaxT set to 5.19D-01
ITU= 0 -1 0 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
ITU= 1 1 0 0 -1 1 -1 1 1 1 1 1 1 1 1 1 0 -1 -1 1
ITU= 1 1 -1 1 0 0 -1 0
Eigenvalues --- 0.00068 0.00111 0.00145 0.00232 0.00275
Eigenvalues --- 0.00533 0.00616 0.00765 0.01237 0.01387
Eigenvalues --- 0.01787 0.01937 0.02171 0.02362 0.02378
Eigenvalues --- 0.02537 0.02683 0.02722 0.03052 0.03097

Eigenvalues --- 0.03280 0.03562 0.03637 0.03981 0.04083
Eigenvalues --- 0.04261 0.04489 0.04740 0.05501 0.05657
Eigenvalues --- 0.05705 0.05762 0.05905 0.07946 0.08691
Eigenvalues --- 0.08996 0.09557 0.10136 0.10628 0.11361
Eigenvalues --- 0.12546 0.13116 0.13226 0.15745 0.15936
Eigenvalues --- 0.15997 0.16002 0.16012 0.16019 0.16129
Eigenvalues --- 0.16253 0.18891 0.21304 0.21712 0.22135
Eigenvalues --- 0.23181 0.23446 0.26080 0.26175 0.27297
Eigenvalues --- 0.28426 0.29595 0.30790 0.31975 0.32724
Eigenvalues --- 0.33660 0.34283 0.34336 0.34407 0.34549
Eigenvalues --- 0.34726 0.34798 0.35129 0.35186 0.35368
Eigenvalues --- 0.35551 0.35661 0.35891 0.35976 0.36418
Eigenvalues --- 0.36627 0.39264 0.41374 0.41976 0.42741
Eigenvalues --- 0.44762 0.45483 0.46481 0.49550 0.54989
Eigenvalues --- 0.58388 0.60641 1.06066
En-DIIS/RFO-DIIS IScMMF= 0 using points: 48 47 46 45 44
RFO step: Lambda=-2.57817862D-09.
DidBck=F Rises=F RFO-DIIS coefs: 1.56443 -0.45108 -0.13509 0.01103 0.01072
Iteration 1 RMS(Cart)= 0.00042766 RMS(Int)= 0.00000006
Iteration 2 RMS(Cart)= 0.00000012 RMS(Int)= 0.00000003

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56495	0.00000	0.00000	0.00000	0.00000	2.56495
R2	2.62132	0.00000	0.00000	0.00000	0.00000	2.62132
R3	2.03396	0.00000	0.00000	0.00000	0.00000	2.03396
R4	2.62515	0.00000	0.00000	0.00000	0.00000	2.62515
R5	2.03073	0.00000	0.00000	0.00000	0.00000	2.03073
R6	2.54366	0.00000	0.00001	0.00000	0.00001	2.54367
R7	2.69883	0.00000	-0.00001	0.00000	-0.00001	2.69882
R8	2.52076	0.00000	-0.00001	0.00000	-0.00001	2.52074
R9	2.09329	0.00000	0.00002	0.00000	0.00001	2.09331
R10	2.78521	0.00000	0.00000	0.00001	0.00000	2.78521
R11	2.89647	0.00000	0.00001	0.00000	0.00001	2.89648
R12	2.05995	0.00000	-0.00001	0.00000	0.00000	2.05995
R13	2.06127	0.00000	0.00000	0.00000	0.00000	2.06127
R14	2.06948	0.00000	0.00001	0.00000	0.00001	2.06949
R15	2.07939	0.00000	0.00001	0.00000	0.00001	2.07940
R16	2.75540	-0.00001	-0.00006	-0.00001	-0.00007	2.75533
R17	4.24844	0.00000	-0.00012	0.00007	-0.00005	4.24840
R18	2.50649	0.00000	0.00000	0.00000	0.00000	2.50649
R19	2.05721	0.00000	0.00000	0.00000	0.00000	2.05720
R20	2.04352	0.00000	0.00000	0.00000	0.00000	2.04352
R21	2.04717	0.00000	0.00000	0.00000	0.00000	2.04717

R22	1.91457	0.00000	-0.00001	0.00000	-0.00001	1.91456
R23	1.92358	0.00000	-0.00001	0.00000	-0.00001	1.92357
R24	4.13656	0.00000	-0.00024	0.00007	-0.00017	4.13639
R25	2.76690	0.00000	0.00002	-0.00002	-0.00001	2.76689
R26	2.73463	0.00001	0.00005	0.00003	0.00008	2.73471
R27	2.05494	0.00000	-0.00001	0.00000	-0.00001	2.05493
R28	2.05194	0.00000	-0.00001	0.00000	-0.00001	2.05193
R29	2.74820	-0.00001	-0.00009	0.00000	-0.00009	2.74811
R30	2.05618	0.00000	0.00000	0.00000	0.00000	2.05618
R31	2.84185	0.00000	0.00002	0.00001	0.00002	2.84187
R32	2.06754	0.00000	0.00000	0.00000	0.00000	2.06754
R33	2.06789	0.00000	0.00000	0.00000	0.00000	2.06788
R34	2.06535	0.00000	0.00000	0.00000	0.00000	2.06536
A1	1.87268	0.00000	0.00000	0.00000	0.00000	1.87268
A2	2.27925	0.00000	-0.00001	0.00000	-0.00001	2.27924
A3	2.13120	0.00000	0.00001	0.00000	0.00001	2.13121
A4	1.86460	0.00000	0.00000	0.00000	0.00000	1.86460
A5	2.27602	0.00000	0.00000	0.00000	0.00000	2.27602
A6	2.14251	0.00000	0.00000	0.00000	0.00000	2.14251
A7	1.89716	0.00000	0.00000	0.00000	0.00000	1.89716
A8	2.25290	0.00000	0.00000	-0.00001	-0.00001	2.25290
A9	2.13308	0.00000	0.00000	0.00001	0.00001	2.13309
A10	1.88989	0.00000	0.00000	0.00000	0.00000	1.88989
A11	2.14667	0.00000	-0.00002	0.00001	-0.00001	2.14666
A12	2.24651	0.00000	0.00002	-0.00001	0.00001	2.24652
A13	1.90043	0.00000	0.00001	0.00000	0.00001	1.90044
A14	2.20479	0.00000	0.00002	-0.00002	0.00000	2.20479
A15	2.17729	0.00000	-0.00002	0.00002	0.00000	2.17728
A16	1.95992	0.00000	-0.00003	0.00000	-0.00003	1.95990
A17	1.87241	0.00000	-0.00003	0.00001	-0.00002	1.87238
A18	1.89035	0.00000	0.00003	-0.00001	0.00002	1.89037
A19	1.90646	0.00000	0.00001	0.00000	0.00001	1.90647
A20	1.92964	0.00000	0.00002	-0.00001	0.00001	1.92965
A21	1.90352	0.00000	0.00000	0.00001	0.00001	1.90353
A22	1.91628	0.00000	-0.00003	0.00000	-0.00003	1.91625
A23	1.89142	0.00000	-0.00003	0.00000	-0.00003	1.89139
A24	1.88081	0.00000	0.00003	0.00000	0.00003	1.88084
A25	1.87588	0.00000	-0.00001	-0.00001	-0.00002	1.87586
A26	1.90002	0.00000	0.00001	0.00000	0.00001	1.90003
A27	1.99881	0.00000	0.00003	0.00001	0.00004	1.99885
A28	2.16125	0.00000	0.00001	0.00000	0.00001	2.16126
A29	1.94582	0.00000	0.00001	0.00000	0.00001	1.94582
A30	2.17612	0.00000	-0.00001	0.00000	-0.00002	2.17610
A31	2.07394	0.00000	0.00000	0.00000	0.00000	2.07393

A32	2.16442	0.00000	0.00000	0.00000	0.00000	2.16442
A33	2.04483	0.00000	0.00000	0.00000	0.00000	2.04483
A34	1.94079	0.00000	0.00003	0.00001	0.00004	1.94083
A35	1.91637	0.00000	0.00001	0.00002	0.00004	1.91640
A36	1.89105	0.00000	0.00003	0.00001	0.00004	1.89109
A37	2.08707	0.00000	-0.00004	-0.00001	-0.00005	2.08702
A38	2.06909	0.00001	-0.00003	0.00002	-0.00001	2.06908
A39	1.99445	0.00000	-0.00003	-0.00002	-0.00005	1.99440
A40	2.00132	0.00000	-0.00005	0.00000	-0.00005	2.00127
A41	2.03764	0.00000	0.00010	0.00001	0.00011	2.03775
A42	2.01676	0.00001	0.00002	0.00002	0.00004	2.01680
A43	2.13745	0.00000	0.00000	0.00000	0.00000	2.13746
A44	1.96166	0.00000	0.00004	0.00000	0.00003	1.96170
A45	2.02877	0.00000	0.00002	0.00002	0.00003	2.02880
A46	2.04379	0.00000	-0.00005	-0.00003	-0.00008	2.04371
A47	2.61548	0.00000	-0.00017	0.00008	-0.00009	2.61540
A48	2.43722	0.00000	0.00018	-0.00034	-0.00016	2.43706
A49	1.93403	0.00000	0.00000	-0.00001	-0.00001	1.93402
A50	1.91729	0.00000	0.00001	0.00000	0.00001	1.91730
A51	1.94208	0.00000	-0.00001	0.00000	-0.00002	1.94207
A52	1.87908	0.00000	0.00000	0.00000	0.00000	1.87909
A53	1.89447	0.00000	0.00000	0.00000	0.00000	1.89447
A54	1.89531	0.00000	0.00001	0.00000	0.00001	1.89532
A55	3.48345	0.00000	-0.00010	-0.00012	-0.00022	3.48323
A56	2.53139	-0.00001	0.00005	-0.00022	-0.00016	2.53122
A57	2.96356	0.00000	0.00002	-0.00061	-0.00058	2.96298
A58	3.10746	0.00000	0.00011	-0.00002	0.00009	3.10755
D1	0.00310	0.00000	0.00001	-0.00002	0.00000	0.00310
D2	-3.12686	0.00000	-0.00005	-0.00008	-0.00012	-3.12699
D3	3.13322	0.00000	-0.00002	0.00000	-0.00001	3.13321
D4	0.00326	0.00000	-0.00007	-0.00006	-0.00013	0.00313
D5	-0.00470	0.00000	-0.00001	0.00002	0.00000	-0.00470
D6	-3.10816	0.00000	-0.00001	0.00002	0.00001	-3.10815
D7	-3.13601	0.00000	0.00002	0.00000	0.00001	-3.13600
D8	0.04371	0.00000	0.00001	0.00001	0.00002	0.04373
D9	-0.00048	0.00000	-0.00001	0.00001	0.00000	-0.00048
D10	-3.13327	0.00000	-0.00005	-0.00003	-0.00008	-3.13335
D11	3.13058	0.00000	0.00004	0.00007	0.00011	3.13069
D12	-0.00221	0.00000	0.00000	0.00003	0.00003	-0.00218
D13	-0.00245	0.00000	0.00000	0.00000	0.00000	-0.00245
D14	-3.12877	0.00000	-0.00003	-0.00016	-0.00019	-3.12897
D15	3.13106	0.00000	0.00004	0.00003	0.00007	3.13114
D16	0.00474	0.00000	0.00001	-0.00013	-0.00012	0.00462
D17	-0.03679	0.00000	0.00015	0.00066	0.00081	-0.03598

D18	3.10536	0.00000	0.00011	0.00063	0.00074	3.10610
D19	3.11466	0.00000	0.00011	0.00062	0.00073	3.11538
D20	-0.02638	0.00000	0.00007	0.00059	0.00066	-0.02572
D21	0.00441	0.00000	0.00000	-0.00001	0.00000	0.00440
D22	3.10861	0.00000	0.00001	-0.00002	-0.00001	3.10860
D23	3.12959	0.00000	0.00004	0.00017	0.00020	3.12979
D24	-0.04939	0.00000	0.00004	0.00016	0.00020	-0.04920
D25	1.34594	0.00000	-0.00024	-0.00024	-0.00048	1.34547
D26	-2.84238	0.00000	-0.00027	-0.00023	-0.00050	-2.84287
D27	-0.78993	0.00000	-0.00027	-0.00022	-0.00048	-0.79042
D28	-1.75174	0.00000	-0.00024	-0.00023	-0.00047	-1.75221
D29	0.34312	0.00000	-0.00027	-0.00022	-0.00049	0.34264
D30	2.39557	0.00000	-0.00027	-0.00021	-0.00048	2.39509
D31	-1.09966	0.00000	-0.00012	0.00008	-0.00004	-1.09970
D32	0.94452	0.00000	-0.00017	0.00007	-0.00010	0.94442
D33	3.11650	0.00000	-0.00013	0.00008	-0.00005	3.11645
D34	3.10855	0.00000	-0.00007	0.00007	0.00000	3.10855
D35	-1.13045	0.00000	-0.00012	0.00006	-0.00006	-1.13051
D36	1.04153	0.00000	-0.00008	0.00007	-0.00001	1.04152
D37	1.01380	0.00000	-0.00009	0.00006	-0.00003	1.01377
D38	3.05798	0.00000	-0.00014	0.00005	-0.00009	3.05789
D39	-1.05322	0.00000	-0.00011	0.00006	-0.00005	-1.05326
D40	2.94404	0.00000	0.00002	-0.00007	-0.00005	2.94399
D41	-1.24646	0.00000	0.00008	-0.00003	0.00004	-1.24642
D42	0.86662	0.00000	0.00003	-0.00007	-0.00004	0.86658
D43	2.95930	0.00000	0.00009	-0.00003	0.00006	2.95936
D44	-1.23329	0.00000	0.00002	-0.00006	-0.00004	-1.23333
D45	0.85939	0.00000	0.00008	-0.00002	0.00005	0.85944
D46	3.13963	0.00000	-0.00001	0.00006	0.00005	3.13969
D47	-0.00247	0.00000	0.00000	0.00006	0.00006	-0.00240
D48	-0.00259	0.00000	0.00003	0.00010	0.00013	-0.00247
D49	3.13849	0.00000	0.00004	0.00010	0.00014	3.13863
D50	2.20714	0.00000	-0.00026	0.00070	0.00044	2.20758
D51	-1.40718	0.00000	-0.00020	-0.00004	-0.00024	-1.40742
D52	-2.08718	0.00000	-0.00022	0.00066	0.00045	-2.08673
D53	0.58169	0.00000	-0.00015	-0.00008	-0.00024	0.58145
D54	-2.71251	0.00000	0.00000	-0.00003	-0.00003	-2.71254
D55	-0.01577	0.00000	-0.00008	-0.00005	-0.00013	-0.01591
D56	-0.02650	0.00000	0.00011	0.00001	0.00012	-0.02638
D57	2.67024	0.00000	0.00003	-0.00002	0.00001	2.67025
D58	0.50835	0.00000	0.00030	-0.00072	-0.00042	0.50793
D59	-1.91111	0.00000	0.00022	-0.00070	-0.00048	-1.91159
D60	1.78337	-0.00001	0.00010	0.00017	0.00026	1.78363
D61	-0.63920	0.00000	0.00012	0.00019	0.00031	-0.63889

D62	2.55521	0.00000	0.00015	0.00011	0.00027	2.55548
D63	-1.65383	0.00000	0.00016	0.00011	0.00027	-1.65356
D64	0.44560	0.00000	0.00017	0.00011	0.00028	0.44588
D65	1.35058	0.00000	0.00010	0.00008	0.00018	1.35077
D66	-2.85846	0.00000	0.00011	0.00008	0.00019	-2.85827
D67	-0.75903	0.00000	0.00012	0.00008	0.00020	-0.75883
D68	-1.03766	0.00000	0.00008	0.00010	0.00018	-1.03748
D69	1.03648	0.00000	0.00009	0.00010	0.00019	1.03667
D70	3.13591	0.00000	0.00010	0.00010	0.00020	3.13611

Item	Value	Threshold	Converged?
Maximum Force	0.000007	0.000450	YES
RMS Force	0.000002	0.000300	YES
Maximum Displacement	0.002236	0.001800	NO
RMS Displacement	0.000428	0.001200	YES

Predicted change in Energy=-1.178840D-08

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.643910	2.100004	-0.197286
2	6	0	-3.535938	1.118408	0.090901
3	7	0	-2.826969	-0.076045	0.111687
4	6	0	-1.534515	0.184477	-0.159513
5	7	0	-1.404078	1.497794	-0.353232
6	6	0	-0.129928	2.182947	-0.635012
7	6	0	0.454689	2.858727	0.610325
8	1	0	-2.783195	3.160993	-0.312939
9	1	0	-4.594399	1.169499	0.269380
10	1	0	0.569865	1.429400	-0.996569
11	1	0	-0.302413	2.916535	-1.423614
12	1	0	-0.226157	3.641186	0.961759
13	1	0	0.533139	2.105754	1.408883
14	35	0	0.137173	-2.666287	-0.214848
15	1	0	-0.758793	-0.604384	-0.214471
16	6	0	-3.301460	-1.400522	0.357130
17	6	0	-4.560995	-1.690310	0.655255
18	1	0	-2.501426	-2.133487	0.268739
19	1	0	-4.832466	-2.723374	0.823981
20	1	0	-5.348346	-0.951428	0.743050
21	7	0	1.721668	3.472098	0.230225
22	1	0	2.064226	4.087037	0.958892

23	1	0	2.419402	2.749217	0.066660
24	6	0	3.332409	-0.425434	-1.138213
25	6	0	3.265708	-0.563974	0.317867
26	8	0	2.735069	0.621142	-0.336901
27	1	0	4.272545	-0.146916	-1.608383
28	1	0	2.629810	-0.987845	-1.745734
29	1	0	2.480400	-1.217812	0.691652
30	6	0	4.462238	-0.354363	1.204405
31	1	0	4.163849	0.077232	2.164476
32	1	0	4.946584	-1.314246	1.408061
33	1	0	5.191329	0.311344	0.735601

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357312	0.000000			
3	N	2.205484	1.389168	0.000000		
4	C	2.213917	2.222753	1.346052	0.000000	
5	N	1.387141	2.210433	2.172035	1.333921	0.000000
6	C	2.553153	3.641579	3.596475	2.488543	1.473870
7	C	3.290777	4.384474	4.430666	3.420701	2.497117
8	H	1.076325	2.214015	3.265063	3.231469	2.160976
9	H	2.210887	1.074618	2.167962	3.243009	3.267043
10	H	3.378892	4.258747	3.877251	2.584359	2.077260
11	H	2.766445	3.997838	4.205481	3.252718	2.090983
12	H	3.092598	4.251760	4.615697	3.862369	2.776838
13	H	3.559980	4.389683	4.211091	3.228989	2.688397
14	Br	5.518357	5.282911	3.949952	3.305217	4.442317
15	H	3.296616	3.282347	2.159368	1.107730	2.203362
16	C	3.604640	2.543790	1.428154	2.429246	3.536228
17	C	4.332264	3.042717	2.430671	3.652157	4.598606
18	H	4.261446	3.417113	2.088950	2.547797	3.844115
19	H	5.394232	4.120398	3.396724	4.505478	5.563986
20	H	4.184428	2.827426	2.742674	4.080466	4.770511
21	N	4.596051	5.762091	5.770049	4.643606	3.742805
22	H	5.239427	6.397500	6.478641	5.425103	4.522718
23	H	5.111582	6.174641	5.958904	4.718316	4.044918
24	C	6.555881	7.146213	6.294621	5.001679	5.171974
25	C	6.502749	7.010301	6.115660	4.881620	5.148608
26	O	5.580317	6.305221	5.623483	4.295520	4.230995
27	H	7.407915	8.090799	7.305255	5.994247	6.041898
28	H	6.304334	6.769489	5.835908	4.607823	4.938594
29	H	6.169009	6.481910	5.459685	4.337101	4.853398
30	C	7.647614	8.208518	7.375909	6.173465	6.345895

31	H	7.484324	8.041796	7.287590	6.154980	6.273648
32	H	8.476429	8.922214	7.977584	6.834333	7.165238
33	H	8.090769	8.788184	8.051859	6.786332	6.789154

		6	7	8	9	10
6	C	0.000000				
7	C	1.532750	0.000000			
8	H	2.846073	3.380484	0.000000		
9	H	4.666530	5.335075	2.754197	0.000000	
10	H	1.090076	2.153682	3.835202	5.323514	0.000000
11	H	1.090777	2.171049	2.729037	4.933509	1.776177
12	H	2.164579	1.095125	2.897221	5.066574	3.059526
13	H	2.150146	1.100372	3.882818	5.335419	2.499000
14	Br	4.874726	5.595311	6.518848	6.110280	4.192012
15	H	2.888173	3.761112	4.276210	4.253545	2.552115
16	C	4.887148	5.684537	4.639506	2.878264	4.982782
17	C	6.025052	6.771472	5.256721	2.885918	6.227908
18	H	5.007232	5.811841	5.333786	3.910276	4.871139
19	H	6.950864	7.691522	6.333867	3.939381	7.053022
20	H	6.241414	6.943350	4.960556	2.300246	6.612098
21	N	2.416393	1.458059	4.548143	6.722812	2.646561
22	H	3.313670	2.054472	5.096332	7.302379	3.622151
23	H	2.704087	2.041485	5.232654	7.192357	2.508616
24	C	4.364017	4.703655	7.137518	8.207279	3.330484
25	C	4.470335	4.438721	7.131797	8.049135	3.601229
26	O	3.276631	3.332290	6.074755	7.374915	2.403445
27	H	5.075183	5.341590	7.899615	9.158692	4.070495
28	H	4.347847	5.007822	6.968959	7.804102	3.263081
29	H	4.487652	4.552833	6.920158	7.478660	3.675319
30	C	5.559622	5.170815	8.194899	9.231420	4.814215
31	H	5.541452	4.889782	7.994285	9.027256	4.973659
32	H	6.494266	6.182816	9.096103	9.924513	5.697851
33	H	5.804933	5.379648	8.533051	9.834341	5.060473

		11	12	13	14	15
11	H	0.000000				
12	H	2.494182	0.000000			
13	H	3.062443	1.770312	0.000000		
14	Br	5.729071	6.426557	5.056251	0.000000	
15	H	3.750625	4.437577	3.413095	2.248155	0.000000
16	C	5.549984	5.936488	5.301350	3.708574	2.725017
17	C	6.609103	6.878199	6.397519	4.876720	4.048752
18	H	5.762156	6.245317	5.336636	2.734947	2.368209
19	H	7.575067	7.857779	7.242396	5.077375	4.707792
20	H	6.716920	6.883078	6.661949	5.826597	4.701200
21	N	2.672216	2.087524	2.160725	6.355194	4.792510

22	H	3.556317	2.333376	2.544052	7.120294	5.599612
23	H	3.107601	2.931858	2.402830	5.883494	4.628887
24	C	4.945922	5.797472	4.553078	4.010431	4.198007
25	C	5.279980	5.503734	3.972996	3.806736	4.059757
26	O	3.959301	4.424482	3.178101	4.191796	3.704588
27	H	5.509003	6.418230	5.306748	5.038895	5.240862
28	H	4.893452	6.075771	4.890602	3.372538	3.738240
29	H	5.413985	5.568508	3.918206	2.900092	3.419024
30	C	6.348792	6.164766	4.640237	5.105435	5.416169
31	H	6.394022	5.781042	4.227040	5.422379	5.509664
32	H	7.312309	7.177238	5.583448	5.252836	5.973931
33	H	6.452164	6.363029	5.037057	5.942569	6.094682

		16	17	18	19	20
16	C	0.000000				
17	C	1.326380	0.000000			
18	H	1.088626	2.141875	0.000000		
19	H	2.076503	1.081382	2.467795	0.000000	
20	H	2.130812	1.083317	3.118845	1.847289	0.000000
21	N	6.999311	8.142663	7.018447	9.038423	8.355577
22	H	7.698442	8.795651	7.747026	9.693516	8.965430
23	H	7.073399	8.293478	6.935141	9.116599	8.630769
24	C	6.869867	8.192818	6.239438	8.706085	8.897827
25	C	6.620352	7.914527	5.977091	8.396403	8.633240
26	O	6.403787	7.717495	5.947744	8.354700	8.305472
27	H	7.924666	9.248651	7.304569	9.770146	9.936701
28	H	6.306529	7.613532	5.630290	8.080907	8.357412
29	H	5.794411	7.057324	5.082903	7.467412	7.833446
30	C	7.879552	9.138110	7.247991	9.599399	9.839558
31	H	7.821835	9.029111	7.273719	9.517037	9.672665
32	H	8.315175	9.544747	7.579054	9.897303	10.322765
33	H	8.671862	9.955947	8.085396	10.473480	10.615055

		21	22	23	24	25
21	N	0.000000				
22	H	1.013140	0.000000			
23	H	1.017911	1.646813	0.000000		
24	C	4.433719	5.135030	3.516207	0.000000	
25	C	4.322224	4.846275	3.428786	1.464175	0.000000
26	O	3.078403	3.760524	2.188883	1.447148	1.454235
27	H	4.794238	5.421618	3.824591	1.087422	2.213164
28	H	4.961878	5.778349	4.158687	1.085834	2.200564
29	H	4.773243	5.327856	4.016423	2.168453	1.088085
30	C	4.806408	5.053392	3.885853	2.601811	1.503852
31	H	4.607677	4.684056	3.818826	3.442632	2.151225
32	H	5.890371	6.138697	4.969682	3.143097	2.139340

33	H	4.720627	4.907595	3.751571	2.740365	2.156084
		26	27	28	29	30
26	O	0.000000				
27	H	2.137853	0.000000			
28	H	2.141198	1.850569	0.000000		
29	H	2.122388	3.106246	2.452765	0.000000	
30	C	2.512041	2.826800	3.530215	2.221743	0.000000
31	H	2.931576	3.781075	4.333290	2.584637	1.094096
32	H	3.417810	3.303926	3.926882	2.569943	1.094277
33	H	2.698045	2.558990	3.795562	3.112777	1.092939
		31	32	33		
31	H	0.000000				
32	H	1.766649	0.000000			
33	H	1.775446	1.776132	0.000000		

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.350956	2.471492	-0.264145
2	6	0	-3.337586	1.589803	0.038313
3	7	0	-2.751173	0.331471	0.088415
4	6	0	-1.437987	0.456360	-0.179542
5	7	0	-1.176553	1.745796	-0.399433
6	6	0	0.160750	2.294711	-0.686844
7	6	0	0.804100	2.935217	0.548135
8	1	0	-2.383379	3.538386	-0.402570
9	1	0	-4.386497	1.749677	0.208692
10	1	0	0.783665	1.467817	-1.028147
11	1	0	0.065742	3.024952	-1.491529
12	1	0	0.202962	3.788776	0.878848
13	1	0	0.803567	2.195255	1.362551
14	35	0	-0.058224	-2.547056	-0.165020
15	1	0	-0.744426	-0.406725	-0.213088
16	6	0	-3.356293	-0.933753	0.357971
17	6	0	-4.639761	-1.090460	0.653668
18	1	0	-2.632824	-1.744358	0.290008
19	1	0	-5.013508	-2.087598	0.841860

20	1	0	-5.350018	-0.275244	0.720996
21	7	0	2.127566	3.411355	0.163859
22	1	0	2.526345	4.004468	0.881943
23	1	0	2.750588	2.619364	0.019855
24	6	0	3.348408	-0.655149	-1.113232
25	6	0	3.261646	-0.755503	0.344921
26	8	0	2.854618	0.462379	-0.337641
27	1	0	4.313724	-0.481531	-1.582814
28	1	0	2.596060	-1.157634	-1.713662
29	1	0	2.413451	-1.319935	0.726905
30	6	0	4.469071	-0.647204	1.234847
31	1	0	4.210790	-0.167839	2.183819
32	1	0	4.854506	-1.645969	1.461453
33	1	0	5.262940	-0.067386	0.757250

Rotational constants (GHZ): 0.4225934 0.2920206 0.1827031

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1312.9524977008 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 3.62D-06 NBF= 482

NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000019 -0.000001 0.000054 Ang= 0.01 deg.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3205.64837898 A.U. after 7 cycles

NFock= 7 Conv=0.57D-08 -V/T= 2.0018

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000002979	0.000001016	-0.000001894
2	6	0.000000860	-0.000000646	0.000001030
3	7	0.000004482	0.000006324	0.000001184
4	6	-0.000006829	-0.000011249	-0.000009004
5	7	0.000002068	0.000000033	-0.000000498
6	6	0.000000698	0.000002908	-0.000001276
7	6	-0.000013363	-0.000004818	0.000004320
8	1	0.000001841	0.000000554	-0.000000366
9	1	0.000000159	0.000001655	-0.000002032
10	1	0.000002540	-0.000001688	0.000001873
11	1	0.000000918	-0.000000047	-0.000000709
12	1	0.000002643	0.000000642	0.000001018
13	1	0.000002315	0.000002587	-0.000001781
14	35	0.000000531	-0.000001608	0.000000420
15	1	-0.000000312	0.000008530	0.000003113
16	6	-0.000001731	-0.000002326	-0.000000108
17	6	0.000000084	0.000001021	-0.000002230
18	1	-0.000000769	0.000002002	0.000001494
19	1	-0.000001398	0.000001550	-0.000000212
20	1	-0.000000467	0.000001264	-0.000001795
21	7	0.000009687	0.000003756	-0.000009661
22	1	-0.000001232	0.000001428	0.000000886
23	1	0.000003220	-0.000006578	0.000001879
24	6	-0.000005657	0.000004028	0.000009038
25	6	0.000007022	-0.000005060	0.000010849
26	8	-0.000007403	0.000000965	-0.000005009
27	1	0.000001843	-0.000002556	-0.000004186
28	1	0.000005372	-0.000001803	-0.000004299
29	1	-0.000001499	0.000003331	0.000003255
30	6	-0.000001057	-0.000002794	0.000001785
31	1	-0.000001437	0.000000374	-0.000000181
32	1	-0.000000825	-0.000001169	0.000001177
33	1	0.000000674	-0.000001626	0.000001919

Cartesian Forces: Max 0.000013363 RMS 0.000003924

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.000010123 RMS 0.000002271
Search for a local minimum.
Step number 49 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 31 32 33 34 35
36 37 38 39 40
41 42 43 44 45
46 47 48 49
DE= -4.14D-08 DEPred=-1.18D-08 R= 3.51D+00
Trust test= 3.51D+00 RLast= 2.44D-03 DXMaxT set to 5.19D-01
ITU= 0 0 -1 0 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1
ITU= 1 1 1 0 0 -1 1 -1 1 1 1 1 1 1 1 1 1 0 -1 -1
ITU= 1 1 1 -1 1 0 0 -1 0
Eigenvalues --- 0.00071 0.00105 0.00140 0.00185 0.00266
Eigenvalues --- 0.00509 0.00535 0.00772 0.01207 0.01368
Eigenvalues --- 0.01829 0.01913 0.02168 0.02352 0.02392
Eigenvalues --- 0.02488 0.02654 0.02689 0.03053 0.03102
Eigenvalues --- 0.03307 0.03550 0.03613 0.03992 0.04131
Eigenvalues --- 0.04297 0.04482 0.04721 0.05512 0.05652
Eigenvalues --- 0.05731 0.05765 0.05902 0.07705 0.08795
Eigenvalues --- 0.08964 0.09564 0.09746 0.11188 0.12036
Eigenvalues --- 0.12610 0.13083 0.13236 0.15754 0.15932
Eigenvalues --- 0.15999 0.16002 0.16013 0.16022 0.16128
Eigenvalues --- 0.16345 0.19365 0.21190 0.21980 0.22134
Eigenvalues --- 0.23168 0.23387 0.25628 0.26102 0.27521
Eigenvalues --- 0.28619 0.29784 0.30809 0.32099 0.32709
Eigenvalues --- 0.33703 0.34290 0.34337 0.34407 0.34549
Eigenvalues --- 0.34725 0.34806 0.35105 0.35173 0.35365
Eigenvalues --- 0.35579 0.35778 0.35854 0.35919 0.36419
Eigenvalues --- 0.36628 0.39714 0.41591 0.42211 0.43612
Eigenvalues --- 0.45259 0.45953 0.46533 0.49566 0.55062
Eigenvalues --- 0.58620 0.60696 1.06659
En-DIIS/RFO-DIIS IScMMF= 0 using points: 49 48 47 46 45
RFO step: Lambda=-1.99887632D-09.
DidBck=F Rises=F RFO-DIIS coefs: 1.57464 -0.53204 -0.18947 0.11390 0.03297
Iteration 1 RMS(Cart)= 0.00055328 RMS(Int)= 0.00000008
Iteration 2 RMS(Cart)= 0.00000018 RMS(Int)= 0.00000001

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56495	0.00000	0.00000	0.00000	0.00000	2.56495
R2	2.62132	0.00000	0.00000	0.00000	0.00000	2.62132

R3	2.03396	0.00000	0.00000	0.00000	0.00000	2.03396
R4	2.62515	0.00000	0.00000	0.00000	0.00000	2.62515
R5	2.03073	0.00000	0.00000	0.00000	0.00000	2.03073
R6	2.54367	0.00000	0.00000	0.00000	0.00000	2.54367
R7	2.69882	0.00000	0.00000	0.00000	0.00000	2.69882
R8	2.52074	0.00000	-0.00001	0.00000	-0.00001	2.52074
R9	2.09331	0.00000	-0.00001	0.00000	-0.00001	2.09330
R10	2.78521	0.00000	0.00001	0.00000	0.00001	2.78522
R11	2.89648	0.00000	0.00000	0.00000	0.00000	2.89648
R12	2.05995	0.00000	0.00000	0.00000	0.00000	2.05994
R13	2.06127	0.00000	0.00000	0.00000	0.00000	2.06127
R14	2.06949	0.00000	0.00000	0.00000	0.00000	2.06949
R15	2.07940	0.00000	0.00001	-0.00001	0.00000	2.07940
R16	2.75533	0.00001	-0.00004	0.00002	-0.00001	2.75532
R17	4.24840	0.00000	0.00003	-0.00001	0.00002	4.24842
R18	2.50649	0.00000	0.00000	0.00000	0.00000	2.50649
R19	2.05720	0.00000	0.00000	0.00000	-0.00001	2.05720
R20	2.04352	0.00000	0.00000	0.00000	0.00000	2.04352
R21	2.04717	0.00000	0.00000	0.00000	0.00000	2.04717
R22	1.91456	0.00000	0.00000	0.00000	0.00000	1.91456
R23	1.92357	0.00000	0.00000	0.00000	0.00000	1.92357
R24	4.13639	0.00000	-0.00007	-0.00010	-0.00017	4.13622
R25	2.76689	0.00001	-0.00002	0.00002	0.00000	2.76689
R26	2.73471	0.00000	0.00006	-0.00001	0.00005	2.73476
R27	2.05493	0.00000	0.00000	0.00000	0.00000	2.05493
R28	2.05193	0.00000	0.00000	0.00000	0.00000	2.05192
R29	2.74811	0.00001	-0.00004	0.00000	-0.00004	2.74807
R30	2.05618	0.00000	0.00000	0.00000	0.00000	2.05618
R31	2.84187	0.00000	0.00002	-0.00001	0.00001	2.84188
R32	2.06754	0.00000	0.00000	0.00000	0.00000	2.06754
R33	2.06788	0.00000	0.00000	0.00000	0.00000	2.06788
R34	2.06536	0.00000	0.00000	0.00000	0.00000	2.06536
A1	1.87268	0.00000	0.00000	0.00000	0.00000	1.87267
A2	2.27924	0.00000	0.00000	0.00000	0.00000	2.27924
A3	2.13121	0.00000	0.00000	0.00000	0.00000	2.13121
A4	1.86460	0.00000	0.00000	0.00000	0.00000	1.86460
A5	2.27602	0.00000	0.00000	0.00000	0.00000	2.27601
A6	2.14251	0.00000	0.00000	0.00000	0.00000	2.14252
A7	1.89716	0.00000	0.00000	0.00000	0.00000	1.89716
A8	2.25290	0.00000	-0.00001	0.00000	0.00000	2.25289
A9	2.13309	0.00000	0.00001	-0.00001	0.00000	2.13310
A10	1.88989	0.00000	0.00000	0.00000	0.00000	1.88989
A11	2.14666	0.00001	0.00003	0.00001	0.00004	2.14670
A12	2.24652	-0.00001	-0.00002	-0.00001	-0.00003	2.24648

A13	1.90044	0.00000	0.00000	0.00000	0.00000	1.90044
A14	2.20479	0.00000	0.00000	0.00000	0.00000	2.20479
A15	2.17728	0.00000	-0.00001	0.00000	0.00000	2.17728
A16	1.95990	0.00001	0.00001	0.00002	0.00002	1.95992
A17	1.87238	0.00000	-0.00003	0.00000	-0.00003	1.87235
A18	1.89037	0.00000	0.00001	0.00000	0.00001	1.89038
A19	1.90647	0.00000	-0.00001	-0.00001	-0.00002	1.90645
A20	1.92965	0.00000	0.00000	0.00000	0.00000	1.92965
A21	1.90353	0.00000	0.00002	0.00000	0.00002	1.90355
A22	1.91625	0.00000	0.00000	0.00002	0.00002	1.91626
A23	1.89139	0.00000	0.00000	0.00001	0.00001	1.89140
A24	1.88084	-0.00001	-0.00001	-0.00002	-0.00003	1.88081
A25	1.87586	0.00000	-0.00001	0.00001	0.00000	1.87586
A26	1.90003	0.00000	0.00001	0.00000	0.00001	1.90004
A27	1.99885	0.00000	0.00002	-0.00001	0.00000	1.99885
A28	2.16126	0.00000	0.00000	0.00000	0.00001	2.16127
A29	1.94582	0.00000	0.00000	0.00000	0.00000	1.94582
A30	2.17610	0.00000	-0.00001	0.00000	-0.00001	2.17610
A31	2.07393	0.00000	0.00000	0.00000	0.00000	2.07394
A32	2.16442	0.00000	0.00000	0.00000	0.00000	2.16442
A33	2.04483	0.00000	0.00000	0.00000	0.00000	2.04483
A34	1.94083	0.00000	0.00002	-0.00002	0.00001	1.94084
A35	1.91640	0.00000	0.00002	-0.00002	0.00000	1.91640
A36	1.89109	0.00000	0.00003	0.00000	0.00002	1.89112
A37	2.08702	0.00000	-0.00004	0.00001	-0.00003	2.08699
A38	2.06908	0.00001	0.00001	0.00000	0.00001	2.06909
A39	1.99440	0.00000	-0.00003	0.00001	-0.00003	1.99437
A40	2.00127	0.00000	-0.00001	0.00001	0.00000	2.00126
A41	2.03775	-0.00001	0.00005	-0.00002	0.00004	2.03779
A42	2.01680	0.00000	0.00001	0.00001	0.00002	2.01682
A43	2.13746	0.00000	0.00002	-0.00002	0.00000	2.13746
A44	1.96170	0.00000	0.00001	-0.00002	-0.00001	1.96169
A45	2.02880	0.00001	0.00003	0.00002	0.00005	2.02885
A46	2.04371	0.00000	-0.00005	0.00001	-0.00005	2.04367
A47	2.61540	0.00000	-0.00002	0.00023	0.00020	2.61560
A48	2.43706	0.00000	-0.00015	-0.00013	-0.00027	2.43679
A49	1.93402	0.00000	-0.00001	0.00001	-0.00001	1.93401
A50	1.91730	0.00000	0.00001	-0.00001	0.00000	1.91730
A51	1.94207	0.00000	0.00000	0.00000	0.00000	1.94207
A52	1.87909	0.00000	0.00001	0.00000	0.00001	1.87910
A53	1.89447	0.00000	0.00000	0.00000	0.00000	1.89447
A54	1.89532	0.00000	0.00000	0.00000	0.00000	1.89531
A55	3.48323	0.00000	0.00000	-0.00023	-0.00023	3.48300
A56	2.53122	0.00000	-0.00012	0.00011	0.00000	2.53122

A57	2.96298	0.00000	-0.00010	-0.00048	-0.00058	2.96240
A58	3.10755	0.00000	0.00006	0.00000	0.00006	3.10761
D1	0.00310	0.00000	0.00000	0.00000	0.00000	0.00310
D2	-3.12699	0.00000	-0.00003	-0.00005	-0.00008	-3.12707
D3	3.13321	0.00000	-0.00001	0.00004	0.00003	3.13324
D4	0.00313	0.00000	-0.00004	-0.00001	-0.00006	0.00307
D5	-0.00470	0.00000	0.00001	0.00000	0.00001	-0.00468
D6	-3.10815	0.00000	-0.00003	0.00001	-0.00001	-3.10817
D7	-3.13600	0.00000	0.00002	-0.00003	-0.00001	-3.13601
D8	0.04373	0.00000	-0.00002	-0.00002	-0.00003	0.04370
D9	-0.00048	0.00000	-0.00001	-0.00001	-0.00002	-0.00050
D10	-3.13335	0.00000	-0.00003	0.00000	-0.00004	-3.13338
D11	3.13069	0.00000	0.00002	0.00004	0.00006	3.13075
D12	-0.00218	0.00000	-0.00001	0.00005	0.00004	-0.00214
D13	-0.00245	0.00000	0.00002	0.00001	0.00003	-0.00242
D14	-3.12897	0.00000	-0.00005	-0.00012	-0.00018	-3.12914
D15	3.13114	0.00000	0.00004	0.00000	0.00004	3.13118
D16	0.00462	0.00000	-0.00003	-0.00013	-0.00016	0.00446
D17	-0.03598	0.00000	0.00020	0.00047	0.00068	-0.03531
D18	3.10610	0.00000	0.00018	0.00044	0.00062	3.10672
D19	3.11538	0.00000	0.00018	0.00048	0.00066	3.11604
D20	-0.02572	0.00000	0.00015	0.00045	0.00060	-0.02512
D21	0.00440	0.00000	-0.00002	-0.00001	-0.00003	0.00438
D22	3.10860	0.00000	0.00002	-0.00002	0.00000	3.10860
D23	3.12979	0.00000	0.00006	0.00014	0.00020	3.12999
D24	-0.04920	0.00000	0.00010	0.00013	0.00022	-0.04897
D25	1.34547	0.00000	-0.00038	-0.00008	-0.00046	1.34501
D26	-2.84287	0.00000	-0.00041	-0.00008	-0.00049	-2.84336
D27	-0.79042	0.00000	-0.00040	-0.00008	-0.00048	-0.79090
D28	-1.75221	0.00000	-0.00042	-0.00007	-0.00049	-1.75270
D29	0.34264	0.00000	-0.00045	-0.00007	-0.00052	0.34212
D30	2.39509	0.00000	-0.00044	-0.00007	-0.00051	2.39458
D31	-1.09970	0.00000	-0.00010	-0.00002	-0.00012	-1.09982
D32	0.94442	0.00000	-0.00011	0.00001	-0.00011	0.94431
D33	3.11645	0.00000	-0.00010	-0.00001	-0.00012	3.11633
D34	3.10855	0.00000	-0.00006	-0.00002	-0.00008	3.10847
D35	-1.13051	0.00000	-0.00007	0.00000	-0.00007	-1.13058
D36	1.04152	0.00000	-0.00006	-0.00002	-0.00008	1.04144
D37	1.01377	0.00000	-0.00008	-0.00001	-0.00009	1.01368
D38	3.05789	0.00000	-0.00009	0.00002	-0.00008	3.05781
D39	-1.05326	0.00000	-0.00008	-0.00001	-0.00009	-1.05335
D40	2.94399	0.00000	-0.00007	-0.00004	-0.00011	2.94388
D41	-1.24642	0.00000	-0.00001	-0.00007	-0.00008	-1.24650
D42	0.86658	0.00000	-0.00007	-0.00005	-0.00012	0.86647

D43	2.95936	0.00000	-0.00001	-0.00007	-0.00008	2.95928
D44	-1.23333	0.00000	-0.00007	-0.00005	-0.00012	-1.23345
D45	0.85944	0.00000	-0.00001	-0.00007	-0.00009	0.85936
D46	3.13969	0.00000	0.00001	0.00001	0.00002	3.13971
D47	-0.00240	0.00000	0.00001	0.00004	0.00005	-0.00235
D48	-0.00247	0.00000	0.00004	0.00005	0.00009	-0.00238
D49	3.13863	0.00000	0.00004	0.00008	0.00012	3.13875
D50	2.20758	0.00000	0.00023	-0.00021	0.00003	2.20761
D51	-1.40742	0.00000	-0.00027	0.00007	-0.00020	-1.40762
D52	-2.08673	0.00000	0.00023	-0.00019	0.00004	-2.08669
D53	0.58145	0.00000	-0.00028	0.00009	-0.00019	0.58126
D54	-2.71254	0.00000	-0.00002	-0.00003	-0.00005	-2.71258
D55	-0.01591	0.00000	-0.00009	-0.00002	-0.00011	-0.01601
D56	-0.02638	0.00000	0.00004	-0.00004	0.00001	-0.02637
D57	2.67025	0.00000	-0.00002	-0.00003	-0.00006	2.67020
D58	0.50793	0.00000	-0.00036	-0.00002	-0.00037	0.50756
D59	-1.91159	0.00000	-0.00039	0.00000	-0.00039	-1.91198
D60	1.78363	0.00000	0.00018	-0.00032	-0.00014	1.78349
D61	-0.63889	0.00000	0.00022	-0.00033	-0.00011	-0.63900
D62	2.55548	0.00000	0.00005	0.00005	0.00010	2.55558
D63	-1.65356	0.00000	0.00006	0.00005	0.00011	-1.65345
D64	0.44588	0.00000	0.00006	0.00005	0.00011	0.44599
D65	1.35077	0.00000	-0.00001	0.00006	0.00004	1.35081
D66	-2.85827	0.00000	-0.00001	0.00006	0.00005	-2.85822
D67	-0.75883	0.00000	0.00000	0.00005	0.00005	-0.75878
D68	-1.03748	0.00000	0.00000	0.00005	0.00006	-1.03742
D69	1.03667	0.00000	0.00001	0.00006	0.00007	1.03673
D70	3.13611	0.00000	0.00001	0.00005	0.00006	3.13617

Item	Value	Threshold	Converged?
Maximum Force	0.000010	0.000450	YES
RMS Force	0.000002	0.000300	YES
Maximum Displacement	0.002436	0.001800	NO
RMS Displacement	0.000553	0.001200	YES

Predicted change in Energy=-6.556588D-09

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.643833	2.100090	-0.196483
2	6	0	-3.535839	1.118451	0.091626
3	7	0	-2.826959	-0.076066	0.111699

4	6	0	-1.534584	0.184455	-0.159868
5	7	0	-1.404105	1.497837	-0.353097
6	6	0	-0.129993	2.182991	-0.635066
7	6	0	0.454821	2.858803	0.610163
8	1	0	-2.783067	3.161139	-0.311650
9	1	0	-4.594223	1.169570	0.270556
10	1	0	0.569739	1.429414	-0.996675
11	1	0	-0.302572	2.916557	-1.423669
12	1	0	-0.225901	3.641357	0.961628
13	1	0	0.533298	2.105883	1.408769
14	35	0	0.137249	-2.666237	-0.215408
15	1	0	-0.758889	-0.604397	-0.215255
16	6	0	-3.301469	-1.400595	0.356825
17	6	0	-4.561067	-1.690476	0.654590
18	1	0	-2.501402	-2.133525	0.268470
19	1	0	-4.832539	-2.723573	0.823113
20	1	0	-5.348478	-0.951642	0.742251
21	7	0	1.721808	3.472008	0.229847
22	1	0	2.064476	4.087055	0.958370
23	1	0	2.419466	2.749044	0.066323
24	6	0	3.332072	-0.426001	-1.137894
25	6	0	3.265647	-0.563846	0.318261
26	8	0	2.734901	0.620968	-0.336923
27	1	0	4.272130	-0.147694	-1.608348
28	1	0	2.629340	-0.988669	-1.745020
29	1	0	2.480398	-1.217477	0.692530
30	6	0	4.462374	-0.353930	1.204471
31	1	0	4.164193	0.078048	2.164433
32	1	0	4.946735	-1.313749	1.408389
33	1	0	5.191386	0.311575	0.735257

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357312	0.000000			
3	N	2.205485	1.389168	0.000000		
4	C	2.213918	2.222752	1.346051	0.000000	
5	N	1.387142	2.210431	2.172031	1.333917	0.000000
6	C	2.553159	3.641582	3.596474	2.488541	1.473874
7	C	3.290591	4.384413	4.430801	3.420938	2.497139
8	H	1.076324	2.214016	3.265064	3.231470	2.160978
9	H	2.210885	1.074618	2.167964	3.243009	3.267041
10	H	3.378929	4.258741	3.877179	2.584249	2.077242
11	H	2.766606	3.997915	4.205434	3.252603	2.090996

12	H	3.092430	4.251782	4.615963	3.862716	2.776930
13	H	3.559639	4.389506	4.211248	3.229341	2.688386
14	Br	5.518392	5.282964	3.950001	3.305231	4.442324
15	H	3.296607	3.282352	2.159385	1.107726	2.203337
16	C	3.604640	2.543787	1.428154	2.429246	3.536225
17	C	4.332262	3.042711	2.430675	3.652165	4.598607
18	H	4.261451	3.417117	2.088948	2.547792	3.844113
19	H	5.394231	4.120395	3.396727	4.505484	5.563986
20	H	4.184423	2.827412	2.742679	4.080481	4.770515
21	N	4.595948	5.762047	5.770101	4.643702	3.742793
22	H	5.239265	6.397452	6.478778	5.425309	4.522726
23	H	5.111478	6.174555	5.958882	4.718345	4.044888
24	C	6.555825	7.145997	6.294251	5.001353	5.171889
25	C	6.502575	7.010115	6.115590	4.881678	5.148577
26	O	5.580171	6.305024	5.623291	4.295392	4.230902
27	H	7.407864	8.090577	7.304845	5.993859	6.041777
28	H	6.304344	6.769244	5.835361	4.607297	4.938506
29	H	6.168820	6.481725	5.459691	4.337289	4.853415
30	C	7.647423	8.208395	7.376024	6.173717	6.345915
31	H	7.484103	8.041732	7.287912	6.155465	6.273731
32	H	8.476240	8.922082	7.977693	6.834584	7.165265
33	H	8.090586	8.788047	8.051890	6.786463	6.789126

		6	7	8	9	10
6	C	0.000000				
7	C	1.532750	0.000000			
8	H	2.846081	3.380099	0.000000		
9	H	4.666532	5.334950	2.754196	0.000000	
10	H	1.090076	2.153669	3.835289	5.323523	0.000000
11	H	1.090778	2.171049	2.729335	4.933623	1.776188
12	H	2.164592	1.095126	2.896713	5.066513	3.059524
13	H	2.150153	1.100372	3.882227	5.335136	2.499020
14	Br	4.874684	5.595398	6.518881	6.110352	4.191871
15	H	2.888129	3.761404	4.276196	4.253558	2.551913
16	C	4.887146	5.684748	4.639505	2.878263	4.982686
17	C	6.025063	6.771783	5.256716	2.885904	6.227805
18	H	5.007222	5.812001	5.333792	3.910286	4.871040
19	H	6.950871	7.691843	6.333865	3.939375	7.052910
20	H	6.241435	6.943718	4.960545	2.300204	6.612003
21	N	2.416361	1.458052	4.547940	6.722732	2.646471
22	H	3.313637	2.054469	5.095974	7.302266	3.622085
23	H	2.704089	2.041479	5.232498	7.192237	2.508561
24	C	4.364123	4.703638	7.137590	8.207054	3.330615
25	C	4.470383	4.438522	7.131567	8.048886	3.601398
26	O	3.276648	3.332212	6.074626	7.374690	2.403494

27	H	5.075240	5.341597	7.899723	9.158476	4.070518
28	H	4.348028	5.007840	6.969190	7.803871	3.263296
29	H	4.487743	4.552560	6.919879	7.478390	3.675604
30	C	5.559649	5.170622	8.194556	9.231208	4.814350
31	H	5.541481	4.889559	7.993801	9.027072	4.973821
32	H	6.494311	6.182608	9.095769	9.924284	5.698015
33	H	5.804917	5.379504	8.532757	9.834137	5.060512

		11	12	13	14	15
11	H	0.000000				
12	H	2.494164	0.000000			
13	H	3.062446	1.770311	0.000000		
14	Br	5.728955	6.426744	5.056474	0.000000	
15	H	3.750414	4.437968	3.413622	2.248165	0.000000
16	C	5.549896	5.936850	5.301641	3.708649	2.725053
17	C	6.608986	6.878690	6.397943	4.876800	4.048796
18	H	5.762076	6.245610	5.336878	2.735032	2.368243
19	H	7.574939	7.858285	7.242848	5.077461	4.707838
20	H	6.716796	6.883645	6.662431	5.826675	4.701246
21	N	2.672219	2.087523	2.160720	6.355087	4.792604
22	H	3.556275	2.333342	2.544094	7.120317	5.599867
23	H	3.107672	2.931852	2.402800	5.883294	4.628908
24	C	4.946211	5.797462	4.552919	4.009555	4.197506
25	C	5.280124	5.503505	3.972706	3.806800	4.059948
26	O	3.959417	4.424402	3.177966	4.191453	3.704442
27	H	5.509232	6.418253	5.306644	5.037915	5.240272
28	H	4.893890	6.075811	4.890401	3.371122	3.737371
29	H	5.414190	5.568190	3.917769	2.900622	3.419492
30	C	6.348851	6.164513	4.640049	5.105833	5.416636
31	H	6.394028	5.780729	4.226883	5.423193	5.510479
32	H	7.312405	7.176966	5.583217	5.253294	5.974408
33	H	6.452167	6.362836	5.036958	5.942679	6.094937

		16	17	18	19	20
16	C	0.000000				
17	C	1.326380	0.000000			
18	H	1.088623	2.141869	0.000000		
19	H	2.076505	1.081382	2.467790	0.000000	
20	H	2.130811	1.083317	3.118839	1.847287	0.000000
21	N	6.999406	8.142860	7.018476	9.038620	8.355847
22	H	7.698670	8.796020	7.747182	9.693904	8.965884
23	H	7.073399	8.293565	6.935076	9.116679	8.630927
24	C	6.869344	8.192286	6.238824	8.705473	8.897370
25	C	6.620321	7.914535	5.977059	8.396423	8.633267
26	O	6.403574	7.717319	5.947487	8.354507	8.305343
27	H	7.924082	9.248051	7.303884	9.769451	9.936184

28	H	6.305706	7.612661	5.629329	8.079903	8.356642
29	H	5.794499	7.057436	5.083041	7.467559	7.833546
30	C	7.879801	9.138447	7.248258	9.599795	9.839905
31	H	7.822399	9.029810	7.274331	9.517847	9.673353
32	H	8.315419	9.545074	7.579327	9.897695	10.323094
33	H	8.671985	9.956157	8.085506	10.473725	10.615296

		21	22	23	24	25
21	N	0.000000				
22	H	1.013139	0.000000			
23	H	1.017912	1.646827	0.000000		
24	C	4.433751	5.135056	3.516234	0.000000	
25	C	4.321965	4.845971	3.428518	1.464173	0.000000
26	O	3.078314	3.760454	2.188792	1.447174	1.454216
27	H	4.794304	5.421704	3.824654	1.087424	2.213146
28	H	4.961991	5.778439	4.158786	1.085831	2.200566
29	H	4.772924	5.327450	4.016109	2.168464	1.088084
30	C	4.806079	5.053002	3.885524	2.601817	1.503858
31	H	4.607259	4.683539	3.818423	3.442653	2.151224
32	H	5.890042	6.138291	4.969358	3.143054	2.139343
33	H	4.720355	4.907300	3.751302	2.740395	2.156089

		26	27	28	29	30
26	O	0.000000				
27	H	2.137858	0.000000			
28	H	2.141217	1.850589	0.000000		
29	H	2.122363	3.106249	2.452792	0.000000	
30	C	2.512068	2.826779	3.530213	2.221716	0.000000
31	H	2.931624	3.781070	4.333299	2.584578	1.094096
32	H	3.417815	3.303858	3.926829	2.569930	1.094276
33	H	2.698076	2.558993	3.795588	3.112761	1.092940

		31	32	33
31	H	0.000000		
32	H	1.766657	0.000000	
33	H	1.775445	1.776130	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-2.350821	2.471620	-0.263515
2	6	0	-3.337450	1.589954	0.039015
3	7	0	-2.751163	0.331543	0.088567
4	6	0	-1.438056	0.456356	-0.179808
5	7	0	-1.176546	1.745825	-0.399398
6	6	0	0.160728	2.294663	-0.687108
7	6	0	0.804327	2.935334	0.547657
8	1	0	-2.383164	3.538559	-0.401604
9	1	0	-4.386275	1.749910	0.209848
10	1	0	0.783548	1.467677	-1.028363
11	1	0	0.065625	3.024780	-1.491895
12	1	0	0.203353	3.789039	0.878294
13	1	0	0.803823	2.195538	1.362224
14	35	0	-0.058227	-2.547043	-0.165102
15	1	0	-0.744546	-0.406750	-0.213678
16	6	0	-3.356335	-0.933683	0.358001
17	6	0	-4.639871	-1.090406	0.653392
18	1	0	-2.632855	-1.744285	0.290169
19	1	0	-5.013644	-2.087544	0.841531
20	1	0	-5.350167	-0.275206	0.720490
21	7	0	2.127788	3.411209	0.163069
22	1	0	2.526724	4.004506	0.880913
23	1	0	2.750701	2.619107	0.019204
24	6	0	3.347959	-0.655920	-1.112777
25	6	0	3.261573	-0.755401	0.345456
26	8	0	2.854429	0.462098	-0.337679
27	1	0	4.313172	-0.482604	-1.582687
28	1	0	2.595423	-1.158702	-1.712718
29	1	0	2.413450	-1.319545	0.728020
30	6	0	4.469251	-0.646735	1.235003
31	1	0	4.211253	-0.166871	2.183799
32	1	0	4.854684	-1.645411	1.462000
33	1	0	5.263028	-0.067207	0.756899

Rotational constants (GHZ): 0.4225993 0.2920272 0.1827045

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1312.9617022014 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 482 RedAO= T EigKep= 3.62D-06 NBF= 482
NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 0.000029 -0.000010 0.000013 Ang= 0.00 deg.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3205.64837901 A.U. after 7 cycles
NFock= 7 Conv=0.68D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000002171	-0.000000303	-0.000003074
2	6	0.000001424	0.000000685	0.000002020
3	7	0.000002211	0.000003628	-0.000000678
4	6	-0.000004302	-0.000006503	-0.000003533
5	7	0.000002307	0.000004316	-0.000001701
6	6	-0.000000784	0.000000480	-0.000000791
7	6	-0.000017055	-0.000007457	0.000004122
8	1	0.000001403	0.000000585	-0.000000167
9	1	0.000000054	0.000001331	-0.000002063
10	1	0.000002729	-0.000000489	0.000000648
11	1	0.000001470	-0.000000602	-0.000001046
12	1	0.000002953	0.000000423	0.000000240
13	1	0.000002039	0.000002291	-0.000002155
14	35	-0.000000333	-0.000001681	0.000000801
15	1	-0.000001369	0.000004074	0.000002988
16	6	-0.000002170	-0.000002875	-0.000002490
17	6	0.000000253	0.000001783	-0.000001708
18	1	0.000000596	0.000001325	0.000001418
19	1	-0.000001086	0.000001433	-0.000000057
20	1	-0.000000713	0.000001393	-0.000001257
21	7	0.000011887	0.000006857	-0.000008853
22	1	0.000000289	0.000000739	0.000000996

23	1	0.000003305	-0.000005026	0.000001784
24	6	-0.000007744	0.000010098	0.000012310
25	6	0.000007270	-0.000011863	0.000014653
26	8	-0.000001740	0.000001046	-0.000008704
27	1	0.000000666	-0.000003332	-0.000004141
28	1	0.000004058	-0.000002253	-0.000002793
29	1	-0.000001217	0.000000900	-0.000001253
30	6	-0.000003373	0.000001779	0.000000002
31	1	-0.000000134	0.000000356	0.000001081
32	1	-0.000001267	-0.000001274	0.000001558
33	1	0.000000541	-0.000001864	0.000001842

Cartesian Forces: Max 0.000017055 RMS 0.000004282

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000014821 RMS 0.000001944
Search for a local minimum.
Step number 50 out of a maximum of 172
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 31 32 33 34 35
36 37 38 39 40
41 42 43 44 45
46 47 48 49 50
DE= -2.44D-08 DEPred=-6.56D-09 R= 3.72D+00
Trust test= 3.72D+00 RLast= 2.11D-03 DXMaxT set to 5.19D-01
ITU= 0 0 0 -1 0 0 1 1 1 1 1 1 1 1 1 1 1 1 1 1
ITU= 1 1 1 1 0 0 -1 1 -1 1 1 1 1 1 1 1 1 1 0 -1
ITU= -1 1 1 1 -1 1 0 0 -1 0

Eigenvalues ---	0.00066	0.00091	0.00139	0.00174	0.00283
Eigenvalues ---	0.00442	0.00535	0.00775	0.01181	0.01367
Eigenvalues ---	0.01868	0.01906	0.02169	0.02315	0.02387
Eigenvalues ---	0.02489	0.02682	0.02701	0.03054	0.03103
Eigenvalues ---	0.03331	0.03475	0.03649	0.03974	0.04089
Eigenvalues ---	0.04350	0.04486	0.04721	0.05526	0.05622
Eigenvalues ---	0.05712	0.05761	0.05908	0.07611	0.08721
Eigenvalues ---	0.08997	0.09568	0.09801	0.11069	0.12147
Eigenvalues ---	0.12448	0.13072	0.13483	0.15782	0.15938
Eigenvalues ---	0.15999	0.16001	0.16002	0.16019	0.16143

Eigenvalues --- 0.16390 0.18787 0.21379 0.21838 0.22125
Eigenvalues --- 0.23241 0.23361 0.25167 0.26129 0.27405
Eigenvalues --- 0.29059 0.30059 0.30843 0.32013 0.32731
Eigenvalues --- 0.33716 0.34300 0.34338 0.34413 0.34551
Eigenvalues --- 0.34726 0.34790 0.35107 0.35186 0.35360
Eigenvalues --- 0.35567 0.35737 0.35881 0.36128 0.36421
Eigenvalues --- 0.36627 0.40158 0.41683 0.42302 0.44392
Eigenvalues --- 0.44967 0.45797 0.46562 0.49582 0.55059
Eigenvalues --- 0.58997 0.60777 1.06570
En-DIIS/RFO-DIIS IScMMF= 0 using points: 50 49 48 47 46
RFO step: Lambda=-1.27103698D-09.
DidBck=F Rises=F RFO-DIIS coefs: 1.65604 -0.50523 -0.48365 0.31235 0.02049
Iteration 1 RMS(Cart)= 0.00039600 RMS(Int)= 0.00000004
Iteration 2 RMS(Cart)= 0.00000010 RMS(Int)= 0.00000001

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56495	0.00000	0.00000	0.00000	0.00000	2.56495
R2	2.62132	0.00000	0.00000	0.00000	0.00000	2.62132
R3	2.03396	0.00000	0.00000	0.00000	0.00000	2.03396
R4	2.62515	0.00000	0.00000	0.00000	0.00000	2.62515
R5	2.03073	0.00000	0.00000	0.00000	0.00000	2.03073
R6	2.54367	0.00000	0.00000	0.00000	-0.00001	2.54366
R7	2.69882	0.00000	0.00000	0.00000	0.00001	2.69882
R8	2.52074	0.00000	0.00000	0.00000	0.00000	2.52074
R9	2.09330	0.00000	-0.00001	0.00000	-0.00001	2.09329
R10	2.78522	0.00000	0.00001	0.00000	0.00000	2.78522
R11	2.89648	0.00000	0.00000	0.00000	0.00000	2.89648
R12	2.05994	0.00000	0.00000	0.00000	0.00000	2.05995
R13	2.06127	0.00000	0.00000	0.00000	0.00000	2.06127
R14	2.06949	0.00000	0.00000	0.00000	0.00000	2.06949
R15	2.07940	0.00000	0.00000	0.00000	-0.00001	2.07939
R16	2.75532	0.00001	0.00001	0.00002	0.00003	2.75535
R17	4.24842	0.00000	0.00009	0.00000	0.00009	4.24851
R18	2.50649	0.00000	0.00000	0.00000	0.00000	2.50649
R19	2.05720	0.00000	0.00000	0.00000	0.00000	2.05720
R20	2.04352	0.00000	0.00000	0.00000	0.00000	2.04352
R21	2.04717	0.00000	0.00000	0.00000	0.00000	2.04717
R22	1.91456	0.00000	0.00000	0.00000	0.00000	1.91456
R23	1.92357	0.00000	0.00000	0.00000	0.00001	1.92358
R24	4.13622	0.00000	-0.00003	-0.00007	-0.00010	4.13611
R25	2.76689	0.00000	-0.00001	0.00000	-0.00001	2.76688
R26	2.73476	-0.00001	0.00002	-0.00002	0.00000	2.73476
R27	2.05493	0.00000	0.00001	0.00000	0.00001	2.05494

R28	2.05192	0.00000	0.00000	0.00000	0.00000	2.05192
R29	2.74807	0.00001	0.00000	0.00001	0.00002	2.74809
R30	2.05618	0.00000	0.00000	0.00000	0.00000	2.05618
R31	2.84188	0.00000	0.00000	0.00000	0.00000	2.84188
R32	2.06754	0.00000	0.00000	0.00000	0.00000	2.06754
R33	2.06788	0.00000	0.00000	0.00000	0.00000	2.06788
R34	2.06536	0.00000	0.00000	0.00000	0.00000	2.06536
A1	1.87267	0.00000	0.00000	0.00000	0.00000	1.87267
A2	2.27924	0.00000	0.00000	0.00000	0.00000	2.27925
A3	2.13121	0.00000	0.00000	0.00000	0.00000	2.13121
A4	1.86460	0.00000	0.00000	0.00000	0.00000	1.86460
A5	2.27601	0.00000	0.00000	0.00000	0.00000	2.27601
A6	2.14252	0.00000	0.00000	0.00000	0.00000	2.14252
A7	1.89716	0.00000	0.00000	0.00000	0.00000	1.89716
A8	2.25289	0.00000	-0.00001	0.00001	0.00000	2.25289
A9	2.13310	0.00000	0.00000	0.00000	0.00000	2.13310
A10	1.88989	0.00000	0.00000	0.00000	0.00000	1.88989
A11	2.14670	0.00000	0.00003	-0.00001	0.00002	2.14672
A12	2.24648	0.00000	-0.00003	0.00001	-0.00002	2.24646
A13	1.90044	0.00000	0.00000	0.00000	0.00000	1.90044
A14	2.20479	0.00000	-0.00001	0.00001	0.00000	2.20479
A15	2.17728	0.00000	0.00001	0.00000	0.00000	2.17728
A16	1.95992	0.00000	0.00002	0.00000	0.00002	1.95994
A17	1.87235	0.00000	-0.00001	-0.00001	-0.00002	1.87234
A18	1.89038	0.00000	0.00000	0.00001	0.00001	1.89039
A19	1.90645	0.00000	-0.00001	-0.00001	-0.00003	1.90643
A20	1.92965	0.00000	-0.00001	0.00001	0.00000	1.92964
A21	1.90355	0.00000	0.00001	0.00000	0.00001	1.90356
A22	1.91626	0.00000	0.00002	0.00001	0.00003	1.91629
A23	1.89140	0.00000	0.00002	0.00000	0.00002	1.89141
A24	1.88081	0.00000	-0.00003	0.00000	-0.00003	1.88078
A25	1.87586	0.00000	0.00000	0.00001	0.00001	1.87586
A26	1.90004	0.00000	0.00000	0.00000	0.00000	1.90003
A27	1.99885	0.00000	-0.00001	-0.00001	-0.00002	1.99883
A28	2.16127	0.00000	0.00000	0.00000	0.00000	2.16127
A29	1.94582	0.00000	0.00000	0.00000	0.00000	1.94582
A30	2.17610	0.00000	0.00000	0.00000	0.00000	2.17610
A31	2.07394	0.00000	0.00000	0.00000	0.00000	2.07394
A32	2.16442	0.00000	0.00000	0.00000	0.00000	2.16442
A33	2.04483	0.00000	0.00000	0.00000	0.00000	2.04482
A34	1.94084	0.00000	0.00000	-0.00001	-0.00001	1.94082
A35	1.91640	0.00000	0.00000	-0.00001	-0.00001	1.91639
A36	1.89112	0.00000	0.00001	-0.00001	0.00001	1.89112
A37	2.08699	0.00000	-0.00001	0.00001	0.00000	2.08700

A38	2.06909	0.00000	0.00003	0.00000	0.00003	2.06912
A39	1.99437	0.00000	-0.00001	0.00001	0.00000	1.99437
A40	2.00126	0.00000	0.00001	0.00000	0.00002	2.00128
A41	2.03779	0.00000	-0.00001	-0.00002	-0.00003	2.03776
A42	2.01682	0.00000	0.00002	-0.00002	0.00000	2.01682
A43	2.13746	0.00000	0.00000	0.00000	0.00001	2.13747
A44	1.96169	0.00000	-0.00002	0.00000	-0.00002	1.96167
A45	2.02885	0.00000	0.00003	-0.00001	0.00002	2.02887
A46	2.04367	0.00000	-0.00003	0.00002	-0.00001	2.04366
A47	2.61560	0.00000	0.00017	-0.00022	-0.00005	2.61554
A48	2.43679	0.00000	-0.00024	0.00009	-0.00015	2.43664
A49	1.93401	0.00000	-0.00001	0.00001	0.00000	1.93401
A50	1.91730	0.00000	-0.00001	-0.00001	-0.00001	1.91729
A51	1.94207	0.00000	0.00001	0.00000	0.00001	1.94207
A52	1.87910	0.00000	0.00001	0.00000	0.00001	1.87911
A53	1.89447	0.00000	0.00000	0.00000	0.00000	1.89447
A54	1.89531	0.00000	0.00000	0.00000	-0.00001	1.89531
A55	3.48300	0.00000	-0.00012	-0.00003	-0.00015	3.48284
A56	2.53122	0.00000	-0.00005	-0.00001	-0.00006	2.53116
A57	2.96240	0.00000	-0.00047	-0.00010	-0.00057	2.96183
A58	3.10761	0.00000	-0.00003	-0.00005	-0.00007	3.10753
D1	0.00310	0.00000	0.00000	-0.00001	-0.00001	0.00309
D2	-3.12707	0.00000	-0.00005	-0.00002	-0.00007	-3.12713
D3	3.13324	0.00000	0.00002	0.00002	0.00004	3.13328
D4	0.00307	0.00000	-0.00002	0.00001	-0.00001	0.00306
D5	-0.00468	0.00000	0.00001	0.00000	0.00001	-0.00467
D6	-3.10817	0.00000	-0.00001	0.00000	-0.00001	-3.10818
D7	-3.13601	0.00000	-0.00001	-0.00002	-0.00004	-3.13604
D8	0.04370	0.00000	-0.00003	-0.00003	-0.00006	0.04363
D9	-0.00050	0.00000	-0.00001	0.00001	0.00001	-0.00050
D10	-3.13338	0.00000	-0.00001	0.00002	0.00000	-3.13338
D11	3.13075	0.00000	0.00003	0.00002	0.00006	3.13080
D12	-0.00214	0.00000	0.00002	0.00003	0.00005	-0.00209
D13	-0.00242	0.00000	0.00002	-0.00001	0.00000	-0.00242
D14	-3.12914	0.00000	-0.00013	-0.00006	-0.00019	-3.12933
D15	3.13118	0.00000	0.00002	-0.00001	0.00001	3.13119
D16	0.00446	0.00000	-0.00013	-0.00006	-0.00018	0.00427
D17	-0.03531	0.00000	0.00047	0.00016	0.00063	-0.03467
D18	3.10672	0.00000	0.00044	0.00016	0.00060	3.10732
D19	3.11604	0.00000	0.00046	0.00017	0.00063	3.11667
D20	-0.02512	0.00000	0.00043	0.00016	0.00059	-0.02452
D21	0.00438	0.00000	-0.00002	0.00001	-0.00001	0.00437
D22	3.10860	0.00000	0.00000	0.00001	0.00002	3.10862
D23	3.12999	0.00000	0.00014	0.00005	0.00019	3.13018

D24	-0.04897	0.00000	0.00016	0.00006	0.00022	-0.04875
D25	1.34501	0.00000	-0.00027	-0.00013	-0.00040	1.34460
D26	-2.84336	0.00000	-0.00028	-0.00015	-0.00043	-2.84379
D27	-0.79090	0.00000	-0.00027	-0.00015	-0.00042	-0.79132
D28	-1.75270	0.00000	-0.00029	-0.00014	-0.00043	-1.75313
D29	0.34212	0.00000	-0.00030	-0.00016	-0.00046	0.34166
D30	2.39458	0.00000	-0.00030	-0.00016	-0.00045	2.39413
D31	-1.09982	0.00000	-0.00002	-0.00005	-0.00007	-1.09990
D32	0.94431	0.00000	0.00000	-0.00004	-0.00004	0.94427
D33	3.11633	0.00000	-0.00002	-0.00005	-0.00007	3.11626
D34	3.10847	0.00000	-0.00002	-0.00003	-0.00005	3.10841
D35	-1.13058	0.00000	0.00000	-0.00002	-0.00002	-1.13061
D36	1.04144	0.00000	-0.00001	-0.00004	-0.00005	1.04139
D37	1.01368	0.00000	-0.00001	-0.00003	-0.00005	1.01363
D38	3.05781	0.00000	0.00001	-0.00002	-0.00001	3.05780
D39	-1.05335	0.00000	-0.00001	-0.00003	-0.00004	-1.05339
D40	2.94388	0.00000	-0.00011	-0.00001	-0.00012	2.94376
D41	-1.24650	0.00000	-0.00009	-0.00003	-0.00012	-1.24662
D42	0.86647	0.00000	-0.00011	-0.00002	-0.00013	0.86633
D43	2.95928	0.00000	-0.00010	-0.00004	-0.00014	2.95913
D44	-1.23345	0.00000	-0.00011	-0.00002	-0.00013	-1.23358
D45	0.85936	0.00000	-0.00010	-0.00004	-0.00013	0.85922
D46	3.13971	0.00000	0.00003	0.00001	0.00003	3.13974
D47	-0.00235	0.00000	0.00004	0.00002	0.00006	-0.00229
D48	-0.00238	0.00000	0.00006	0.00001	0.00007	-0.00231
D49	3.13875	0.00000	0.00007	0.00002	0.00010	3.13884
D50	2.20761	0.00000	0.00026	0.00027	0.00053	2.20814
D51	-1.40762	0.00000	0.00004	-0.00013	-0.00009	-1.40772
D52	-2.08669	0.00000	0.00027	0.00026	0.00052	-2.08617
D53	0.58126	0.00000	0.00004	-0.00015	-0.00011	0.58116
D54	-2.71258	0.00000	-0.00004	0.00002	-0.00002	-2.71261
D55	-0.01601	0.00000	-0.00005	0.00003	-0.00002	-0.01603
D56	-0.02637	0.00000	-0.00003	-0.00001	-0.00004	-0.02641
D57	2.67020	0.00000	-0.00005	0.00001	-0.00004	2.67016
D58	0.50756	0.00000	-0.00037	-0.00006	-0.00043	0.50713
D59	-1.91198	0.00000	-0.00035	-0.00004	-0.00040	-1.91238
D60	1.78349	0.00000	-0.00011	0.00034	0.00023	1.78372
D61	-0.63900	0.00000	-0.00008	0.00032	0.00024	-0.63876
D62	2.55558	0.00000	0.00001	0.00001	0.00002	2.55560
D63	-1.65345	0.00000	0.00001	0.00001	0.00002	-1.65343
D64	0.44599	0.00000	0.00001	0.00000	0.00001	0.44600
D65	1.35081	0.00000	-0.00002	0.00003	0.00001	1.35082
D66	-2.85822	0.00000	-0.00001	0.00003	0.00001	-2.85821
D67	-0.75878	0.00000	-0.00002	0.00002	0.00000	-0.75878

D68	-1.03742	0.00000	0.00001	0.00001	0.00002	-1.03740
D69	1.03673	0.00000	0.00001	0.00002	0.00003	1.03676
D70	3.13617	0.00000	0.00001	0.00001	0.00002	3.13619

Item	Value	Threshold	Converged?
Maximum Force	0.000015	0.000450	YES
RMS Force	0.000002	0.000300	YES
Maximum Displacement	0.002033	0.001800	NO
RMS Displacement	0.000396	0.001200	YES

Predicted change in Energy=-3.905885D-09

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.643732	2.100134	-0.195797
2	6	0	-3.535720	1.118474	0.092297
3	7	0	-2.826920	-0.076100	0.111801
4	6	0	-1.534611	0.184407	-0.160078
5	7	0	-1.404091	1.497839	-0.352952
6	6	0	-0.130015	2.182984	-0.635119
7	6	0	0.454967	2.858902	0.609971
8	1	0	-2.782916	3.161231	-0.310574
9	1	0	-4.594037	1.169626	0.271608
10	1	0	0.569678	1.429370	-0.996727
11	1	0	-0.302675	2.916482	-1.423769
12	1	0	-0.225652	3.641541	0.961443
13	1	0	0.533521	2.106075	1.408652
14	35	0	0.137223	-2.666323	-0.215507
15	1	0	-0.758947	-0.604443	-0.215767
16	6	0	-3.301452	-1.400669	0.356682
17	6	0	-4.561123	-1.690622	0.654069
18	1	0	-2.501340	-2.133564	0.268455
19	1	0	-4.832600	-2.723739	0.822458
20	1	0	-5.348597	-0.951832	0.741523
21	7	0	1.721953	3.471989	0.229408
22	1	0	2.064692	4.087188	0.957772
23	1	0	2.419571	2.748955	0.066000
24	6	0	3.332004	-0.426216	-1.137783
25	6	0	3.265528	-0.563819	0.318389
26	8	0	2.734723	0.620854	-0.337027
27	1	0	4.272065	-0.147922	-1.608248
28	1	0	2.629358	-0.989036	-1.744867

29	1	0	2.480296	-1.217422	0.692738
30	6	0	4.462201	-0.353697	1.204621
31	1	0	4.163954	0.078408	2.164505
32	1	0	4.946603	-1.313462	1.408697
33	1	0	5.191203	0.311773	0.735341

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357312	0.000000			
3	N	2.205485	1.389167	0.000000		
4	C	2.213918	2.222748	1.346048	0.000000	
5	N	1.387144	2.210431	2.172032	1.333918	0.000000
6	C	2.553163	3.641585	3.596477	2.488546	1.473876
7	C	3.290430	4.384365	4.430936	3.421157	2.497160
8	H	1.076324	2.214017	3.265064	3.231469	2.160979
9	H	2.210882	1.074618	2.167965	3.243007	3.267041
10	H	3.378967	4.258746	3.877132	2.584172	2.077233
11	H	2.766747	3.997983	4.205394	3.252509	2.091008
12	H	3.092289	4.251803	4.616204	3.863024	2.777015
13	H	3.559386	4.389404	4.211446	3.229689	2.688409
14	Br	5.518443	5.282986	3.950004	3.305263	4.442385
15	H	3.296597	3.282349	2.159389	1.107719	2.203320
16	C	3.604642	2.543789	1.428156	2.429246	3.536228
17	C	4.332261	3.042706	2.430678	3.652170	4.598611
18	H	4.261455	3.417123	2.088948	2.547783	3.844111
19	H	5.394232	4.120393	3.396731	4.505489	5.563990
20	H	4.184418	2.827399	2.742683	4.080492	4.770523
21	N	4.595867	5.762027	5.770183	4.643824	3.742801
22	H	5.239118	6.397414	6.478927	5.425519	4.522740
23	H	5.111413	6.174516	5.958918	4.718429	4.044898
24	C	6.555853	7.145964	6.294155	5.001271	5.171899
25	C	6.502337	7.009864	6.115429	4.881609	5.148443
26	O	5.579963	6.304791	5.623083	4.295231	4.230737
27	H	7.407903	8.090557	7.304746	5.993757	6.041775
28	H	6.304607	6.769413	5.835378	4.607295	4.938693
29	H	6.168576	6.481465	5.459546	4.337268	4.853305
30	C	7.647009	8.208002	7.375812	6.173631	6.345676
31	H	7.483514	8.041191	7.287646	6.155369	6.273396
32	H	8.475861	8.921717	7.977510	6.834530	7.165063
33	H	8.090207	8.787687	8.051679	6.786351	6.788890

		6	7	8	9	10
6	C	0.000000				
7	C	1.532749	0.000000			

8	H	2.846082	3.379748	0.000000		
9	H	4.666534	5.334846	2.754193	0.000000	
10	H	1.090076	2.153648	3.835367	5.323541	0.000000
11	H	1.090779	2.171045	2.729598	4.933720	1.776195
12	H	2.164612	1.095125	2.896261	5.066460	3.059523
13	H	2.150162	1.100368	3.881733	5.334947	2.499017
14	Br	4.874759	5.595577	6.518944	6.110369	4.191899
15	H	2.888107	3.761674	4.276183	4.253560	2.551772
16	C	4.887152	5.684961	4.639508	2.878268	4.982618
17	C	6.025076	6.772095	5.256713	2.885893	6.227728
18	H	5.007217	5.812151	5.333799	3.910301	4.870969
19	H	6.950883	7.692165	6.333865	3.939371	7.052826
20	H	6.241459	6.944088	4.960535	2.300166	6.611930
21	N	2.416345	1.458066	4.547747	6.722677	2.646400
22	H	3.313612	2.054474	5.095626	7.302167	3.622033
23	H	2.704123	2.041485	5.232366	7.192166	2.508545
24	C	4.364192	4.703614	7.137668	8.207023	3.330697
25	C	4.470326	4.438388	7.131288	8.048588	3.601380
26	O	3.276558	3.332109	6.074418	7.374436	2.403398
27	H	5.075275	5.341510	7.899824	9.158469	4.070562
28	H	4.348264	5.007981	6.969550	7.804065	3.263538
29	H	4.487727	4.552496	6.919584	7.478070	3.675630
30	C	5.559483	5.170331	8.194038	9.230735	4.814249
31	H	5.541237	4.889203	7.993048	9.026418	4.973661
32	H	6.494180	6.182344	9.095287	9.923835	5.697952
33	H	5.804735	5.379174	8.532287	9.833711	5.060392

		11	12	13	14	15
11	H	0.000000				
12	H	2.494169	0.000000			
13	H	3.062449	1.770310	0.000000		
14	Br	5.728972	6.426978	5.056751	0.000000	
15	H	3.750249	4.438312	3.414106	2.248215	0.000000
16	C	5.549817	5.937185	5.301973	3.708608	2.725070
17	C	6.608873	6.879153	6.398414	4.876742	4.048820
18	H	5.762006	6.245865	5.337132	2.734971	2.368251
19	H	7.574817	7.858759	7.243341	5.077382	4.707863
20	H	6.716671	6.884185	6.662970	5.826630	4.701273
21	N	2.672209	2.087532	2.160719	6.355170	4.792739
22	H	3.556221	2.333300	2.544127	7.120507	5.600136
23	H	3.107748	2.931848	2.402747	5.883332	4.629001
24	C	4.946343	5.797440	4.552839	4.009401	4.197352
25	C	5.280121	5.503354	3.972514	3.806817	4.059972
26	O	3.959382	4.424296	3.177824	4.191336	3.704293
27	H	5.509342	6.418162	5.306496	5.037756	5.240086

28	H	4.894179	6.075973	4.890494	3.370900	3.737201
29	H	5.414212	5.568113	3.917665	2.900727	3.419623
30	C	6.348744	6.164173	4.639680	5.105922	5.416712
31	H	6.393837	5.780304	4.226439	5.423336	5.510620
32	H	7.312333	7.176651	5.582878	5.253418	5.974520
33	H	6.452050	6.362452	5.036553	5.942716	6.094944

		16	17	18	19	20
16	C	0.000000				
17	C	1.326379	0.000000			
18	H	1.088623	2.141869	0.000000		
19	H	2.076506	1.081382	2.467793	0.000000	
20	H	2.130812	1.083316	3.118839	1.847285	0.000000
21	N	6.999542	8.143091	7.018543	9.038856	8.356143
22	H	7.698920	8.796405	7.747358	9.694311	8.966344
23	H	7.073471	8.293718	6.935081	9.116831	8.631141
24	C	6.869187	8.192125	6.238625	8.705281	8.897241
25	C	6.620197	7.914470	5.976902	8.396369	8.633235
26	O	6.403374	7.717160	5.947250	8.354345	8.305219
27	H	7.923919	9.247876	7.303684	9.769242	9.936037
28	H	6.305590	7.612499	5.629163	8.079677	8.356512
29	H	5.794405	7.057407	5.082915	7.467548	7.833549
30	C	7.879687	9.138428	7.248120	9.599817	9.839918
31	H	7.822288	9.029831	7.274199	9.517936	9.673412
32	H	8.315333	9.545081	7.579220	9.897746	10.323132
33	H	8.671853	9.956106	8.085349	10.473707	10.615277

		21	22	23	24	25
21	N	0.000000				
22	H	1.013140	0.000000			
23	H	1.017914	1.646833	0.000000		
24	C	4.433675	5.135002	3.516154	0.000000	
25	C	4.321838	4.845893	3.428384	1.464169	0.000000
26	O	3.078233	3.760441	2.188737	1.447173	1.454226
27	H	4.794143	5.421542	3.824493	1.087428	2.213147
28	H	4.962045	5.778508	4.158826	1.085831	2.200579
29	H	4.772874	5.327462	4.016047	2.168461	1.088082
30	C	4.805816	5.052766	3.885260	2.601819	1.503857
31	H	4.606990	4.683313	3.818169	3.442658	2.151226
32	H	5.889790	6.138059	4.969100	3.143039	2.139334
33	H	4.720024	4.906965	3.750975	2.740409	2.156092

		26	27	28	29	30
26	O	0.000000				
27	H	2.137859	0.000000			
28	H	2.141229	1.850574	0.000000		
29	H	2.122358	3.106253	2.452815	0.000000	

30	C	2.512092	2.826788	3.530220	2.221710	0.000000
31	H	2.931657	3.781082	4.333315	2.584565	1.094095
32	H	3.417827	3.303853	3.926811	2.569921	1.094277
33	H	2.698110	2.559013	3.795601	3.112759	1.092940

		31	32	33
31	H	0.000000		
32	H	1.766661	0.000000	
33	H	1.775446	1.776127	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.350512	2.471870	-0.262938
2	6	0	-3.337196	1.590271	0.039607
3	7	0	-2.751091	0.331756	0.088650
4	6	0	-1.438038	0.456441	-0.180032
5	7	0	-1.176382	1.745932	-0.399322
6	6	0	0.160901	2.294645	-0.687244
7	6	0	0.804719	2.935405	0.547358
8	1	0	-2.382718	3.538857	-0.400684
9	1	0	-4.385942	1.750351	0.210808
10	1	0	0.783618	1.467563	-1.028457
11	1	0	0.065774	3.024674	-1.492109
12	1	0	0.203921	3.789245	0.877959
13	1	0	0.804239	2.195731	1.362031
14	35	0	-0.058446	-2.547101	-0.165076
15	1	0	-0.744623	-0.406722	-0.214163
16	6	0	-3.356388	-0.933455	0.357890
17	6	0	-4.640016	-1.090138	0.652902
18	1	0	-2.632922	-1.744083	0.290225
19	1	0	-5.013874	-2.087261	0.840948
20	1	0	-5.350315	-0.274920	0.719753
21	7	0	2.128210	3.411037	0.162515
22	1	0	2.527272	4.004474	0.880174
23	1	0	2.751015	2.618818	0.018805
24	6	0	3.347838	-0.656404	-1.112595
25	6	0	3.261408	-0.755569	0.345653

26	8	0	2.854292	0.461792	-0.337766
27	1	0	4.313070	-0.483197	-1.582517
28	1	0	2.595338	-1.159312	-1.712475
29	1	0	2.413257	-1.319602	0.728315
30	6	0	4.469055	-0.646747	1.235221
31	1	0	4.211035	-0.166692	2.183913
32	1	0	4.854453	-1.645391	1.462421
33	1	0	5.262867	-0.067338	0.757032

Rotational constants (GHZ): 0.4225892 0.2920386 0.1827051

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 499 symmetry adapted cartesian basis functions of A symmetry.

There are 482 symmetry adapted basis functions of A symmetry.

482 basis functions, 760 primitive gaussians, 499 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1312.9653576991 Hartrees.

NAtoms= 33 NActive= 33 NUniq= 33 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 482 RedAO= T EigKep= 3.62D-06 NBF= 482

NBsUse= 482 1.00D-06 EigRej= -1.00D+00 NBFU= 482

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2po/nh2po.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000014 0.000000 0.000041 Ang= 0.00 deg.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3205.64837903 A.U. after 7 cycles

NFock= 7 Conv=0.51D-08 -V/T= 2.0018

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000000415	-0.000000512	-0.000002393
2	6	0.000001134	0.000001331	0.000000386
3	7	-0.000000175	0.000000697	-0.000000957

4	6	-0.000000496	-0.000001203	-0.000000726
5	7	0.000001165	0.000005204	-0.000001226
6	6	-0.000000666	-0.000001175	-0.000000916
7	6	-0.000010035	-0.000005077	0.000001693
8	1	0.000000786	0.000000576	-0.000000670
9	1	0.000000007	0.000000962	-0.000001929
10	1	0.000001752	0.000000061	-0.000000410
11	1	0.000001305	-0.000000922	-0.000001180
12	1	0.000002081	0.000000407	-0.000000754
13	1	0.000000754	0.000001033	-0.000001428
14	35	0.000000048	-0.000001117	0.000001102
15	1	-0.000002310	0.000000559	0.000001881
16	6	-0.000001952	-0.000001564	-0.000002400
17	6	0.000000010	0.000002149	-0.000001179
18	1	0.000000893	0.000000576	0.000000735
19	1	-0.000000782	0.000001337	-0.000000156
20	1	-0.000000820	0.000001528	-0.000000972
21	7	0.000007714	0.000005166	-0.000004364
22	1	0.000000862	-0.000000013	0.000000332
23	1	0.000001743	-0.000003000	0.000000750
24	6	-0.000004007	0.000010408	0.000006656
25	6	0.000003846	-0.000010285	0.000013773
26	8	0.000001865	-0.000001703	-0.000006156
27	1	-0.000000097	-0.000003128	-0.000001768
28	1	0.000001387	-0.000001972	0.000000049
29	1	-0.000001417	-0.000000413	-0.000001899
30	6	-0.000003248	0.000002540	-0.000001441
31	1	0.000000069	0.000000194	0.000001580
32	1	-0.000001290	-0.000001026	0.000002307
33	1	0.000000289	-0.000001619	0.000001681

Cartesian Forces: Max 0.000013773 RMS 0.000003075

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000009397 RMS 0.000001359

Search for a local minimum.

Step number 51 out of a maximum of 172

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 31 32 33 34 35

36 37 38 39 40
41 42 43 44 45
46 47 48 49 50
51

DE= -2.49D-08 DEPred=-3.91D-09 R= 6.38D+00
Trust test= 6.38D+00 RLast= 2.10D-03 DXMaxT set to 5.19D-01
ITU= 0 0 0 0 -1 0 0 1 1 1 1 1 1 1 1 1 1 1 1 1
ITU= 1 1 1 1 1 0 0 -1 1 -1 1 1 1 1 1 1 1 1 1 0
ITU= -1 -1 1 1 1 -1 1 0 0 -1 0

Eigenvalues ---	0.00070	0.00094	0.00141	0.00151	0.00277
Eigenvalues ---	0.00411	0.00537	0.00769	0.01191	0.01361
Eigenvalues ---	0.01840	0.01905	0.02174	0.02249	0.02380
Eigenvalues ---	0.02485	0.02678	0.02712	0.03059	0.03100
Eigenvalues ---	0.03328	0.03373	0.03699	0.03929	0.04072
Eigenvalues ---	0.04325	0.04488	0.04734	0.05518	0.05632
Eigenvalues ---	0.05707	0.05754	0.05913	0.07683	0.08527
Eigenvalues ---	0.08978	0.09569	0.09612	0.10692	0.11594
Eigenvalues ---	0.12568	0.13053	0.13412	0.15786	0.15936
Eigenvalues ---	0.15988	0.16002	0.16005	0.16022	0.16151
Eigenvalues ---	0.16290	0.19021	0.21411	0.21669	0.22146
Eigenvalues ---	0.23235	0.23454	0.25491	0.26119	0.27488
Eigenvalues ---	0.29021	0.29925	0.30851	0.31866	0.32970
Eigenvalues ---	0.33676	0.34300	0.34335	0.34411	0.34550
Eigenvalues ---	0.34727	0.34772	0.35108	0.35198	0.35372
Eigenvalues ---	0.35546	0.35684	0.35886	0.36246	0.36423
Eigenvalues ---	0.36626	0.39981	0.41699	0.42043	0.42691
Eigenvalues ---	0.44708	0.45486	0.46492	0.49557	0.54970
Eigenvalues ---	0.58789	0.60696	1.07281		

En-DIIS/RFO-DIIS IScMMF= 0 using points: 51 50 49 48 47
RFO step: Lambda=-6.28858268D-10.
DidBck=F Rises=F RFO-DIIS coefs: 1.79909 -1.05163 0.01004 0.36681 -0.12430
Iteration 1 RMS(Cart)= 0.00016491 RMS(Int)= 0.00000001
Iteration 2 RMS(Cart)= 0.00000003 RMS(Int)= 0.00000001

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56495	0.00000	0.00000	0.00000	0.00000	2.56495
R2	2.62132	0.00000	0.00000	0.00000	0.00000	2.62132
R3	2.03396	0.00000	0.00000	0.00000	0.00000	2.03396
R4	2.62515	0.00000	0.00000	0.00000	0.00000	2.62514
R5	2.03073	0.00000	0.00000	0.00000	0.00000	2.03073
R6	2.54366	0.00000	-0.00001	0.00000	0.00000	2.54366
R7	2.69882	0.00000	0.00000	0.00000	0.00001	2.69883
R8	2.52074	0.00000	0.00000	0.00000	0.00001	2.52075

R9	2.09329	0.00000	-0.00001	0.00000	-0.00001	2.09328
R10	2.78522	0.00000	0.00000	0.00000	0.00000	2.78522
R11	2.89648	0.00000	0.00000	0.00000	0.00000	2.89647
R12	2.05995	0.00000	0.00000	0.00000	0.00000	2.05995
R13	2.06127	0.00000	0.00000	0.00000	0.00000	2.06127
R14	2.06949	0.00000	0.00000	0.00000	0.00000	2.06948
R15	2.07939	0.00000	-0.00001	0.00000	-0.00001	2.07939
R16	2.75535	0.00001	0.00003	0.00000	0.00004	2.75538
R17	4.24851	0.00000	0.00005	0.00002	0.00007	4.24858
R18	2.50649	0.00000	0.00000	0.00000	0.00000	2.50649
R19	2.05720	0.00000	0.00000	0.00000	0.00000	2.05720
R20	2.04352	0.00000	0.00000	0.00000	0.00000	2.04352
R21	2.04717	0.00000	0.00000	0.00000	0.00000	2.04717
R22	1.91456	0.00000	0.00000	0.00000	0.00000	1.91456
R23	1.92358	0.00000	0.00000	0.00000	0.00000	1.92358
R24	4.13611	0.00000	-0.00004	-0.00008	-0.00012	4.13599
R25	2.76688	0.00000	0.00000	0.00001	0.00001	2.76689
R26	2.73476	-0.00001	-0.00002	-0.00001	-0.00004	2.73473
R27	2.05494	0.00000	0.00001	0.00000	0.00000	2.05495
R28	2.05192	0.00000	0.00000	0.00000	0.00000	2.05193
R29	2.74809	0.00000	0.00003	0.00000	0.00003	2.74812
R30	2.05618	0.00000	0.00000	0.00000	0.00000	2.05618
R31	2.84188	0.00000	-0.00001	-0.00001	-0.00001	2.84187
R32	2.06754	0.00000	0.00000	0.00000	0.00000	2.06754
R33	2.06788	0.00000	0.00000	0.00000	0.00000	2.06788
R34	2.06536	0.00000	0.00000	0.00000	0.00000	2.06536
A1	1.87267	0.00000	0.00000	0.00000	0.00000	1.87267
A2	2.27925	0.00000	0.00000	0.00000	0.00000	2.27925
A3	2.13121	0.00000	0.00000	0.00000	0.00000	2.13121
A4	1.86460	0.00000	0.00000	0.00000	0.00000	1.86460
A5	2.27601	0.00000	0.00000	0.00000	0.00000	2.27601
A6	2.14252	0.00000	0.00000	0.00000	0.00000	2.14252
A7	1.89716	0.00000	0.00000	0.00000	0.00000	1.89716
A8	2.25289	0.00000	0.00000	0.00000	0.00001	2.25290
A9	2.13310	0.00000	0.00000	0.00000	0.00000	2.13309
A10	1.88989	0.00000	0.00000	0.00000	0.00000	1.88990
A11	2.14672	0.00000	0.00001	-0.00001	-0.00001	2.14671
A12	2.24646	0.00000	-0.00001	0.00001	0.00000	2.24647
A13	1.90044	0.00000	0.00000	0.00000	-0.00001	1.90043
A14	2.20479	0.00000	0.00000	0.00000	0.00001	2.20480
A15	2.17728	0.00000	0.00000	0.00000	0.00000	2.17728
A16	1.95994	0.00000	0.00002	-0.00001	0.00001	1.95995
A17	1.87234	0.00000	-0.00001	0.00001	0.00000	1.87234
A18	1.89039	0.00000	0.00001	-0.00001	0.00000	1.89039

A19	1.90643	0.00000	-0.00002	0.00001	-0.00001	1.90642
A20	1.92964	0.00000	0.00000	0.00000	0.00000	1.92964
A21	1.90356	0.00000	0.00000	-0.00001	0.00000	1.90355
A22	1.91629	0.00000	0.00002	0.00000	0.00002	1.91631
A23	1.89141	0.00000	0.00001	0.00000	0.00001	1.89142
A24	1.88078	0.00000	-0.00002	0.00001	-0.00001	1.88077
A25	1.87586	0.00000	0.00001	0.00000	0.00001	1.87587
A26	1.90003	0.00000	-0.00001	0.00000	-0.00001	1.90002
A27	1.99883	0.00000	-0.00002	0.00000	-0.00002	1.99882
A28	2.16127	0.00000	0.00000	0.00000	0.00000	2.16126
A29	1.94582	0.00000	0.00000	0.00000	0.00000	1.94582
A30	2.17610	0.00000	0.00000	0.00000	0.00001	2.17611
A31	2.07394	0.00000	0.00000	0.00000	0.00000	2.07394
A32	2.16442	0.00000	0.00000	0.00000	0.00000	2.16442
A33	2.04482	0.00000	0.00000	0.00000	0.00000	2.04482
A34	1.94082	0.00000	-0.00002	0.00000	-0.00002	1.94081
A35	1.91639	0.00000	-0.00002	0.00000	-0.00002	1.91637
A36	1.89112	0.00000	-0.00001	0.00000	-0.00001	1.89111
A37	2.08700	0.00000	0.00001	0.00000	0.00002	2.08701
A38	2.06912	0.00000	0.00001	-0.00001	0.00000	2.06912
A39	1.99437	0.00000	0.00001	0.00001	0.00002	1.99439
A40	2.00128	0.00000	0.00002	0.00000	0.00002	2.00130
A41	2.03776	0.00000	-0.00004	0.00000	-0.00004	2.03772
A42	2.01682	0.00000	-0.00002	0.00001	-0.00001	2.01681
A43	2.13747	0.00000	0.00001	-0.00001	0.00000	2.13747
A44	1.96167	0.00000	-0.00002	0.00000	-0.00002	1.96165
A45	2.02887	0.00000	0.00000	-0.00001	-0.00001	2.02887
A46	2.04366	0.00000	0.00002	0.00001	0.00003	2.04369
A47	2.61554	0.00000	-0.00009	0.00001	-0.00008	2.61546
A48	2.43664	0.00000	0.00000	0.00004	0.00004	2.43668
A49	1.93401	0.00000	0.00001	0.00000	0.00001	1.93402
A50	1.91729	0.00000	-0.00001	0.00000	-0.00001	1.91728
A51	1.94207	0.00000	0.00001	0.00000	0.00000	1.94208
A52	1.87911	0.00000	0.00000	0.00000	0.00000	1.87911
A53	1.89447	0.00000	0.00000	0.00000	0.00000	1.89447
A54	1.89531	0.00000	-0.00001	0.00000	0.00000	1.89530
A55	3.48284	0.00000	-0.00003	-0.00007	-0.00010	3.48274
A56	2.53116	0.00000	0.00000	0.00000	0.00000	2.53115
A57	2.96183	0.00000	-0.00016	-0.00012	-0.00028	2.96155
A58	3.10753	0.00000	-0.00006	0.00005	-0.00001	3.10752
D1	0.00309	0.00000	-0.00001	0.00000	-0.00001	0.00308
D2	-3.12713	0.00000	-0.00001	-0.00001	-0.00002	-3.12716
D3	3.13328	0.00000	0.00003	0.00001	0.00004	3.13332
D4	0.00306	0.00000	0.00003	-0.00001	0.00002	0.00308

D5	-0.00467	0.00000	0.00001	0.00000	0.00000	-0.00467
D6	-3.10818	0.00000	-0.00001	-0.00001	-0.00002	-3.10820
D7	-3.13604	0.00000	-0.00003	-0.00001	-0.00003	-3.13608
D8	0.04363	0.00000	-0.00004	-0.00001	-0.00005	0.04358
D9	-0.00050	0.00000	0.00001	0.00000	0.00001	-0.00049
D10	-3.13338	0.00000	0.00002	-0.00001	0.00001	-3.13337
D11	3.13080	0.00000	0.00001	0.00001	0.00002	3.13082
D12	-0.00209	0.00000	0.00002	0.00000	0.00003	-0.00206
D13	-0.00242	0.00000	0.00000	0.00000	-0.00001	-0.00243
D14	-3.12933	0.00000	-0.00006	-0.00004	-0.00010	-3.12943
D15	3.13119	0.00000	-0.00002	0.00001	-0.00001	3.13118
D16	0.00427	0.00000	-0.00007	-0.00003	-0.00010	0.00417
D17	-0.03467	0.00000	0.00016	0.00010	0.00027	-0.03441
D18	3.10732	0.00000	0.00016	0.00012	0.00028	3.10760
D19	3.11667	0.00000	0.00018	0.00009	0.00027	3.11694
D20	-0.02452	0.00000	0.00018	0.00011	0.00028	-0.02424
D21	0.00437	0.00000	0.00000	0.00000	0.00000	0.00437
D22	3.10862	0.00000	0.00001	0.00001	0.00002	3.10864
D23	3.13018	0.00000	0.00006	0.00004	0.00010	3.13028
D24	-0.04875	0.00000	0.00008	0.00004	0.00012	-0.04863
D25	1.34460	0.00000	-0.00013	0.00000	-0.00013	1.34447
D26	-2.84379	0.00000	-0.00015	0.00001	-0.00014	-2.84393
D27	-0.79132	0.00000	-0.00014	0.00000	-0.00014	-0.79146
D28	-1.75313	0.00000	-0.00015	-0.00001	-0.00016	-1.75329
D29	0.34166	0.00000	-0.00016	0.00000	-0.00016	0.34149
D30	2.39413	0.00000	-0.00016	0.00000	-0.00017	2.39396
D31	-1.09990	0.00000	-0.00005	0.00001	-0.00003	-1.09993
D32	0.94427	0.00000	-0.00001	0.00001	0.00000	0.94427
D33	3.11626	0.00000	-0.00004	0.00002	-0.00003	3.11624
D34	3.10841	0.00000	-0.00004	0.00000	-0.00003	3.10838
D35	-1.13061	0.00000	-0.00001	0.00000	0.00000	-1.13061
D36	1.04139	0.00000	-0.00003	0.00001	-0.00003	1.04136
D37	1.01363	0.00000	-0.00003	0.00001	-0.00002	1.01361
D38	3.05780	0.00000	0.00000	0.00000	0.00001	3.05781
D39	-1.05339	0.00000	-0.00002	0.00001	-0.00001	-1.05341
D40	2.94376	0.00000	-0.00004	-0.00003	-0.00007	2.94369
D41	-1.24662	0.00000	-0.00007	-0.00003	-0.00011	-1.24673
D42	0.86633	0.00000	-0.00006	-0.00003	-0.00009	0.86625
D43	2.95913	0.00000	-0.00009	-0.00003	-0.00012	2.95901
D44	-1.23358	0.00000	-0.00005	-0.00003	-0.00008	-1.23366
D45	0.85922	0.00000	-0.00008	-0.00003	-0.00012	0.85911
D46	3.13974	0.00000	0.00001	0.00003	0.00003	3.13977
D47	-0.00229	0.00000	0.00002	0.00002	0.00003	-0.00226
D48	-0.00231	0.00000	0.00001	0.00001	0.00002	-0.00228

D49	3.13884	0.00000	0.00002	0.00000	0.00002	3.13886
D50	2.20814	0.00000	0.00024	-0.00015	0.00010	2.20824
D51	-1.40772	0.00000	-0.00005	0.00006	0.00000	-1.40772
D52	-2.08617	0.00000	0.00023	-0.00016	0.00007	-2.08610
D53	0.58116	0.00000	-0.00007	0.00004	-0.00002	0.58113
D54	-2.71261	0.00000	0.00000	0.00000	0.00000	-2.71260
D55	-0.01603	0.00000	0.00003	0.00002	0.00005	-0.01599
D56	-0.02641	0.00000	-0.00004	-0.00001	-0.00005	-0.02647
D57	2.67016	0.00000	-0.00001	0.00000	-0.00001	2.67015
D58	0.50713	0.00000	-0.00013	0.00013	-0.00001	0.50712
D59	-1.91238	0.00000	-0.00010	0.00011	0.00001	-1.91237
D60	1.78372	0.00000	0.00018	-0.00007	0.00011	1.78383
D61	-0.63876	0.00000	0.00017	-0.00008	0.00009	-0.63866
D62	2.55560	0.00000	-0.00004	-0.00003	-0.00008	2.55553
D63	-1.65343	0.00000	-0.00004	-0.00004	-0.00008	-1.65350
D64	0.44600	0.00000	-0.00005	-0.00003	-0.00009	0.44591
D65	1.35082	0.00000	-0.00002	-0.00002	-0.00004	1.35078
D66	-2.85821	0.00000	-0.00002	-0.00002	-0.00005	-2.85825
D67	-0.75878	0.00000	-0.00003	-0.00002	-0.00005	-0.75883
D68	-1.03740	0.00000	-0.00002	-0.00002	-0.00004	-1.03744
D69	1.03676	0.00000	-0.00002	-0.00002	-0.00004	1.03672
D70	3.13619	0.00000	-0.00003	-0.00002	-0.00005	3.13614

Item	Value	Threshold	Converged?
Maximum Force	0.000009	0.000450	YES
RMS Force	0.000001	0.000300	YES
Maximum Displacement	0.000851	0.001800	YES
RMS Displacement	0.000165	0.001200	YES

Predicted change in Energy=-1.191704D-09

Optimization completed.

-- Stationary point found.

! Optimized Parameters !

! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.	
! R1	R(1,2)	1.3573	-DE/DX =	0.0 !
! R2	R(1,5)	1.3871	-DE/DX =	0.0 !
! R3	R(1,8)	1.0763	-DE/DX =	0.0 !
! R4	R(2,3)	1.3892	-DE/DX =	0.0 !
! R5	R(2,9)	1.0746	-DE/DX =	0.0 !
! R6	R(3,4)	1.346	-DE/DX =	0.0 !
! R7	R(3,16)	1.4282	-DE/DX =	0.0 !
! R8	R(4,5)	1.3339	-DE/DX =	0.0 !

! R9	R(4,15)	1.1077	-DE/DX =	0.0	!
! R10	R(5,6)	1.4739	-DE/DX =	0.0	!
! R11	R(6,7)	1.5327	-DE/DX =	0.0	!
! R12	R(6,10)	1.0901	-DE/DX =	0.0	!
! R13	R(6,11)	1.0908	-DE/DX =	0.0	!
! R14	R(7,12)	1.0951	-DE/DX =	0.0	!
! R15	R(7,13)	1.1004	-DE/DX =	0.0	!
! R16	R(7,21)	1.4581	-DE/DX =	0.0	!
! R17	R(14,15)	2.2482	-DE/DX =	0.0	!
! R18	R(16,17)	1.3264	-DE/DX =	0.0	!
! R19	R(16,18)	1.0886	-DE/DX =	0.0	!
! R20	R(17,19)	1.0814	-DE/DX =	0.0	!
! R21	R(17,20)	1.0833	-DE/DX =	0.0	!
! R22	R(21,22)	1.0131	-DE/DX =	0.0	!
! R23	R(21,23)	1.0179	-DE/DX =	0.0	!
! R24	R(23,26)	2.1887	-DE/DX =	0.0	!
! R25	R(24,25)	1.4642	-DE/DX =	0.0	!
! R26	R(24,26)	1.4472	-DE/DX =	0.0	!
! R27	R(24,27)	1.0874	-DE/DX =	0.0	!
! R28	R(24,28)	1.0858	-DE/DX =	0.0	!
! R29	R(25,26)	1.4542	-DE/DX =	0.0	!
! R30	R(25,29)	1.0881	-DE/DX =	0.0	!
! R31	R(25,30)	1.5039	-DE/DX =	0.0	!
! R32	R(30,31)	1.0941	-DE/DX =	0.0	!
! R33	R(30,32)	1.0943	-DE/DX =	0.0	!
! R34	R(30,33)	1.0929	-DE/DX =	0.0	!
! A1	A(2,1,5)	107.2961	-DE/DX =	0.0	!
! A2	A(2,1,8)	130.5913	-DE/DX =	0.0	!
! A3	A(5,1,8)	122.1094	-DE/DX =	0.0	!
! A4	A(1,2,3)	106.8338	-DE/DX =	0.0	!
! A5	A(1,2,9)	130.4056	-DE/DX =	0.0	!
! A6	A(3,2,9)	122.7574	-DE/DX =	0.0	!
! A7	A(2,3,4)	108.6994	-DE/DX =	0.0	!
! A8	A(2,3,16)	129.0813	-DE/DX =	0.0	!
! A9	A(4,3,16)	122.2175	-DE/DX =	0.0	!
! A10	A(3,4,5)	108.2829	-DE/DX =	0.0	!
! A11	A(3,4,15)	122.998	-DE/DX =	0.0	!
! A12	A(5,4,15)	128.7128	-DE/DX =	0.0	!
! A13	A(1,5,4)	108.8871	-DE/DX =	0.0	!
! A14	A(1,5,6)	126.3252	-DE/DX =	0.0	!
! A15	A(4,5,6)	124.7491	-DE/DX =	0.0	!
! A16	A(5,6,7)	112.2964	-DE/DX =	0.0	!
! A17	A(5,6,10)	107.2771	-DE/DX =	0.0	!
! A18	A(5,6,11)	108.3114	-DE/DX =	0.0	!

! A19	A(7,6,10)	109.2302	-DE/DX =	0.0	!
! A20	A(7,6,11)	110.5604	-DE/DX =	0.0	!
! A21	A(10,6,11)	109.0658	-DE/DX =	0.0	!
! A22	A(6,7,12)	109.7954	-DE/DX =	0.0	!
! A23	A(6,7,13)	108.3701	-DE/DX =	0.0	!
! A24	A(6,7,21)	107.7607	-DE/DX =	0.0	!
! A25	A(12,7,13)	107.4791	-DE/DX =	0.0	!
! A26	A(12,7,21)	108.8638	-DE/DX =	0.0	!
! A27	A(13,7,21)	114.5248	-DE/DX =	0.0	!
! A28	A(3,16,17)	123.8314	-DE/DX =	0.0	!
! A29	A(3,16,18)	111.4873	-DE/DX =	0.0	!
! A30	A(17,16,18)	124.6813	-DE/DX =	0.0	!
! A31	A(16,17,19)	118.828	-DE/DX =	0.0	!
! A32	A(16,17,20)	124.0122	-DE/DX =	0.0	!
! A33	A(19,17,20)	117.1598	-DE/DX =	0.0	!
! A34	A(7,21,22)	111.2011	-DE/DX =	0.0	!
! A35	A(7,21,23)	109.8011	-DE/DX =	0.0	!
! A36	A(22,21,23)	108.3534	-DE/DX =	0.0	!
! A37	A(25,24,27)	119.576	-DE/DX =	0.0	!
! A38	A(25,24,28)	118.5516	-DE/DX =	0.0	!
! A39	A(26,24,27)	114.2688	-DE/DX =	0.0	!
! A40	A(26,24,28)	114.6651	-DE/DX =	0.0	!
! A41	A(27,24,28)	116.7548	-DE/DX =	0.0	!
! A42	A(24,25,29)	115.5555	-DE/DX =	0.0	!
! A43	A(24,25,30)	122.468	-DE/DX =	0.0	!
! A44	A(26,25,29)	112.3953	-DE/DX =	0.0	!
! A45	A(26,25,30)	116.246	-DE/DX =	0.0	!
! A46	A(29,25,30)	117.0931	-DE/DX =	0.0	!
! A47	A(23,26,24)	149.8596	-DE/DX =	0.0	!
! A48	A(23,26,25)	139.609	-DE/DX =	0.0	!
! A49	A(25,30,31)	110.8108	-DE/DX =	0.0	!
! A50	A(25,30,32)	109.8526	-DE/DX =	0.0	!
! A51	A(25,30,33)	111.2726	-DE/DX =	0.0	!
! A52	A(31,30,32)	107.6649	-DE/DX =	0.0	!
! A53	A(31,30,33)	108.5454	-DE/DX =	0.0	!
! A54	A(32,30,33)	108.5932	-DE/DX =	0.0	!
! A55	L(4,15,14,7,-1)	199.5523	-DE/DX =	0.0	!
! A56	L(21,23,26,3,-1)	145.0246	-DE/DX =	0.0	!
! A57	L(4,15,14,7,-2)	169.7002	-DE/DX =	0.0	!
! A58	L(21,23,26,3,-2)	178.0485	-DE/DX =	0.0	!
! D1	D(5,1,2,3)	0.177	-DE/DX =	0.0	!
! D2	D(5,1,2,9)	-179.1715	-DE/DX =	0.0	!
! D3	D(8,1,2,3)	179.5238	-DE/DX =	0.0	!
! D4	D(8,1,2,9)	0.1753	-DE/DX =	0.0	!

! D5	D(2,1,5,4)	-0.2675	-DE/DX =	0.0	!
! D6	D(2,1,5,6)	-178.0855	-DE/DX =	0.0	!
! D7	D(8,1,5,4)	-179.6819	-DE/DX =	0.0	!
! D8	D(8,1,5,6)	2.5001	-DE/DX =	0.0	!
! D9	D(1,2,3,4)	-0.0284	-DE/DX =	0.0	!
! D10	D(1,2,3,16)	-179.5296	-DE/DX =	0.0	!
! D11	D(9,2,3,4)	179.3817	-DE/DX =	0.0	!
! D12	D(9,2,3,16)	-0.1195	-DE/DX =	0.0	!
! D13	D(2,3,4,5)	-0.1385	-DE/DX =	0.0	!
! D14	D(2,3,4,15)	-179.2975	-DE/DX =	0.0	!
! D15	D(16,3,4,5)	179.4038	-DE/DX =	0.0	!
! D16	D(16,3,4,15)	0.2449	-DE/DX =	0.0	!
! D17	D(2,3,16,17)	-1.9866	-DE/DX =	0.0	!
! D18	D(2,3,16,18)	178.0364	-DE/DX =	0.0	!
! D19	D(4,3,16,17)	178.5718	-DE/DX =	0.0	!
! D20	D(4,3,16,18)	-1.4052	-DE/DX =	0.0	!
! D21	D(3,4,5,1)	0.2503	-DE/DX =	0.0	!
! D22	D(3,4,5,6)	178.1108	-DE/DX =	0.0	!
! D23	D(15,4,5,1)	179.3463	-DE/DX =	0.0	!
! D24	D(15,4,5,6)	-2.7933	-DE/DX =	0.0	!
! D25	D(1,5,6,7)	77.0402	-DE/DX =	0.0	!
! D26	D(1,5,6,10)	-162.9374	-DE/DX =	0.0	!
! D27	D(1,5,6,11)	-45.3393	-DE/DX =	0.0	!
! D28	D(4,5,6,7)	-100.447	-DE/DX =	0.0	!
! D29	D(4,5,6,10)	19.5755	-DE/DX =	0.0	!
! D30	D(4,5,6,11)	137.1735	-DE/DX =	0.0	!
! D31	D(5,6,7,12)	-63.0194	-DE/DX =	0.0	!
! D32	D(5,6,7,13)	54.1026	-DE/DX =	0.0	!
! D33	D(5,6,7,21)	178.5488	-DE/DX =	0.0	!
! D34	D(10,6,7,12)	178.099	-DE/DX =	0.0	!
! D35	D(10,6,7,13)	-64.7789	-DE/DX =	0.0	!
! D36	D(10,6,7,21)	59.6672	-DE/DX =	0.0	!
! D37	D(11,6,7,12)	58.0769	-DE/DX =	0.0	!
! D38	D(11,6,7,13)	175.199	-DE/DX =	0.0	!
! D39	D(11,6,7,21)	-60.3549	-DE/DX =	0.0	!
! D40	D(6,7,21,22)	168.6652	-DE/DX =	0.0	!
! D41	D(6,7,21,23)	-71.4262	-DE/DX =	0.0	!
! D42	D(12,7,21,22)	49.6372	-DE/DX =	0.0	!
! D43	D(12,7,21,23)	169.5459	-DE/DX =	0.0	!
! D44	D(13,7,21,22)	-70.6788	-DE/DX =	0.0	!
! D45	D(13,7,21,23)	49.2298	-DE/DX =	0.0	!
! D46	D(3,16,17,19)	179.8938	-DE/DX =	0.0	!
! D47	D(3,16,17,20)	-0.1315	-DE/DX =	0.0	!
! D48	D(18,16,17,19)	-0.1322	-DE/DX =	0.0	!

! D49	D(18,16,17,20)	179.8425	-DE/DX =	0.0 !
! D50	D(7,21,26,24)	126.5172	-DE/DX =	0.0 !
! D51	D(7,21,26,25)	-80.6563	-DE/DX =	0.0 !
! D52	D(22,21,26,24)	-119.5285	-DE/DX =	0.0 !
! D53	D(22,21,26,25)	33.2979	-DE/DX =	0.0 !
! D54	D(27,24,25,29)	-155.4209	-DE/DX =	0.0 !
! D55	D(27,24,25,30)	-0.9186	-DE/DX =	0.0 !
! D56	D(28,24,25,29)	-1.5134	-DE/DX =	0.0 !
! D57	D(28,24,25,30)	152.9889	-DE/DX =	0.0 !
! D58	D(27,24,26,23)	29.0562	-DE/DX =	0.0 !
! D59	D(28,24,26,23)	-109.5714	-DE/DX =	0.0 !
! D60	D(29,25,26,23)	102.1997	-DE/DX =	0.0 !
! D61	D(30,25,26,23)	-36.598	-DE/DX =	0.0 !
! D62	D(24,25,30,31)	146.4252	-DE/DX =	0.0 !
! D63	D(24,25,30,32)	-94.7344	-DE/DX =	0.0 !
! D64	D(24,25,30,33)	25.5539	-DE/DX =	0.0 !
! D65	D(26,25,30,31)	77.3963	-DE/DX =	0.0 !
! D66	D(26,25,30,32)	-163.7633	-DE/DX =	0.0 !
! D67	D(26,25,30,33)	-43.4749	-DE/DX =	0.0 !
! D68	D(29,25,30,31)	-59.4384	-DE/DX =	0.0 !
! D69	D(29,25,30,32)	59.402	-DE/DX =	0.0 !
! D70	D(29,25,30,33)	179.6904	-DE/DX =	0.0 !

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.643732	2.100134	-0.195797
2	6	0	-3.535720	1.118474	0.092297
3	7	0	-2.826920	-0.076100	0.111801
4	6	0	-1.534611	0.184407	-0.160078
5	7	0	-1.404091	1.497839	-0.352952
6	6	0	-0.130015	2.182984	-0.635119
7	6	0	0.454967	2.858902	0.609971
8	1	0	-2.782916	3.161231	-0.310574
9	1	0	-4.594037	1.169626	0.271608
10	1	0	0.569678	1.429370	-0.996727
11	1	0	-0.302675	2.916482	-1.423769
12	1	0	-0.225652	3.641541	0.961443
13	1	0	0.533521	2.106075	1.408652
14	35	0	0.137223	-2.666323	-0.215507

15	1	0	-0.758947	-0.604443	-0.215767
16	6	0	-3.301452	-1.400669	0.356682
17	6	0	-4.561123	-1.690622	0.654069
18	1	0	-2.501340	-2.133564	0.268455
19	1	0	-4.832600	-2.723739	0.822458
20	1	0	-5.348597	-0.951832	0.741523
21	7	0	1.721953	3.471989	0.229408
22	1	0	2.064692	4.087188	0.957772
23	1	0	2.419571	2.748955	0.066000
24	6	0	3.332004	-0.426216	-1.137783
25	6	0	3.265528	-0.563819	0.318389
26	8	0	2.734723	0.620854	-0.337027
27	1	0	4.272065	-0.147922	-1.608248
28	1	0	2.629358	-0.989036	-1.744867
29	1	0	2.480296	-1.217422	0.692738
30	6	0	4.462201	-0.353697	1.204621
31	1	0	4.163954	0.078408	2.164505
32	1	0	4.946603	-1.313462	1.408697
33	1	0	5.191203	0.311773	0.735341

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357312	0.000000			
3	N	2.205485	1.389167	0.000000		
4	C	2.213918	2.222748	1.346048	0.000000	
5	N	1.387144	2.210431	2.172032	1.333918	0.000000
6	C	2.553163	3.641585	3.596477	2.488546	1.473876
7	C	3.290430	4.384365	4.430936	3.421157	2.497160
8	H	1.076324	2.214017	3.265064	3.231469	2.160979
9	H	2.210882	1.074618	2.167965	3.243007	3.267041
10	H	3.378967	4.258746	3.877132	2.584172	2.077233
11	H	2.766747	3.997983	4.205394	3.252509	2.091008
12	H	3.092289	4.251803	4.616204	3.863024	2.777015
13	H	3.559386	4.389404	4.211446	3.229689	2.688409
14	Br	5.518443	5.282986	3.950004	3.305263	4.442385
15	H	3.296597	3.282349	2.159389	1.107719	2.203320
16	C	3.604642	2.543789	1.428156	2.429246	3.536228
17	C	4.332261	3.042706	2.430678	3.652170	4.598611
18	H	4.261455	3.417123	2.088948	2.547783	3.844111
19	H	5.394232	4.120393	3.396731	4.505489	5.563990
20	H	4.184418	2.827399	2.742683	4.080492	4.770523
21	N	4.595867	5.762027	5.770183	4.643824	3.742801
22	H	5.239118	6.397414	6.478927	5.425519	4.522740

23	H	5.111413	6.174516	5.958918	4.718429	4.044898
24	C	6.555853	7.145964	6.294155	5.001271	5.171899
25	C	6.502337	7.009864	6.115429	4.881609	5.148443
26	O	5.579963	6.304791	5.623083	4.295231	4.230737
27	H	7.407903	8.090557	7.304746	5.993757	6.041775
28	H	6.304607	6.769413	5.835378	4.607295	4.938693
29	H	6.168576	6.481465	5.459546	4.337268	4.853305
30	C	7.647009	8.208002	7.375812	6.173631	6.345676
31	H	7.483514	8.041191	7.287646	6.155369	6.273396
32	H	8.475861	8.921717	7.977510	6.834530	7.165063
33	H	8.090207	8.787687	8.051679	6.786351	6.788890

		6	7	8	9	10
6	C	0.000000				
7	C	1.532749	0.000000			
8	H	2.846082	3.379748	0.000000		
9	H	4.666534	5.334846	2.754193	0.000000	
10	H	1.090076	2.153648	3.835367	5.323541	0.000000
11	H	1.090779	2.171045	2.729598	4.933720	1.776195
12	H	2.164612	1.095125	2.896261	5.066460	3.059523
13	H	2.150162	1.100368	3.881733	5.334947	2.499017
14	Br	4.874759	5.595577	6.518944	6.110369	4.191899
15	H	2.888107	3.761674	4.276183	4.253560	2.551772
16	C	4.887152	5.684961	4.639508	2.878268	4.982618
17	C	6.025076	6.772095	5.256713	2.885893	6.227728
18	H	5.007217	5.812151	5.333799	3.910301	4.870969
19	H	6.950883	7.692165	6.333865	3.939371	7.052826
20	H	6.241459	6.944088	4.960535	2.300166	6.611930
21	N	2.416345	1.458066	4.547747	6.722677	2.646400
22	H	3.313612	2.054474	5.095626	7.302167	3.622033
23	H	2.704123	2.041485	5.232366	7.192166	2.508545
24	C	4.364192	4.703614	7.137668	8.207023	3.330697
25	C	4.470326	4.438388	7.131288	8.048588	3.601380
26	O	3.276558	3.332109	6.074418	7.374436	2.403398
27	H	5.075275	5.341510	7.899824	9.158469	4.070562
28	H	4.348264	5.007981	6.969550	7.804065	3.263538
29	H	4.487727	4.552496	6.919584	7.478070	3.675630
30	C	5.559483	5.170331	8.194038	9.230735	4.814249
31	H	5.541237	4.889203	7.993048	9.026418	4.973661
32	H	6.494180	6.182344	9.095287	9.923835	5.697952
33	H	5.804735	5.379174	8.532287	9.833711	5.060392

		11	12	13	14	15
11	H	0.000000				
12	H	2.494169	0.000000			
13	H	3.062449	1.770310	0.000000		

14	Br	5.728972	6.426978	5.056751	0.000000	
15	H	3.750249	4.438312	3.414106	2.248215	0.000000
16	C	5.549817	5.937185	5.301973	3.708608	2.725070
17	C	6.608873	6.879153	6.398414	4.876742	4.048820
18	H	5.762006	6.245865	5.337132	2.734971	2.368251
19	H	7.574817	7.858759	7.243341	5.077382	4.707863
20	H	6.716671	6.884185	6.662970	5.826630	4.701273
21	N	2.672209	2.087532	2.160719	6.355170	4.792739
22	H	3.556221	2.333300	2.544127	7.120507	5.600136
23	H	3.107748	2.931848	2.402747	5.883332	4.629001
24	C	4.946343	5.797440	4.552839	4.009401	4.197352
25	C	5.280121	5.503354	3.972514	3.806817	4.059972
26	O	3.959382	4.424296	3.177824	4.191336	3.704293
27	H	5.509342	6.418162	5.306496	5.037756	5.240086
28	H	4.894179	6.075973	4.890494	3.370900	3.737201
29	H	5.414212	5.568113	3.917665	2.900727	3.419623
30	C	6.348744	6.164173	4.639680	5.105922	5.416712
31	H	6.393837	5.780304	4.226439	5.423336	5.510620
32	H	7.312333	7.176651	5.582878	5.253418	5.974520
33	H	6.452050	6.362452	5.036553	5.942716	6.094944

		16	17	18	19	20
16	C	0.000000				
17	C	1.326379	0.000000			
18	H	1.088623	2.141869	0.000000		
19	H	2.076506	1.081382	2.467793	0.000000	
20	H	2.130812	1.083316	3.118839	1.847285	0.000000
21	N	6.999542	8.143091	7.018543	9.038856	8.356143
22	H	7.698920	8.796405	7.747358	9.694311	8.966344
23	H	7.073471	8.293718	6.935081	9.116831	8.631141
24	C	6.869187	8.192125	6.238625	8.705281	8.897241
25	C	6.620197	7.914470	5.976902	8.396369	8.633235
26	O	6.403374	7.717160	5.947250	8.354345	8.305219
27	H	7.923919	9.247876	7.303684	9.769242	9.936037
28	H	6.305590	7.612499	5.629163	8.079677	8.356512
29	H	5.794405	7.057407	5.082915	7.467548	7.833549
30	C	7.879687	9.138428	7.248120	9.599817	9.839918
31	H	7.822288	9.029831	7.274199	9.517936	9.673412
32	H	8.315333	9.545081	7.579220	9.897746	10.323132
33	H	8.671853	9.956106	8.085349	10.473707	10.615277

		21	22	23	24	25
21	N	0.000000				
22	H	1.013140	0.000000			
23	H	1.017914	1.646833	0.000000		
24	C	4.433675	5.135002	3.516154	0.000000	

25	C	4.321838	4.845893	3.428384	1.464169	0.000000
26	O	3.078233	3.760441	2.188737	1.447173	1.454226
27	H	4.794143	5.421542	3.824493	1.087428	2.213147
28	H	4.962045	5.778508	4.158826	1.085831	2.200579
29	H	4.772874	5.327462	4.016047	2.168461	1.088082
30	C	4.805816	5.052766	3.885260	2.601819	1.503857
31	H	4.606990	4.683313	3.818169	3.442658	2.151226
32	H	5.889790	6.138059	4.969100	3.143039	2.139334
33	H	4.720024	4.906965	3.750975	2.740409	2.156092

		26	27	28	29	30
26	O	0.000000				
27	H	2.137859	0.000000			
28	H	2.141229	1.850574	0.000000		
29	H	2.122358	3.106253	2.452815	0.000000	
30	C	2.512092	2.826788	3.530220	2.221710	0.000000
31	H	2.931657	3.781082	4.333315	2.584565	1.094095
32	H	3.417827	3.303853	3.926811	2.569921	1.094277
33	H	2.698110	2.559013	3.795601	3.112759	1.092940

		31	32	33
31	H	0.000000		
32	H	1.766661	0.000000	
33	H	1.775446	1.776127	0.000000

Stoichiometry C10H18BrN3O
Framework group C1[X(C10H18BrN3O)]
Deg. of freedom 93
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.350512	2.471870	-0.262938
2	6	0	-3.337196	1.590271	0.039607
3	7	0	-2.751091	0.331756	0.088650
4	6	0	-1.438038	0.456441	-0.180032
5	7	0	-1.176382	1.745932	-0.399322
6	6	0	0.160901	2.294645	-0.687244
7	6	0	0.804719	2.935405	0.547358
8	1	0	-2.382718	3.538857	-0.400684
9	1	0	-4.385942	1.750351	0.210808
10	1	0	0.783618	1.467563	-1.028457
11	1	0	0.065774	3.024674	-1.492109

12	1	0	0.203921	3.789245	0.877959
13	1	0	0.804239	2.195731	1.362031
14	35	0	-0.058446	-2.547101	-0.165076
15	1	0	-0.744623	-0.406722	-0.214163
16	6	0	-3.356388	-0.933455	0.357890
17	6	0	-4.640016	-1.090138	0.652902
18	1	0	-2.632922	-1.744083	0.290225
19	1	0	-5.013874	-2.087261	0.840948
20	1	0	-5.350315	-0.274920	0.719753
21	7	0	2.128210	3.411037	0.162515
22	1	0	2.527272	4.004474	0.880174
23	1	0	2.751015	2.618818	0.018805
24	6	0	3.347838	-0.656404	-1.112595
25	6	0	3.261408	-0.755569	0.345653
26	8	0	2.854292	0.461792	-0.337766
27	1	0	4.313070	-0.483197	-1.582517
28	1	0	2.595338	-1.159312	-1.712475
29	1	0	2.413257	-1.319602	0.728315
30	6	0	4.469055	-0.646747	1.235221
31	1	0	4.211035	-0.166692	2.183913
32	1	0	4.854453	-1.645391	1.462421
33	1	0	5.262867	-0.067338	0.757032

Rotational constants (GHZ): 0.4225892 0.2920386 0.1827051

****

Population analysis using the SCF density.

****

Orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A)

The electronic state is 1-A.

Alpha occ. eigenvalues -- -482.69206 -62.34546 -56.16322 -56.16316 -56.16311
Alpha occ. eigenvalues -- -19.13089 -14.44359 -14.43854 -14.30468 -10.29053
Alpha occ. eigenvalues -- -10.26756 -10.26653 -10.24700 -10.24396 -10.22275
Alpha occ. eigenvalues -- -10.21501 -10.21034 -10.20378 -10.16394 -8.55458
Alpha occ. eigenvalues -- -6.37776 -6.37738 -6.37710 -2.49022 -2.49010
Alpha occ. eigenvalues -- -2.48986 -2.48957 -2.48954 -1.11023 -1.06171
Alpha occ. eigenvalues -- -0.99546 -0.90293 -0.84486 -0.81501 -0.77289
Alpha occ. eigenvalues -- -0.74277 -0.70338 -0.68061 -0.65917 -0.64782
Alpha occ. eigenvalues -- -0.62983 -0.62526 -0.58794 -0.57523 -0.53595
Alpha occ. eigenvalues -- -0.53235 -0.51714 -0.50743 -0.49932 -0.49863
Alpha occ. eigenvalues -- -0.48991 -0.46914 -0.46458 -0.45526 -0.44483
Alpha occ. eigenvalues -- -0.43382 -0.42258 -0.41752 -0.40308 -0.38521
Alpha occ. eigenvalues -- -0.37556 -0.37024 -0.35994 -0.31177 -0.30329
Alpha occ. eigenvalues -- -0.28999 -0.27406 -0.25909 -0.19584 -0.19275

Alpha occ. eigenvalues --	-0.18951				
Alpha virt. eigenvalues --	-0.07253	-0.04265	-0.02812	-0.01540	-0.00618
Alpha virt. eigenvalues --	0.00386	0.00544	0.00687	0.00986	0.01665
Alpha virt. eigenvalues --	0.02265	0.02715	0.03462	0.03717	0.04405
Alpha virt. eigenvalues --	0.04878	0.05060	0.05485	0.05666	0.06186
Alpha virt. eigenvalues --	0.06688	0.07035	0.07339	0.07737	0.08270
Alpha virt. eigenvalues --	0.08428	0.08663	0.09078	0.09142	0.09655
Alpha virt. eigenvalues --	0.09957	0.10111	0.10539	0.10865	0.11188
Alpha virt. eigenvalues --	0.11543	0.11745	0.12116	0.12275	0.12506
Alpha virt. eigenvalues --	0.13023	0.13052	0.13360	0.13542	0.13946
Alpha virt. eigenvalues --	0.14594	0.14684	0.14812	0.15282	0.15633
Alpha virt. eigenvalues --	0.15995	0.16026	0.16272	0.16371	0.16767
Alpha virt. eigenvalues --	0.17035	0.17431	0.17813	0.18140	0.18545
Alpha virt. eigenvalues --	0.18762	0.19136	0.19503	0.20066	0.20191
Alpha virt. eigenvalues --	0.20434	0.20727	0.20793	0.21351	0.21671
Alpha virt. eigenvalues --	0.21896	0.22308	0.22535	0.22864	0.22973
Alpha virt. eigenvalues --	0.23802	0.24146	0.24509	0.24947	0.24960
Alpha virt. eigenvalues --	0.25475	0.26001	0.26311	0.26815	0.27221
Alpha virt. eigenvalues --	0.27570	0.28057	0.28388	0.28993	0.29372
Alpha virt. eigenvalues --	0.30018	0.30216	0.30415	0.31004	0.31992
Alpha virt. eigenvalues --	0.33085	0.33821	0.34477	0.34567	0.34631
Alpha virt. eigenvalues --	0.35632	0.35787	0.36595	0.37215	0.38514
Alpha virt. eigenvalues --	0.38755	0.39305	0.40577	0.41697	0.42255
Alpha virt. eigenvalues --	0.43270	0.44203	0.45178	0.47466	0.47940
Alpha virt. eigenvalues --	0.48734	0.50204	0.50883	0.51448	0.52254
Alpha virt. eigenvalues --	0.53324	0.53614	0.54737	0.55793	0.56020
Alpha virt. eigenvalues --	0.56629	0.57149	0.57462	0.58034	0.58722
Alpha virt. eigenvalues --	0.59183	0.60343	0.60897	0.61614	0.62311
Alpha virt. eigenvalues --	0.63047	0.63252	0.63750	0.64287	0.64863
Alpha virt. eigenvalues --	0.66290	0.66461	0.66837	0.67501	0.68668
Alpha virt. eigenvalues --	0.69344	0.69704	0.70020	0.70535	0.71067
Alpha virt. eigenvalues --	0.71417	0.72182	0.73010	0.74092	0.74649
Alpha virt. eigenvalues --	0.74815	0.75459	0.75943	0.76978	0.77035
Alpha virt. eigenvalues --	0.77937	0.78614	0.79184	0.79323	0.80388
Alpha virt. eigenvalues --	0.81671	0.82492	0.84321	0.85149	0.86497
Alpha virt. eigenvalues --	0.87282	0.88181	0.89128	0.90265	0.91622
Alpha virt. eigenvalues --	0.92287	0.93669	0.94919	0.95753	0.97054
Alpha virt. eigenvalues --	0.97483	0.99474	1.01456	1.01968	1.02546
Alpha virt. eigenvalues --	1.04253	1.04893	1.05425	1.06317	1.07956
Alpha virt. eigenvalues --	1.10891	1.11433	1.11898	1.12390	1.14143
Alpha virt. eigenvalues --	1.15721	1.17186	1.19284	1.19973	1.21048
Alpha virt. eigenvalues --	1.23370	1.25953	1.27722	1.29666	1.30543
Alpha virt. eigenvalues --	1.32464	1.33330	1.37739	1.39154	1.40271
Alpha virt. eigenvalues --	1.42669	1.43699	1.46111	1.46659	1.47824

Alpha virt. eigenvalues --	1.49443	1.50303	1.50421	1.52481	1.53292	
Alpha virt. eigenvalues --	1.54628	1.54782	1.55945	1.57311	1.59018	
Alpha virt. eigenvalues --	1.59114	1.59789	1.60274	1.60586	1.61172	
Alpha virt. eigenvalues --	1.62206	1.63520	1.65967	1.67347	1.67557	
Alpha virt. eigenvalues --	1.67849	1.69390	1.69875	1.70945	1.71415	
Alpha virt. eigenvalues --	1.72281	1.72836	1.73581	1.74640	1.75329	
Alpha virt. eigenvalues --	1.75592	1.77553	1.79412	1.80099	1.81031	
Alpha virt. eigenvalues --	1.81742	1.83727	1.85945	1.86307	1.88313	
Alpha virt. eigenvalues --	1.89637	1.90358	1.92349	1.93015	1.95489	
Alpha virt. eigenvalues --	1.97463	1.99010	2.00882	2.03034	2.05012	
Alpha virt. eigenvalues --	2.05207	2.06100	2.08019	2.08800	2.09334	
Alpha virt. eigenvalues --	2.10765	2.11973	2.12869	2.13156	2.14933	
Alpha virt. eigenvalues --	2.17433	2.19265	2.19846	2.21351	2.21565	
Alpha virt. eigenvalues --	2.23549	2.26971	2.28763	2.28949	2.31126	
Alpha virt. eigenvalues --	2.33819	2.35298	2.37746	2.40916	2.42198	
Alpha virt. eigenvalues --	2.43644	2.47115	2.47702	2.48152	2.48253	
Alpha virt. eigenvalues --	2.50504	2.52300	2.52817	2.53865	2.55233	
Alpha virt. eigenvalues --	2.55652	2.56571	2.57517	2.58687	2.59452	
Alpha virt. eigenvalues --	2.61173	2.61470	2.62659	2.63582	2.65575	
Alpha virt. eigenvalues --	2.66446	2.67344	2.69516	2.71096	2.72319	
Alpha virt. eigenvalues --	2.72957	2.73225	2.75003	2.76658	2.77013	
Alpha virt. eigenvalues --	2.77331	2.78519	2.79418	2.80453	2.81351	
Alpha virt. eigenvalues --	2.82593	2.82969	2.83433	2.85098	2.86270	
Alpha virt. eigenvalues --	2.87593	2.88158	2.89541	2.92799	2.93624	
Alpha virt. eigenvalues --	2.95073	2.96529	2.98449	3.02974	3.09241	
Alpha virt. eigenvalues --	3.10497	3.15016	3.15813	3.19226	3.21153	
Alpha virt. eigenvalues --	3.22911	3.27196	3.27915	3.37625	3.38844	
Alpha virt. eigenvalues --	3.51150	3.53229	3.56428	3.59910	3.65417	
Alpha virt. eigenvalues --	3.68051	3.71003	3.73581	3.75462	3.76963	
Alpha virt. eigenvalues --	3.78619	3.81189	3.81692	3.82953	3.84013	
Alpha virt. eigenvalues --	3.87034	3.89022	3.97525	4.06390	4.08181	
Alpha virt. eigenvalues --	4.09498	4.13602	4.24770	4.26979	4.29150	
Alpha virt. eigenvalues --	4.32078	4.35350	4.44858	4.51722	4.69668	
Alpha virt. eigenvalues --	4.74623	4.82852	4.93862	5.03320	5.12971	
Alpha virt. eigenvalues --	5.23144	5.49425	5.60822	6.78298	7.68794	
Alpha virt. eigenvalues --	7.75715	7.78479	23.71034	23.75946	23.83544	
Alpha virt. eigenvalues --	23.87168	23.88045	23.88680	23.92717	23.98184	
Alpha virt. eigenvalues --	24.14256	24.24320	35.44307	35.57421	35.61300	
Alpha virt. eigenvalues --	48.06721	49.92510	289.89583	289.96089	289.99392	
Alpha virt. eigenvalues --	1020.85736					

Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	6.943726	-1.103967	0.211967	-0.036279	-0.062971	0.083868
2	C	-1.103967	6.687210	0.063888	0.091145	0.254014	-0.435799

3	N	0.211967	0.063888	6.651186	0.458523	-0.394890	-0.163127
4	C	-0.036279	0.091145	0.458523	7.467643	0.165096	-0.895217
5	N	-0.062971	0.254014	-0.394890	0.165096	7.068269	0.097217
6	C	0.083868	-0.435799	-0.163127	-0.895217	0.097217	7.602303
7	C	-0.064864	0.197870	-0.011329	0.111771	0.069517	-0.949982
8	H	0.503337	-0.114770	0.036043	0.012429	-0.072689	-0.026554
9	H	-0.138056	0.531122	-0.075406	0.003416	0.026590	-0.008227
10	H	0.057307	-0.078612	-0.005979	-0.022571	-0.048417	0.480798
11	H	-0.013412	0.003347	-0.013890	-0.057939	-0.009845	0.520496
12	H	0.017508	-0.037212	0.009858	0.007606	-0.042062	-0.003912
13	H	-0.002775	0.020097	-0.006983	-0.016712	0.075041	-0.117667
14	Br	-0.002217	-0.014434	-0.025508	-0.074326	0.010305	0.014646
15	H	-0.220017	0.064946	-0.084964	-0.853215	0.039957	0.276918
16	C	0.213689	-0.209571	0.268703	0.086283	-0.257175	-0.198066
17	C	-0.165919	0.144071	0.045738	-0.392997	-0.098830	-0.064206
18	H	0.042574	-0.044401	-0.126438	0.169305	0.081181	0.065977
19	H	-0.007267	0.010783	0.026822	-0.018091	-0.003241	-0.003000
20	H	0.009394	-0.000778	-0.044024	0.014315	0.001044	0.000583
21	N	-0.006404	-0.009777	0.007143	0.067049	-0.017541	-0.047392
22	H	-0.000349	0.000663	0.000385	-0.001157	-0.004830	0.018439
23	H	-0.000802	-0.000713	-0.001047	-0.010528	0.000164	0.021416
24	C	-0.012259	0.004032	-0.003350	-0.034240	-0.014291	0.079694
25	C	0.011753	-0.002346	0.005201	0.046237	0.013618	-0.066396
26	O	-0.001249	0.003635	0.001832	-0.020552	0.001133	0.036877
27	H	-0.000397	0.000569	0.000416	0.000755	0.000447	0.003194
28	H	0.000448	0.000073	-0.002301	0.021342	0.001377	-0.021097
29	H	0.000006	0.000064	0.002034	0.007793	0.000384	-0.021036
30	C	0.000975	0.000433	0.001364	0.016094	-0.003005	-0.014988
31	H	-0.000153	0.000054	0.000119	0.000172	-0.000813	0.001948
32	H	-0.000043	-0.000006	-0.000108	0.000449	0.000113	-0.001366
33	H	0.000277	-0.000118	0.000001	0.000410	0.000157	-0.000313

		7	8	9	10	11	12
1	C	-0.064864	0.503337	-0.138056	0.057307	-0.013412	0.017508
2	C	0.197870	-0.114770	0.531122	-0.078612	0.003347	-0.037212
3	N	-0.011329	0.036043	-0.075406	-0.005979	-0.013890	0.009858
4	C	0.111771	0.012429	0.003416	-0.022571	-0.057939	0.007606
5	N	0.069517	-0.072689	0.026590	-0.048417	-0.009845	-0.042062
6	C	-0.949982	-0.026554	-0.008227	0.480798	0.520496	-0.003912
7	C	6.636703	-0.003450	0.003449	-0.112750	-0.157026	0.411698
8	H	-0.003450	0.492135	-0.011184	0.007217	-0.005576	-0.004124
9	H	0.003449	-0.011184	0.499434	-0.001371	0.001023	-0.000035
10	H	-0.112750	0.007217	-0.001371	0.576475	-0.033062	0.004454
11	H	-0.157026	-0.005576	0.001023	-0.033062	0.536948	-0.015492
12	H	0.411698	-0.004124	-0.000035	0.004454	-0.015492	0.631191

13	H	0.367327	0.001329	0.000193	-0.012840	0.020816	-0.088528
14	Br	-0.008237	-0.000420	-0.001498	-0.007025	-0.000467	0.000407
15	H	-0.089899	-0.000503	0.000185	-0.050063	0.006635	0.004172
16	C	0.004387	0.002573	-0.009973	-0.017368	-0.009422	0.004174
17	C	-0.003977	0.000791	0.013314	-0.007163	-0.001092	-0.000250
18	H	-0.000900	0.001325	-0.005587	0.013402	-0.000008	0.000130
19	H	0.000139	-0.000144	0.000170	-0.000481	-0.000028	-0.000022
20	H	-0.000208	0.000609	0.005251	0.000292	-0.000120	0.000012
21	N	0.042863	0.000524	-0.000120	0.020889	0.008432	-0.049274
22	H	-0.023385	-0.000862	0.000040	-0.006102	0.003865	-0.010135
23	H	-0.088057	0.000388	-0.000058	0.002705	0.000535	0.007171
24	C	0.061415	-0.001284	0.000072	-0.081116	0.006533	0.002782
25	C	-0.076439	0.001356	-0.000071	0.059367	-0.006083	-0.004712
26	O	-0.028035	0.000296	0.000012	-0.013464	0.004302	0.000275
27	H	-0.010558	0.000005	0.000004	-0.000203	-0.000335	-0.000355
28	H	0.025121	-0.000258	0.000058	-0.013566	0.000739	0.000494
29	H	-0.008226	0.000146	0.000007	0.009654	-0.000542	-0.000420
30	C	0.016918	-0.000019	0.000058	-0.003890	-0.000301	0.000353
31	H	-0.001921	-0.000002	0.000002	-0.000451	-0.000084	0.000307
32	H	0.001325	-0.000006	0.000000	0.000201	-0.000002	-0.000055
33	H	0.001287	0.000016	0.000000	0.000695	0.000031	-0.000007

		13	14	15	16	17	18
1	C	-0.002775	-0.002217	-0.220017	0.213689	-0.165919	0.042574
2	C	0.020097	-0.014434	0.064946	-0.209571	0.144071	-0.044401
3	N	-0.006983	-0.025508	-0.084964	0.268703	0.045738	-0.126438
4	C	-0.016712	-0.074326	-0.853215	0.086283	-0.392997	0.169305
5	N	0.075041	0.010305	0.039957	-0.257175	-0.098830	0.081181
6	C	-0.117667	0.014646	0.276918	-0.198066	-0.064206	0.065977
7	C	0.367327	-0.008237	-0.089899	0.004387	-0.003977	-0.000900
8	H	0.001329	-0.000420	-0.000503	0.002573	0.000791	0.001325
9	H	0.000193	-0.001498	0.000185	-0.009973	0.013314	-0.005587
10	H	-0.012840	-0.007025	-0.050063	-0.017368	-0.007163	0.013402
11	H	0.020816	-0.000467	0.006635	-0.009422	-0.001092	-0.000008
12	H	-0.088528	0.000407	0.004172	0.004174	-0.000250	0.000130
13	H	0.712332	-0.004064	-0.042802	-0.003200	-0.002323	-0.001874
14	Br	-0.004064	35.588779	0.233571	-0.156268	-0.038647	0.169794
15	H	-0.042802	0.233571	1.834981	-0.231326	0.117390	-0.066577
16	C	-0.003200	-0.156268	-0.231326	6.327542	-0.050734	0.023056
17	C	-0.002323	-0.038647	0.117390	-0.050734	6.239804	-0.130209
18	H	-0.001874	0.169794	-0.066577	0.023056	-0.130209	0.778177
19	H	0.000099	-0.007577	0.004230	-0.091717	0.476755	-0.032590
20	H	-0.000021	0.001780	-0.001459	0.125963	0.240956	0.004633
21	N	-0.081666	0.002065	-0.020514	0.006256	0.000433	-0.000364
22	H	-0.005281	0.000069	-0.000801	0.000222	0.000015	-0.000040

23	H	0.007984	-0.000352	0.007049	-0.001129	-0.000089	0.000274
24	C	-0.006861	-0.031249	0.037863	-0.007264	-0.000970	0.002186
25	C	0.017771	-0.021776	-0.043065	0.008518	0.000960	0.002881
26	O	-0.000959	-0.004053	0.025590	0.001152	0.000253	-0.000306
27	H	0.002129	0.004648	0.006638	0.000905	0.000102	-0.000407
28	H	0.000345	0.007543	-0.025862	0.000088	-0.000827	-0.002241
29	H	0.003914	0.033127	-0.004572	0.008612	0.000887	-0.007713
30	C	-0.007109	0.020964	-0.008906	0.003692	0.000148	-0.004910
31	H	-0.003497	0.001336	0.002164	0.000211	0.000060	0.000002
32	H	0.000444	0.000209	-0.001584	-0.000160	-0.000026	0.000027
33	H	0.000068	0.000641	-0.001359	-0.000032	-0.000008	0.000040

		19	20	21	22	23	24
1	C	-0.007267	0.009394	-0.006404	-0.000349	-0.000802	-0.012259
2	C	0.010783	-0.000778	-0.009777	0.000663	-0.000713	0.004032
3	N	0.026822	-0.044024	0.007143	0.000385	-0.001047	-0.003350
4	C	-0.018091	0.014315	0.067049	-0.001157	-0.010528	-0.034240
5	N	-0.003241	0.001044	-0.017541	-0.004830	0.000164	-0.014291
6	C	-0.003000	0.000583	-0.047392	0.018439	0.021416	0.079694
7	C	0.000139	-0.000208	0.042863	-0.023385	-0.088057	0.061415
8	H	-0.000144	0.000609	0.000524	-0.000862	0.000388	-0.001284
9	H	0.000170	0.005251	-0.000120	0.000040	-0.000058	0.000072
10	H	-0.000481	0.000292	0.020889	-0.006102	0.002705	-0.081116
11	H	-0.000028	-0.000120	0.008432	0.003865	0.000535	0.006533
12	H	-0.000022	0.000012	-0.049274	-0.010135	0.007171	0.002782
13	H	0.000099	-0.000021	-0.081666	-0.005281	0.007984	-0.006861
14	Br	-0.007577	0.001780	0.002065	0.000069	-0.000352	-0.031249
15	H	0.004230	-0.001459	-0.020514	-0.000801	0.007049	0.037863
16	C	-0.091717	0.125963	0.006256	0.000222	-0.001129	-0.007264
17	C	0.476755	0.240956	0.000433	0.000015	-0.000089	-0.000970
18	H	-0.032590	0.004633	-0.000364	-0.000040	0.000274	0.002186
19	H	0.461803	-0.022205	0.000001	0.000001	-0.000005	-0.000041
20	H	-0.022205	0.549154	0.000007	-0.000004	0.000005	-0.000014
21	N	0.000001	0.000007	6.730564	0.359707	0.401154	-0.009821
22	H	0.000001	-0.000004	0.359707	0.481032	-0.043990	0.003633
23	H	-0.000005	0.000005	0.401154	-0.043990	0.397746	0.005717
24	C	-0.000041	-0.000014	-0.009821	0.003633	0.005717	7.164062
25	C	0.000018	0.000024	0.006830	-0.005913	-0.000686	-1.568205
26	O	0.000008	-0.000001	-0.021254	-0.000502	0.012441	0.078128
27	H	0.000006	0.000000	-0.000679	-0.000334	-0.000207	0.175007
28	H	0.000033	-0.000024	-0.000224	0.000290	-0.000692	0.474201
29	H	0.000172	-0.000016	0.002313	-0.000521	-0.000626	-0.093052
30	C	0.000062	-0.000023	0.005096	0.000806	-0.004946	-0.048554
31	H	0.000000	-0.000001	0.001053	0.000124	0.000520	-0.012773
32	H	-0.000001	0.000000	-0.000007	0.000053	-0.000463	0.021915

33	H	0.000000	0.000000	-0.000826	-0.000246	0.000112	0.028350
		25	26	27	28	29	30
1	C	0.011753	-0.001249	-0.000397	0.000448	0.000006	0.000975
2	C	-0.002346	0.003635	0.000569	0.000073	0.000064	0.000433
3	N	0.005201	0.001832	0.000416	-0.002301	0.002034	0.001364
4	C	0.046237	-0.020552	0.000755	0.021342	0.007793	0.016094
5	N	0.013618	0.001133	0.000447	0.001377	0.000384	-0.003005
6	C	-0.066396	0.036877	0.003194	-0.021097	-0.021036	-0.014988
7	C	-0.076439	-0.028035	-0.010558	0.025121	-0.008226	0.016918
8	H	0.001356	0.000296	0.000005	-0.000258	0.000146	-0.000019
9	H	-0.000071	0.000012	0.000004	0.000058	0.000007	0.000058
10	H	0.059367	-0.013464	-0.000203	-0.013566	0.009654	-0.003890
11	H	-0.006083	0.004302	-0.000335	0.000739	-0.000542	-0.000301
12	H	-0.004712	0.000275	-0.000355	0.000494	-0.000420	0.000353
13	H	0.017771	-0.000959	0.002129	0.000345	0.003914	-0.007109
14	Br	-0.021776	-0.004053	0.004648	0.007543	0.033127	0.020964
15	H	-0.043065	0.025590	0.006638	-0.025862	-0.004572	-0.008906
16	C	0.008518	0.001152	0.000905	0.000088	0.008612	0.003692
17	C	0.000960	0.000253	0.000102	-0.000827	0.000887	0.000148
18	H	0.002881	-0.000306	-0.000407	-0.002241	-0.007713	-0.004910
19	H	0.000018	0.000008	0.000006	0.000033	0.000172	0.000062
20	H	0.000024	-0.000001	0.000000	-0.000024	-0.000016	-0.000023
21	N	0.006830	-0.021254	-0.000679	-0.000224	0.002313	0.005096
22	H	-0.005913	-0.000502	-0.000334	0.000290	-0.000521	0.000806
23	H	-0.000686	0.012441	-0.000207	-0.000692	-0.000626	-0.004946
24	C	-1.568205	0.078128	0.175007	0.474201	-0.093052	-0.048554
25	C	7.240425	0.128340	0.158258	-0.103058	0.413993	-0.246838
26	O	0.128340	8.207364	-0.059080	-0.051218	-0.003800	-0.087894
27	H	0.158258	-0.059080	0.628770	-0.063381	0.003477	0.010188
28	H	-0.103058	-0.051218	-0.063381	0.562680	0.006980	-0.001997
29	H	0.413993	-0.003800	0.003477	0.006980	0.457140	0.010480
30	C	-0.246838	-0.087894	0.010188	-0.001997	0.010480	5.890774
31	H	0.013564	-0.016478	-0.000495	-0.002600	0.002499	0.367532
32	H	-0.087860	0.011512	-0.005875	0.003240	0.005286	0.409097
33	H	-0.074631	0.013510	-0.001248	0.004510	-0.009557	0.390415

		31	32	33
1	C	-0.000153	-0.000043	0.000277
2	C	0.000054	-0.000006	-0.000118
3	N	0.000119	-0.000108	0.000001
4	C	0.000172	0.000449	0.000410
5	N	-0.000813	0.000113	0.000157
6	C	0.001948	-0.001366	-0.000313
7	C	-0.001921	0.001325	0.001287
8	H	-0.000002	-0.000006	0.000016

9	H	0.000002	0.000000	0.000000
10	H	-0.000451	0.000201	0.000695
11	H	-0.000084	-0.000002	0.000031
12	H	0.000307	-0.000055	-0.000007
13	H	-0.003497	0.000444	0.000068
14	Br	0.001336	0.000209	0.000641
15	H	0.002164	-0.001584	-0.001359
16	C	0.000211	-0.000160	-0.000032
17	C	0.000060	-0.000026	-0.000008
18	H	0.000002	0.000027	0.000040
19	H	0.000000	-0.000001	0.000000
20	H	-0.000001	0.000000	0.000000
21	N	0.001053	-0.000007	-0.000826
22	H	0.000124	0.000053	-0.000246
23	H	0.000520	-0.000463	0.000112
24	C	-0.012773	0.021915	0.028350
25	C	0.013564	-0.087860	-0.074631
26	O	-0.016478	0.011512	0.013510
27	H	-0.000495	-0.005875	-0.001248
28	H	-0.002600	0.003240	0.004510
29	H	0.002499	0.005286	-0.009557
30	C	0.367532	0.409097	0.390415
31	H	0.579110	-0.039615	-0.038038
32	H	-0.039615	0.555000	-0.020563
33	H	-0.038038	-0.020563	0.573415

Mulliken charges:

		1
1	C	-0.257428
2	C	-0.025509
3	N	0.168124
4	C	-0.314010
5	N	0.124976
6	C	-0.266028
7	C	-0.312548
8	H	0.181322
9	H	0.167185
10	H	0.283037
11	H	0.211023
12	H	0.154005
13	H	0.175272
14	Br	-0.691764
15	H	0.085201
16	C	0.157379
17	C	-0.323411

18	H	0.069599
19	H	0.205308
20	H	0.114874
21	N	-0.396517
22	H	0.235109
23	H	0.289011
24	C	-0.220248
25	C	0.178965
26	O	-0.217816
27	H	0.148035
28	H	0.179788
29	H	0.181116
30	C	-0.712069
31	H	0.146143
32	H	0.148869
33	H	0.133008

Sum of Mulliken charges = 0.00000

Mulliken charges with hydrogens summed into heavy atoms:

		1
1	C	-0.076106
2	C	0.141676
3	N	0.168124
4	C	-0.228809
5	N	0.124976
6	C	0.228031
7	C	0.016729
14	Br	-0.691764
16	C	0.226978
17	C	-0.003229
21	N	0.127604
24	C	0.107575
25	C	0.360082
26	O	-0.217816
30	C	-0.284049

Electronic spatial extent (au): <R**2>= 5752.8926

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= -4.3752 Y= 9.3760 Z= 1.3047

Tot= 10.4285

Quadrupole moment (field-independent basis, Debye-Ang):

XX= -74.4078 YY= -118.7914 ZZ= -107.4286

XY= -10.0634 XZ= 0.4371 YZ= 1.1965

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

XX= 25.8015 YY= -18.5821 ZZ= -7.2194

XY= -10.0634 XZ= 0.4371 YZ= 1.1965

Octapole moment (field-independent basis, Debye-Ang**2):

XXX= -54.5552 YYY= 28.6230 ZZZ= -9.0884 XYY= -28.7173

XXY= -22.4836 XXZ= 17.6718 XZZ= 19.6578 YZZ= -13.3733

YYZ= 20.4913 XYZ= 18.2442

Hexadecapole moment (field-independent basis, Debye-Ang**3):

XXXX= -3930.0041 YYYY= -2677.5264 ZZZZ= -375.0517 XXXY= -47.7286

XXXZ= -81.5090 YYYX= -64.2762 YYYZ= 65.3550 ZZZX= 3.6786

ZZZY= 15.5056 XXYY= -1088.5570 XXZZ= -839.0831 YYZZ= -494.4729

XXYZ= 15.4446 YYXZ= 52.7584 ZZXY= 4.1953

N-N= 1.312965357699D+03 E-N=-1.025042093304D+04 KE= 3.199826207045D+03

1\1\GINC-NODE12\FOpt\RB3LYP\6-311++G(d,p)\C10H18Br1N3O1\SUQIAN\25-Jul-2024\0\\# opt b3lyp/6-311++g(d,p)\\oh\\0,1\C,-2.6437319714,2.1001336706,-0.1957968334\C,-3.5357196916,1.118474492,0.0922967896\N,-2.8269201213,-0.0760997348,0.1118008106\C,-1.5346108679,0.1844074801,-0.160077938\N,-1.4040906803,1.4978389249,-0.3529521214\C,-0.1300151494,2.1829844081,-0.6351188294\C,0.4549671306,2.8589020616,0.6099714112\H,-2.782916387,3.161230884,-0.3105737018\H,-4.5940366158,1.1696263686,0.2716080265\H,0.5696782172,1.4293698196,-0.9967265536\H,-0.3026746801,2.9164821488,-1.423768713\H,-0.2256519313,3.6415413838,0.9614426919\H,0.5335213614,2.1060752983,1.4086521908\Br,0.1372232984,-2.6663228028,-0.2155074815\H,-0.7589469703,-0.6044431828,-0.2157667194\C,-3.3014522846,-1.4006687603,0.3566821935\C,-4.561123082,-1.6906216693,0.6540689913\H,-2.5013398905,-2.1335641692,0.2684546807\H,-4.8325999692,-2.7237393977,0.8224583098\H,-5.3485970089,-0.9518315044,0.7415227729\N,1.7219532752,3.4719885811,0.2294080036\H,2.0646917396,4.087187503,0.9577715733\H,2.4195712147,2.7489553289,0.0660004313\C,3.3320042699,-0.4262157644,-1.1377833284\C,3.2655277897,-0.5638190728,0.3183888028\O,2.7347229019,0.620853666,-0.3370267756\H,4.2720650913,-0.1479224523,-1.6082484784\H,2.6293579956,-0.9890360456,-1.7448674801\H,2.4802959374,-1.2174216409,0.6927382572\C,4.4622012262,-0.3536968612,1.2046212078\H,4.1639539953,0.0784082343,2.1645052581\H,4.9466031687,-1.313462184,1.4086966065\H,5.1912026886,0.311772989,0.7353409445\\Version=EM64L-G09RevD.01\State=1-A\HF=-3205.648379\RMSD=5.094e-09\RMSF=3.075e-06\Dipole=-2.0766096,3.4873639,0.5997317\Quadrupole=20.3400652,-15.0057745,-5.3342907,-4.0588622,-0.0198161,0.7438296\PG=C01 [X(C10H18Br1N3O1)]\\@

"THE ACADEMIC HIERARCHY"

THE PRESIDENT:
LEAPS TALL BUILDINGS IN A SINGLE BOUND,
IS MORE POWERFUL THAN A LOCOMOTIVE,
IS FASTER THAN A SPEEDING BULLET,
WALKS ON WATER,
GIVES POLICY TO GOD.

THE VICE PRESIDENT FOR ACADEMIC AFFAIRS:
LEAPS SHORT BUILDINGS IN A SINGLE BOUND,
IS MORE POWERFUL THAN A SWITCH ENGINE,
IS JUST AS FAST AS A SPEEDING BULLET,
WALKS ON WATER IF SEA IS CALM,
TALKS WITH GOD.

PROFESSOR:
LEAPS SHORT BUILDINGS WITH A RUNNING START AND FAVORABLE WINDS,
IS ALMOST AS POWERFUL AS A SWITCH ENGINE,
CAN FIRE A SPEEDING BULLET,
WALKS ON WATER IN AN INDOOR SWIMMING POOL,
TALKS WITH GOD IF SPECIAL REQUEST IS APPROVED.

ASSOCIATE PROFESSOR:
BARELY CLEARS A QUONSET HUT,
LOSES TUG OF WAR WITH LOCOMOTIVE,
MISFIRES FREQUENTLY,
SWIMS WELL,
IS OCCASIONALLY ADDRESSED BY GOD.

ASSISTANT PROFESSOR:
MAKES HIGH MARKS ON WALLS WHEN TRYING TO LEAP TALL BUILDINGS,
IS RUN OVER BY LOCOMOTIVES,
CAN SOMETIMES HANDLE A GUN WITHOUT INFLICTING SELF INJURY,
DOG PADDLES,
TALKS TO ANIMALS.

GRADUATE STUDENT:
RUNS INTO BUILDINGS,
RECOGNIZES LOCOMOTIVES TWO OUT OF THREE TIMES,
IS NOT ISSUED AMMUNITION,
CAN STAY AFLOAT WITH A LIFE JACKET,
TALKS TO WALLS.

UNDERGRADUATE AND WORK STUDY STUDENT:
FALLS OVER DOORSTEP WHEN TRYING TO ENTER BUILDINGS,
SAYS, "LOOK AT THE CHOO-CHOO,"
WETS HIMSELF WITH A WATER PISTOL,
PLAYS IN MUD PUDDLES,
MUMBLES TO HIMSELF.

DEPARTMENT SECRETARY:
LIFTS TALL BUILDINGS AND WALKS UNDER THEM,
KICKS LOCOMOTIVES OFF THE TRACKS,
CATCHES SPEEDING BULLETS IN HER TEETH AND EATS THEM,
FREEZES WATER WITH A SINGLE GLANCE,
IS GOD.

Job cpu time: 1 days 9 hours 35 minutes 1.9 seconds.
File lengths (MBytes): RWF= 138 Int= 0 D2E= 0 Chk= 17 Scr= 1
Normal termination of Gaussian 09 at Thu Jul 25 16:02:10 2024.

Entering Gaussian System, Link 0=/opt/gaussian/g09/g09
Initial command:
/opt/gaussian/g09/l1.exe "/tmp/Gau-29071.inp" -scrdir="/tmp/"
Entering Link 1 = /opt/gaussian/g09/l1.exe PID= 29072.

Cite this work as:
Gaussian 09, Revision D.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci,
G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian,
A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada,
M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima,
Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr.,
J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers,
K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand,
K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi,
M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross,
V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,
O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,
R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth,
P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels,

O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski,
and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

****
Gaussian 09: EM64L-G09RevD.01 24-Apr-2013
                20-Jul-2024
****
%chk=/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk
%mem=1000MB
%nprocl=1
Will use up to 1 processors via Linda.
%nprocs=8
Will use up to 8 processors via shared memory.
---
opt b3lyp/6-311++g(d,p)

1/14=-1,18=20,19=15,26=3,38=1/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=4,6=6,7=1111,11=2,16=1,25=1,30=1,71=1,74=-5/1,2,3;
4//1;
5/5=2,38=5/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(2);
2/9=110/2;
99//99;
2/9=110/2;
3/5=4,6=6,7=1111,11=2,16=1,25=1,30=1,71=1,74=-5/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;
--
oh
--
Symbolic Z-matrix:
Charge = 0 Multiplicity = 1
C -1.85298 -2.00477 0.26195
C -2.84494 -1.10868 0.02227
N -2.2526 0.1497 0.01266
C -0.93264 0.00637 0.24353

N	-0.67446	-1.292	0.4013
C	0.68899	-1.82956	0.59657
C	1.47835	-1.92564	-0.73551
H	-1.88574	-3.07712	0.34901
H	-3.89688	-1.25872	-0.13791
H	1.21191	-1.1335	1.25067
H	0.59178	-2.79327	1.09741
H	1.34487	-2.9108	-1.19079
H	1.08962	-1.16668	-1.42475
Br	2.0255	1.47738	0.09935
H	-0.1445	0.78154	0.25732
C	-2.86233	1.41676	-0.19872
C	-4.16281	1.61048	-0.37392
H	-2.13902	2.2222	-0.2043
H	-4.52894	2.61515	-0.53341
H	-4.89412	0.81234	-0.36723
N	2.91644	-1.74142	-0.49289
H	3.35148	-2.63397	-0.3742
H	3.32852	-1.27085	-1.27311

Add virtual bond connecting atoms H15 and Br14 Dist= 4.32D+00.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.

! Initial Parameters !
! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.	!
! R1	R(1,2)	1.3581	estimate D2E/DX2	!
! R2	R(1,5)	1.3843	estimate D2E/DX2	!
! R3	R(1,8)	1.0764	estimate D2E/DX2	!
! R4	R(2,3)	1.3909	estimate D2E/DX2	!
! R5	R(2,9)	1.0746	estimate D2E/DX2	!
! R6	R(3,4)	1.3476	estimate D2E/DX2	!
! R7	R(3,16)	1.4219	estimate D2E/DX2	!
! R8	R(4,5)	1.3332	estimate D2E/DX2	!
! R9	R(4,15)	1.1056	estimate D2E/DX2	!
! R10	R(5,6)	1.4785	estimate D2E/DX2	!
! R11	R(6,7)	1.5514	estimate D2E/DX2	!
! R12	R(6,10)	1.0889	estimate D2E/DX2	!
! R13	R(6,11)	1.0904	estimate D2E/DX2	!

! R14	R(7,12)	1.0935	estimate D2E/DX2	!
! R15	R(7,13)	1.0964	estimate D2E/DX2	!
! R16	R(7,21)	1.47	estimate D2E/DX2	!
! R17	R(14,15)	2.2843	estimate D2E/DX2	!
! R18	R(16,17)	1.3265	estimate D2E/DX2	!
! R19	R(16,18)	1.0826	estimate D2E/DX2	!
! R20	R(17,19)	1.0811	estimate D2E/DX2	!
! R21	R(17,20)	1.0825	estimate D2E/DX2	!
! R22	R(21,22)	1.0	estimate D2E/DX2	!
! R23	R(21,23)	1.0	estimate D2E/DX2	!
! A1	A(2,1,5)	107.4487	estimate D2E/DX2	!
! A2	A(2,1,8)	130.4957	estimate D2E/DX2	!
! A3	A(5,1,8)	122.0547	estimate D2E/DX2	!
! A4	A(1,2,3)	106.6857	estimate D2E/DX2	!
! A5	A(1,2,9)	130.4812	estimate D2E/DX2	!
! A6	A(3,2,9)	122.8331	estimate D2E/DX2	!
! A7	A(2,3,4)	108.6462	estimate D2E/DX2	!
! A8	A(2,3,16)	128.6538	estimate D2E/DX2	!
! A9	A(4,3,16)	122.6999	estimate D2E/DX2	!
! A10	A(3,4,5)	108.2726	estimate D2E/DX2	!
! A11	A(3,4,15)	128.7417	estimate D2E/DX2	!
! A12	A(5,4,15)	122.9107	estimate D2E/DX2	!
! A13	A(1,5,4)	108.9455	estimate D2E/DX2	!
! A14	A(1,5,6)	127.6728	estimate D2E/DX2	!
! A15	A(4,5,6)	123.2506	estimate D2E/DX2	!
! A16	A(5,6,7)	112.2301	estimate D2E/DX2	!
! A17	A(5,6,10)	106.8437	estimate D2E/DX2	!
! A18	A(5,6,11)	107.4442	estimate D2E/DX2	!
! A19	A(7,6,10)	108.1204	estimate D2E/DX2	!
! A20	A(7,6,11)	112.6443	estimate D2E/DX2	!
! A21	A(10,6,11)	109.3802	estimate D2E/DX2	!
! A22	A(6,7,12)	110.5609	estimate D2E/DX2	!
! A23	A(6,7,13)	108.4511	estimate D2E/DX2	!
! A24	A(6,7,21)	110.3829	estimate D2E/DX2	!
! A25	A(12,7,13)	108.5799	estimate D2E/DX2	!
! A26	A(12,7,21)	107.5209	estimate D2E/DX2	!
! A27	A(13,7,21)	111.3365	estimate D2E/DX2	!
! A28	A(4,15,14)	152.8661	estimate D2E/DX2	!
! A29	A(3,16,17)	124.7632	estimate D2E/DX2	!
! A30	A(3,16,18)	112.1624	estimate D2E/DX2	!
! A31	A(17,16,18)	123.0742	estimate D2E/DX2	!
! A32	A(16,17,19)	119.1583	estimate D2E/DX2	!
! A33	A(16,17,20)	123.6301	estimate D2E/DX2	!
! A34	A(19,17,20)	117.2116	estimate D2E/DX2	!

! A35	A(7,21,22)	109.4712	estimate D2E/DX2 !
! A36	A(7,21,23)	109.4712	estimate D2E/DX2 !
! A37	A(22,21,23)	109.4713	estimate D2E/DX2 !
! D1	D(5,1,2,3)	0.2541	estimate D2E/DX2 !
! D2	D(5,1,2,9)	-179.7257	estimate D2E/DX2 !
! D3	D(8,1,2,3)	179.9213	estimate D2E/DX2 !
! D4	D(8,1,2,9)	-0.0585	estimate D2E/DX2 !
! D5	D(2,1,5,4)	-0.3687	estimate D2E/DX2 !
! D6	D(2,1,5,6)	-176.2729	estimate D2E/DX2 !
! D7	D(8,1,5,4)	179.9299	estimate D2E/DX2 !
! D8	D(8,1,5,6)	4.0256	estimate D2E/DX2 !
! D9	D(1,2,3,4)	-0.0562	estimate D2E/DX2 !
! D10	D(1,2,3,16)	179.8446	estimate D2E/DX2 !
! D11	D(9,2,3,4)	179.9255	estimate D2E/DX2 !
! D12	D(9,2,3,16)	-0.1737	estimate D2E/DX2 !
! D13	D(2,3,4,5)	-0.1729	estimate D2E/DX2 !
! D14	D(2,3,4,15)	176.707	estimate D2E/DX2 !
! D15	D(16,3,4,5)	179.9192	estimate D2E/DX2 !
! D16	D(16,3,4,15)	-3.2009	estimate D2E/DX2 !
! D17	D(2,3,16,17)	3.0504	estimate D2E/DX2 !
! D18	D(2,3,16,18)	-176.7973	estimate D2E/DX2 !
! D19	D(4,3,16,17)	-177.0614	estimate D2E/DX2 !
! D20	D(4,3,16,18)	3.0909	estimate D2E/DX2 !
! D21	D(3,4,5,1)	0.3336	estimate D2E/DX2 !
! D22	D(3,4,5,6)	176.4574	estimate D2E/DX2 !
! D23	D(15,4,5,1)	-176.7678	estimate D2E/DX2 !
! D24	D(15,4,5,6)	-0.644	estimate D2E/DX2 !
! D25	D(3,4,15,14)	-157.7623	estimate D2E/DX2 !
! D26	D(5,4,15,14)	18.7081	estimate D2E/DX2 !
! D27	D(1,5,6,7)	96.5542	estimate D2E/DX2 !
! D28	D(1,5,6,10)	-145.1004	estimate D2E/DX2 !
! D29	D(1,5,6,11)	-27.8065	estimate D2E/DX2 !
! D30	D(4,5,6,7)	-78.8125	estimate D2E/DX2 !
! D31	D(4,5,6,10)	39.5329	estimate D2E/DX2 !
! D32	D(4,5,6,11)	156.8268	estimate D2E/DX2 !
! D33	D(5,6,7,12)	-91.7943	estimate D2E/DX2 !
! D34	D(5,6,7,13)	27.1459	estimate D2E/DX2 !
! D35	D(5,6,7,21)	149.3646	estimate D2E/DX2 !
! D36	D(10,6,7,12)	150.6177	estimate D2E/DX2 !
! D37	D(10,6,7,13)	-90.4421	estimate D2E/DX2 !
! D38	D(10,6,7,21)	31.7765	estimate D2E/DX2 !
! D39	D(11,6,7,12)	29.6316	estimate D2E/DX2 !
! D40	D(11,6,7,13)	148.5719	estimate D2E/DX2 !
! D41	D(11,6,7,21)	-89.2095	estimate D2E/DX2 !

! D42	D(6,7,21,22)	93.8039	estimate D2E/DX2	!
! D43	D(6,7,21,23)	-146.1961	estimate D2E/DX2	!
! D44	D(12,7,21,22)	-26.8726	estimate D2E/DX2	!
! D45	D(12,7,21,23)	93.1274	estimate D2E/DX2	!
! D46	D(13,7,21,22)	-145.6908	estimate D2E/DX2	!
! D47	D(13,7,21,23)	-25.6908	estimate D2E/DX2	!
! D48	D(3,16,17,19)	-179.6544	estimate D2E/DX2	!
! D49	D(3,16,17,20)	0.3485	estimate D2E/DX2	!
! D50	D(18,16,17,19)	0.1773	estimate D2E/DX2	!
! D51	D(18,16,17,20)	-179.8198	estimate D2E/DX2	!

Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-06

Number of steps in this run= 121 maximum allowed number of steps= 138.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.852977	-2.004770	0.261946
2	6	0	-2.844936	-1.108684	0.022270
3	7	0	-2.252596	0.149697	0.012664
4	6	0	-0.932640	0.006366	0.243529
5	7	0	-0.674460	-1.291997	0.401298
6	6	0	0.688990	-1.829559	0.596565
7	6	0	1.478350	-1.925642	-0.735506
8	1	0	-1.885737	-3.077123	0.349012
9	1	0	-3.896876	-1.258715	-0.137907
10	1	0	1.211914	-1.133502	1.250666
11	1	0	0.591782	-2.793267	1.097412
12	1	0	1.344868	-2.910804	-1.190791
13	1	0	1.089622	-1.166684	-1.424751
14	35	0	2.025502	1.477383	0.099347
15	1	0	-0.144502	0.781540	0.257320
16	6	0	-2.862333	1.416758	-0.198718
17	6	0	-4.162812	1.610481	-0.373924
18	1	0	-2.139017	2.222199	-0.204304
19	1	0	-4.528939	2.615146	-0.533412
20	1	0	-4.894120	0.812340	-0.367232
21	7	0	2.916438	-1.741420	-0.492886
22	1	0	3.351482	-2.633973	-0.374200
23	1	0	3.328520	-1.270853	-1.273113

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.358086	0.000000			
3	N	2.205349	1.390856	0.000000		
4	C	2.211793	2.224673	1.347637	0.000000	
5	N	1.384329	2.210935	2.172563	1.333152	0.000000
6	C	2.569876	3.652138	3.593233	2.474861	1.478546
7	C	3.478349	4.464577	4.334368	3.240993	2.515635
8	H	1.076380	2.213950	3.264978	3.229152	2.157916
9	H	2.212240	1.074590	2.170243	3.245400	3.267387
10	H	3.336200	4.238821	3.896419	2.629208	2.074838
11	H	2.701218	3.975523	4.234171	3.300140	2.083688
12	H	3.627334	4.719493	4.874086	3.969156	3.038580
13	H	3.493741	4.192610	3.869036	2.872063	2.542075
14	Br	5.214828	5.514966	4.480222	3.306854	3.879489
15	H	3.268399	3.304624	2.214304	1.105553	2.145027
16	C	3.596924	2.535152	1.421937	2.430741	3.533293
17	C	4.337016	3.047561	2.435624	3.659022	4.603688
18	H	4.262215	3.412395	2.086921	2.562385	3.855030
19	H	5.397869	4.124507	3.399761	4.510292	5.567446
20	H	4.192914	2.835701	2.749739	4.088514	4.777489
21	N	4.835953	5.818864	5.527280	4.290975	3.727747
22	H	5.280812	6.393692	6.269304	5.070176	4.313990
23	H	5.453710	6.309982	5.900851	4.699891	4.339118

		6	7	8	9	10
6	C	0.000000				
7	C	1.551365	0.000000			
8	H	2.871745	3.717414	0.000000		
9	H	4.679261	5.449309	2.754701	0.000000	
10	H	1.088941	2.154844	3.766442	5.295616	0.000000
11	H	1.090427	2.213225	2.603608	4.901930	1.778446
12	H	2.189500	1.093456	3.582662	5.595877	3.022779
13	H	2.164631	1.096442	3.955853	5.150689	2.678416
14	Br	3.601299	3.546397	6.008631	6.528176	2.967184
15	H	2.761817	3.308804	4.234334	4.289424	2.548330
16	C	4.876776	5.504662	4.631276	2.869169	5.020361
17	C	6.026251	6.667654	5.261306	2.891144	6.249513
18	H	5.005573	5.529205	5.334147	3.900159	4.960484
19	H	6.946872	7.533068	6.337753	3.944962	7.084680
20	H	6.251372	6.945541	4.969034	2.310055	6.609656
21	N	2.481168	1.470000	5.055075	6.839610	2.512954
22	H	2.945901	2.034920	5.305458	7.381454	3.077232
23	H	3.282525	2.034920	5.751728	7.314040	3.296718

		11	12	13	14	15
11	H	0.000000				
12	H	2.411810	0.000000			
13	H	3.042191	1.778157	0.000000		
14	Br	4.614124	4.624273	3.192152	0.000000	
15	H	3.745279	4.236585	2.854470	2.284310	0.000000
16	C	5.597783	6.116579	4.878040	4.897290	2.828087
17	C	6.645599	7.172435	6.033651	6.207812	4.151196
18	H	5.857186	6.281587	4.837161	4.241482	2.503335
19	H	7.624454	8.091346	6.831175	6.682483	4.817744
20	H	6.726121	7.311978	6.390622	6.967148	4.790604
21	N	3.006569	2.079510	2.129778	3.391932	4.037015
22	H	3.131607	2.184023	2.893546	4.345770	4.928129
23	H	3.927705	2.575090	2.246444	3.336811	4.314676

		16	17	18	19	20
16	C	0.000000				
17	C	1.326451	0.000000			
18	H	1.082568	2.121018	0.000000		
19	H	2.079839	1.081128	2.444268	0.000000	
20	H	2.126470	1.082536	3.099168	1.846912	0.000000
21	N	6.592027	7.833593	6.430489	8.626410	8.218412
22	H	7.419617	8.630180	7.331907	9.469933	8.936838
23	H	6.834050	8.076551	6.575540	8.797034	8.530658

		21	22	23
21	N	0.000000		
22	H	1.000000	0.000000	
23	H	1.000000	1.632993	0.000000

Stoichiometry C7H12BrN3
Framework group C1[X(C7H12BrN3)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.826300	2.028395	-0.268732
2	6	0	-2.834594	1.153500	-0.019135
3	7	0	-2.267411	-0.116390	-0.006277
4	6	0	-0.946147	-0.000593	-0.244976
5	7	0	-0.663007	1.291551	-0.410777
6	6	0	0.709796	1.800805	-0.616131

7	6	0	1.508209	1.887786	0.711161
8	1	0	-1.838155	3.100738	-0.361109
9	1	0	-3.882440	1.325299	0.145933
10	1	0	1.215146	1.091180	-1.269467
11	1	0	0.629072	2.763740	-1.121374
12	1	0	1.396890	2.877685	1.162110
13	1	0	1.108216	1.140201	1.406365
14	35	0	1.982832	-1.529623	-0.109195
15	1	0	-0.173704	-0.791404	-0.259042
16	6	0	-2.901115	-1.369953	0.214867
17	6	0	-4.204217	-1.536799	0.398062
18	1	0	-2.193978	-2.189633	0.220682
19	1	0	-4.589417	-2.533144	0.564660
20	1	0	-4.919495	-0.724263	0.391222
21	7	0	2.940987	1.673682	0.461748
22	1	0	3.393079	2.556768	0.336155
23	1	0	3.347880	1.198899	1.242144

Rotational constants (GHZ): 0.9756806 0.4464398 0.3176721

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 365 symmetry adapted cartesian basis functions of A symmetry.

There are 352 symmetry adapted basis functions of A symmetry.

352 basis functions, 562 primitive gaussians, 365 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 847.8093262862 Hartrees.

NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 352 RedAO= T EigKep= 4.36D-06 NBF= 352

NBsUse= 352 1.00D-06 EigRej= -1.00D+00 NBFU= 352

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
EnCoef did 4 forward-backward iterations
SCF Done: E(RB3LYP) = -3012.45025632 A.U. after 16 cycles
NFock= 16 Conv=0.81D-08 -V/T= 2.0016

****

Population analysis using the SCF density.

****

Orbital symmetries:
Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A)
Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A)
The electronic state is 1-A.
Alpha occ. eigenvalues -- -482.67888 -62.33222 -56.15006 -56.15001 -56.14973
Alpha occ. eigenvalues -- -14.45342 -14.43968 -14.28546 -10.29441 -10.27247
Alpha occ. eigenvalues -- -10.27173 -10.27051 -10.23716 -10.22176 -10.21057
Alpha occ. eigenvalues -- -8.54128 -6.36467 -6.36424 -6.36344 -2.47716
Alpha occ. eigenvalues -- -2.47707 -2.47645 -2.47610 -2.47598 -1.11582
Alpha occ. eigenvalues -- -1.00147 -0.88843 -0.85228 -0.82471 -0.77316
Alpha occ. eigenvalues -- -0.71356 -0.67850 -0.64781 -0.63119 -0.61670
Alpha occ. eigenvalues -- -0.58467 -0.54157 -0.52944 -0.52213 -0.51182
Alpha occ. eigenvalues -- -0.49340 -0.49021 -0.48346 -0.46186 -0.44462
Alpha occ. eigenvalues -- -0.43731 -0.41237 -0.38164 -0.36994 -0.31642
Alpha occ. eigenvalues -- -0.30360 -0.24100 -0.18386 -0.17772 -0.17314
Alpha virt. eigenvalues -- -0.08425 -0.04557 -0.03256 -0.02036 -0.00835
Alpha virt. eigenvalues -- -0.00687 0.00006 0.00617 0.01124 0.01608
Alpha virt. eigenvalues -- 0.03401 0.03613 0.04427 0.04961 0.05212
Alpha virt. eigenvalues -- 0.05516 0.06343 0.07098 0.07630 0.07817
Alpha virt. eigenvalues -- 0.08125 0.08518 0.09024 0.09280 0.09362
Alpha virt. eigenvalues -- 0.10149 0.10822 0.11123 0.11478 0.12117
Alpha virt. eigenvalues -- 0.12465 0.12648 0.12957 0.13305 0.13421
Alpha virt. eigenvalues -- 0.13823 0.14070 0.14818 0.15278 0.15509
Alpha virt. eigenvalues -- 0.15964 0.16516 0.16765 0.17235 0.17572
Alpha virt. eigenvalues -- 0.18814 0.19004 0.19262 0.19807 0.20739
Alpha virt. eigenvalues -- 0.21162 0.21286 0.22060 0.22429 0.22699
Alpha virt. eigenvalues -- 0.23379 0.23873 0.24291 0.24669 0.25217
Alpha virt. eigenvalues -- 0.25949 0.26104 0.26990 0.27212 0.27909
Alpha virt. eigenvalues -- 0.28979 0.29240 0.29813 0.30538 0.31106
Alpha virt. eigenvalues -- 0.31538 0.33492 0.33580 0.34725 0.35809
Alpha virt. eigenvalues -- 0.36278 0.36649 0.39065 0.40039 0.40923
Alpha virt. eigenvalues -- 0.43144 0.46311 0.46903 0.49410 0.49543
Alpha virt. eigenvalues -- 0.51477 0.51954 0.53191 0.53658 0.54721
Alpha virt. eigenvalues -- 0.54836 0.56024 0.56807 0.56869 0.57768
Alpha virt. eigenvalues -- 0.59934 0.60993 0.61926 0.62533 0.63360
Alpha virt. eigenvalues -- 0.64008 0.65204 0.65802 0.66191 0.66430
Alpha virt. eigenvalues -- 0.67984 0.69334 0.69444 0.70855 0.72814
Alpha virt. eigenvalues -- 0.73352 0.74691 0.75477 0.75637 0.77001
Alpha virt. eigenvalues -- 0.77372 0.78585 0.79492 0.79873 0.80979
Alpha virt. eigenvalues -- 0.81564 0.81839 0.83347 0.85288 0.86363
Alpha virt. eigenvalues -- 0.87505 0.89674 0.89869 0.90173 0.92919
Alpha virt. eigenvalues -- 0.93778 0.95624 0.98592 0.99527 0.99709
Alpha virt. eigenvalues -- 1.01227 1.03389 1.04131 1.05882 1.08829
Alpha virt. eigenvalues -- 1.09186 1.10726 1.11750 1.12940 1.14620
Alpha virt. eigenvalues -- 1.21020 1.25842 1.27157 1.27890 1.32218

Alpha virt. eigenvalues --	1.33372	1.37794	1.39113	1.43960	1.44460	
Alpha virt. eigenvalues --	1.47059	1.48037	1.48959	1.50729	1.53710	
Alpha virt. eigenvalues --	1.54714	1.54878	1.57692	1.58899	1.59973	
Alpha virt. eigenvalues --	1.60732	1.61963	1.65614	1.67161	1.68292	
Alpha virt. eigenvalues --	1.69021	1.69946	1.70720	1.71222	1.72030	
Alpha virt. eigenvalues --	1.73338	1.75687	1.76183	1.77549	1.79517	
Alpha virt. eigenvalues --	1.83800	1.83841	1.85965	1.87369	1.89379	
Alpha virt. eigenvalues --	1.89882	1.94749	1.97374	2.00781	2.03354	
Alpha virt. eigenvalues --	2.03698	2.05576	2.07067	2.09464	2.10090	
Alpha virt. eigenvalues --	2.10467	2.12212	2.12505	2.15704	2.16480	
Alpha virt. eigenvalues --	2.18513	2.19750	2.21852	2.26146	2.28911	
Alpha virt. eigenvalues --	2.29890	2.35985	2.39141	2.42382	2.44266	
Alpha virt. eigenvalues --	2.44891	2.45146	2.47195	2.50683	2.53511	
Alpha virt. eigenvalues --	2.53880	2.56244	2.56418	2.57501	2.60020	
Alpha virt. eigenvalues --	2.61263	2.63239	2.64109	2.65469	2.69363	
Alpha virt. eigenvalues --	2.70377	2.70976	2.71736	2.73233	2.73892	
Alpha virt. eigenvalues --	2.75392	2.76971	2.77637	2.79521	2.81370	
Alpha virt. eigenvalues --	2.83026	2.84047	2.86220	2.87859	2.90772	
Alpha virt. eigenvalues --	2.93754	2.96174	2.97212	3.03191	3.08613	
Alpha virt. eigenvalues --	3.13969	3.16667	3.19535	3.25970	3.37112	
Alpha virt. eigenvalues --	3.48880	3.49156	3.54507	3.59470	3.63225	
Alpha virt. eigenvalues --	3.64181	3.71286	3.75325	3.76663	3.81941	
Alpha virt. eigenvalues --	3.84496	3.86893	3.87771	4.04996	4.05355	
Alpha virt. eigenvalues --	4.08335	4.26125	4.28591	4.31367	4.32971	
Alpha virt. eigenvalues --	4.36757	4.42934	4.68876	4.81740	4.85213	
Alpha virt. eigenvalues --	4.91740	5.02232	5.22555	6.78956	7.70185	
Alpha virt. eigenvalues --	7.74225	7.75848	23.69327	23.74245	23.82586	
Alpha virt. eigenvalues --	23.87606	23.88574	24.13337	24.22214	35.43696	
Alpha virt. eigenvalues --	35.56750	35.63382	48.07473	289.91010	289.94885	
Alpha virt. eigenvalues --	289.963701	020.86357				

Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	7.529670	-1.774388	0.508591	-0.503132	-0.408430	0.328875
2	C	-1.774388	7.461129	-0.267506	0.449499	0.610601	-0.483667
3	N	0.508591	-0.267506	6.950461	-0.157916	-0.478005	-0.099104
4	C	-0.503132	0.449499	-0.157916	7.201866	0.883688	-0.494917
5	N	-0.408430	0.610601	-0.478005	0.883688	7.025985	-0.071339
6	C	0.328875	-0.483667	-0.099104	-0.494917	-0.071339	7.136808
7	C	-0.139490	0.165371	-0.021827	0.017494	0.076015	-0.608939
8	H	0.474859	-0.098166	0.035409	0.027183	-0.062079	-0.028250
9	H	-0.135256	0.539073	-0.077976	-0.006365	0.026378	-0.010174
10	H	0.032271	-0.037128	0.013681	0.009520	-0.020958	0.448869
11	H	-0.046640	0.065881	0.008521	0.018790	-0.086310	0.285207
12	H	0.091108	-0.099395	0.022037	-0.045186	-0.043672	0.063538

13	H	-0.120213	0.114551	-0.031106	0.076777	0.052754	-0.163098
14	Br	-0.002198	-0.010110	-0.003068	-0.142105	-0.026051	0.008522
15	H	0.139806	-0.292710	0.120211	-0.641201	-0.234510	0.122464
16	C	0.310060	-0.286887	0.367830	-0.487610	-0.189456	-0.116897
17	C	-0.078570	0.007509	0.015778	-0.282996	-0.107805	-0.041568
18	H	-0.028040	0.042948	-0.092454	0.145742	0.029977	0.004724
19	H	-0.000635	0.002347	0.022658	-0.012269	-0.001047	-0.000217
20	H	-0.003518	0.008357	-0.033662	0.005930	-0.000291	-0.001478
21	N	-0.028437	0.024638	-0.013178	0.045002	0.020414	-0.078126
22	H	-0.001561	0.004518	-0.001208	0.001263	0.000124	-0.015161
23	H	-0.001141	-0.000096	0.000382	0.004178	0.003091	-0.025167

		7	8	9	10	11	12
1	C	-0.139490	0.474859	-0.135256	0.032271	-0.046640	0.091108
2	C	0.165371	-0.098166	0.539073	-0.037128	0.065881	-0.099395
3	N	-0.021827	0.035409	-0.077976	0.013681	0.008521	0.022037
4	C	0.017494	0.027183	-0.006365	0.009520	0.018790	-0.045186
5	N	0.076015	-0.062079	0.026378	-0.020958	-0.086310	-0.043672
6	C	-0.608939	-0.028250	-0.010174	0.448869	0.285207	0.063538
7	C	6.534791	0.005661	0.003929	-0.126068	-0.058827	0.414267
8	H	0.005661	0.493000	-0.011026	0.005356	-0.020772	0.002032
9	H	0.003929	-0.011026	0.502089	-0.000223	0.003133	-0.000490
10	H	-0.126068	0.005356	-0.000223	0.441891	-0.053636	0.009188
11	H	-0.058827	-0.020772	0.003133	-0.053636	0.693538	-0.021021
12	H	0.414267	0.002032	-0.000490	0.009188	-0.021021	0.789213
13	H	0.386729	-0.003896	0.001145	-0.011742	0.019936	-0.129546
14	Br	0.103146	-0.001552	-0.000906	-0.025030	0.018478	0.017013
15	H	-0.058306	-0.001034	-0.005805	-0.001802	0.016136	0.029018
16	C	-0.011837	0.002340	0.004059	0.003545	0.010896	0.004683
17	C	-0.000980	0.002496	0.001339	-0.003600	0.002027	0.000544
18	H	-0.002648	-0.000196	0.001536	0.000414	-0.001331	-0.001338
19	H	0.000107	-0.000095	-0.000594	-0.000032	0.000089	0.000043
20	H	-0.000280	0.000680	0.005729	-0.000053	-0.000112	-0.000098
21	N	-0.066086	-0.002737	0.000121	0.018324	0.005295	-0.208814
22	H	-0.043104	-0.000289	0.000034	-0.011020	0.007030	-0.026610
23	H	0.006326	0.000365	0.000044	0.012863	-0.004353	0.021904

		13	14	15	16	17	18
1	C	-0.120213	-0.002198	0.139806	0.310060	-0.078570	-0.028040
2	C	0.114551	-0.010110	-0.292710	-0.286887	0.007509	0.042948
3	N	-0.031106	-0.003068	0.120211	0.367830	0.015778	-0.092454
4	C	0.076777	-0.142105	-0.641201	-0.487610	-0.282996	0.145742
5	N	0.052754	-0.026051	-0.234510	-0.189456	-0.107805	0.029977
6	C	-0.163098	0.008522	0.122464	-0.116897	-0.041568	0.004724
7	C	0.386729	0.103146	-0.058306	-0.011837	-0.000980	-0.002648
8	H	-0.003896	-0.001552	-0.001034	0.002340	0.002496	-0.000196

9	H	0.001145	-0.000906	-0.005805	0.004059	0.001339	0.001536
10	H	-0.011742	-0.025030	-0.001802	0.003545	-0.003600	0.000414
11	H	0.019936	0.018478	0.016136	0.010896	0.002027	-0.001331
12	H	-0.129546	0.017013	0.029018	0.004683	0.000544	-0.001338
13	H	0.616509	-0.033579	-0.081378	-0.006044	-0.002179	0.003939
14	Br	-0.033579	35.576258	0.285770	-0.006997	0.015508	-0.005084
15	H	-0.081378	0.285770	1.545526	0.028331	0.134679	-0.074775
16	C	-0.006044	-0.006997	0.028331	5.983603	-0.052335	0.413354
17	C	-0.002179	0.015508	0.134679	-0.052335	6.153130	-0.117786
18	H	0.003939	-0.005084	-0.074775	0.413354	-0.117786	0.464057
19	H	-0.000102	-0.000271	0.004919	-0.095990	0.457431	-0.009437
20	H	0.000102	0.000078	0.002139	0.080512	0.294496	0.003183
21	N	0.059250	-0.093932	-0.040447	-0.004936	-0.001325	0.001550
22	H	0.019997	0.002574	-0.006290	-0.000519	-0.000147	0.000115
23	H	-0.025250	-0.003031	-0.001556	0.000118	-0.000039	0.000019

		19	20	21	22	23
1	C	-0.000635	-0.003518	-0.028437	-0.001561	-0.001141
2	C	0.002347	0.008357	0.024638	0.004518	-0.000096
3	N	0.022658	-0.033662	-0.013178	-0.001208	0.000382
4	C	-0.012269	0.005930	0.045002	0.001263	0.004178
5	N	-0.001047	-0.000291	0.020414	0.000124	0.003091
6	C	-0.000217	-0.001478	-0.078126	-0.015161	-0.025167
7	C	0.000107	-0.000280	-0.066086	-0.043104	0.006326
8	H	-0.000095	0.000680	-0.002737	-0.000289	0.000365
9	H	-0.000594	0.005729	0.000121	0.000034	0.000044
10	H	-0.000032	-0.000053	0.018324	-0.011020	0.012863
11	H	0.000089	-0.000112	0.005295	0.007030	-0.004353
12	H	0.000043	-0.000098	-0.208814	-0.026610	0.021904
13	H	-0.000102	0.000102	0.059250	0.019997	-0.025250
14	Br	-0.000271	0.000078	-0.093932	0.002574	-0.003031
15	H	0.004919	0.002139	-0.040447	-0.006290	-0.001556
16	C	-0.095990	0.080512	-0.004936	-0.000519	0.000118
17	C	0.457431	0.294496	-0.001325	-0.000147	-0.000039
18	H	-0.009437	0.003183	0.001550	0.000115	0.000019
19	H	0.464131	-0.021019	-0.000031	-0.000002	-0.000002
20	H	-0.021019	0.534171	-0.000014	-0.000001	-0.000002
21	N	-0.000031	-0.000014	6.774210	0.402452	0.390255
22	H	-0.000002	-0.000001	0.402452	0.509593	-0.057064
23	H	-0.000002	-0.000002	0.390255	-0.057064	0.433833

Mulliken charges:

		1
1	C	-0.143590
2	C	-0.146369
3	N	0.211452

4	C	-0.113236
5	N	0.000929
6	C	-0.160906
7	C	-0.575443
8	H	0.180713
9	H	0.160208
10	H	0.295369
11	H	0.138044
12	H	0.111583
13	H	0.256446
14	Br	-0.673434
15	H	0.010814
16	C	0.050177
17	C	-0.395606
18	H	0.221530
19	H	0.190020
20	H	0.125150
21	N	-0.203448
22	H	0.215274
23	H	0.244323

Sum of Mulliken charges = 0.00000

Mulliken charges with hydrogens summed into heavy atoms:

		1
1	C	0.037123
2	C	0.013840
3	N	0.211452
4	C	-0.102421
5	N	0.000929
6	C	0.272507
7	C	-0.207414
14	Br	-0.673434
16	C	0.271707
17	C	-0.080437
21	N	0.256148

Electronic spatial extent (au): <R**2>= 3249.7365

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= -11.0054 Y= 8.0897 Z= 0.9463 Tot= 13.6915

Quadrupole moment (field-independent basis, Debye-Ang):

XX= -72.8182 YY= -75.4590 ZZ= -83.7358

XY= 15.8709 XZ= 2.7620 YZ= -2.0155

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

XX= 4.5195 YY= 1.8787 ZZ= -6.3982

XY= 15.8709 XZ= 2.7620 YZ= -2.0155

Octapole moment (field-independent basis, Debye-Ang**2):

XXX= -47.9584 YYY= 11.9079 ZZZ= -2.1368 XYY= -14.3038

XXY= 19.6521 XXZ= 23.2949 XZZ= 27.5983 YZZ= -6.3772

YYZ= -2.1578 XYZ= 5.8929

Hexadecapole moment (field-independent basis, Debye-Ang**3):

XXXX= -2360.3628 YYYY= -1154.7652 ZZZZ= -196.2757 XXXY= 55.8759

XXXZ= 6.4048 YYYX= 20.4644 YYYZ= -22.2358 ZZZX= 8.7697

ZZZY= 4.7528 XXYY= -581.0423 XXZZ= -508.8367 YYZZ= -253.4576

XXYZ= -1.9872 YYXZ= -3.9241 ZZXY= -16.5449

N-N= 8.478093262862D+02 E-N=-8.869220074409D+03 KE= 3.007500483407D+03

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000257627	0.000042709	-0.000080648
2	6	-0.000530682	-0.000388920	0.000052937
3	7	-0.000312578	-0.000113566	-0.000170000
4	6	0.000092517	0.000076739	0.000702379
5	7	-0.000456123	-0.001143191	-0.000781594
6	6	0.003726615	0.002630660	-0.001865437
7	6	0.006202833	-0.004756327	0.001679991
8	1	-0.000054020	0.000049586	-0.000029458
9	1	-0.000017511	-0.000028311	-0.000012081
10	1	0.001912272	0.001083458	-0.001152964
11	1	-0.000949463	-0.000458320	-0.000012598
12	1	-0.011190958	-0.001705931	-0.002248394
13	1	0.005553131	-0.001005651	0.003711516
14	35	-0.005594546	0.004703429	-0.000490633
15	1	0.002893715	0.001807329	-0.000115642
16	6	0.000397015	-0.000290832	0.000110760
17	6	-0.000217664	-0.000007875	-0.000046106
18	1	0.000215784	-0.000037522	0.000050253
19	1	0.000012655	0.000002474	0.000001965
20	1	-0.000028765	-0.000023435	0.000033730
21	7	-0.017533973	0.000479410	0.005542242

22	1	0.008329080	-0.009843925	-0.000779043
23	1	0.007808292	0.008928012	-0.004101173

Cartesian Forces: Max 0.017533973 RMS 0.003818412

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.025835512 RMS 0.005760474
Search for a local minimum.
Step number 1 out of a maximum of 121
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Second derivative matrix not updated -- first step.
ITU= 0

Eigenvalues ---	0.00230	0.00230	0.00653	0.00766	0.01402
Eigenvalues ---	0.01512	0.01860	0.01898	0.02144	0.02169
Eigenvalues ---	0.02314	0.02385	0.02431	0.03062	0.03062
Eigenvalues ---	0.03704	0.04129	0.04248	0.04363	0.05307
Eigenvalues ---	0.05451	0.09016	0.09375	0.12569	0.12750
Eigenvalues ---	0.15965	0.16000	0.16000	0.16000	0.16000
Eigenvalues ---	0.16000	0.16000	0.16000	0.21960	0.22000
Eigenvalues ---	0.22034	0.22817	0.23539	0.24903	0.25000
Eigenvalues ---	0.25000	0.27535	0.33075	0.34079	0.34416
Eigenvalues ---	0.34737	0.34763	0.34935	0.35686	0.35690
Eigenvalues ---	0.35740	0.35858	0.36435	0.36656	0.42170
Eigenvalues ---	0.42774	0.45890	0.47688	0.47688	0.49289
Eigenvalues ---	0.54376	0.56818	0.60352		

RFO step: Lambda=-2.18576896D-02 EMin= 2.30000000D-03
Linear search not attempted -- first point.
Iteration 1 RMS(Cart)= 0.21045399 RMS(Int)= 0.01638783
Iteration 2 RMS(Cart)= 0.02983508 RMS(Int)= 0.00062105
Iteration 3 RMS(Cart)= 0.00055827 RMS(Int)= 0.00053974
Iteration 4 RMS(Cart)= 0.00000036 RMS(Int)= 0.00053974

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56641	-0.00335	0.00000	-0.00752	-0.00755	2.55886
R2	2.61600	0.00206	0.00000	0.00443	0.00445	2.62045
R3	2.03406	-0.00005	0.00000	-0.00013	-0.00013	2.03394
R4	2.62834	-0.00319	0.00000	-0.00781	-0.00785	2.62049
R5	2.03068	0.00002	0.00000	0.00006	0.00006	2.03074
R6	2.54667	0.00140	0.00000	0.00314	0.00315	2.54982
R7	2.68707	-0.00051	0.00000	-0.00114	-0.00114	2.68593
R8	2.51929	0.01058	0.00000	0.01888	0.01893	2.53822

R9	2.08919	0.00263	0.00000	0.00746	0.00746	2.09665
R10	2.79405	0.00536	0.00000	0.01451	0.01451	2.80855
R11	2.93166	-0.00321	0.00000	-0.01080	-0.01080	2.92086
R12	2.05780	0.00092	0.00000	0.00247	0.00247	2.06027
R13	2.06061	0.00048	0.00000	0.00131	0.00131	2.06192
R14	2.06633	0.00384	0.00000	0.01048	0.01048	2.07681
R15	2.07198	-0.00500	0.00000	-0.01378	-0.01378	2.05819
R16	2.77790	-0.00130	0.00000	-0.00343	-0.00343	2.77447
R17	4.31672	-0.00385	0.00000	-0.06537	-0.06537	4.25135
R18	2.50663	0.00023	0.00000	0.00037	0.00037	2.50699
R19	2.04576	0.00011	0.00000	0.00030	0.00030	2.04606
R20	2.04304	0.00000	0.00000	-0.00001	-0.00001	2.04303
R21	2.04570	0.00004	0.00000	0.00010	0.00010	2.04580
R22	1.88973	0.01232	0.00000	0.02469	0.02469	1.91442
R23	1.88973	0.01062	0.00000	0.02129	0.02129	1.91101
A1	1.87533	0.00421	0.00000	0.01481	0.01482	1.89016
A2	2.27758	-0.00217	0.00000	-0.00775	-0.00776	2.26982
A3	2.13026	-0.00204	0.00000	-0.00706	-0.00707	2.12319
A4	1.86202	-0.00083	0.00000	-0.00924	-0.00928	1.85273
A5	2.27733	0.00039	0.00000	0.00447	0.00448	2.28181
A6	2.14384	0.00044	0.00000	0.00476	0.00477	2.14861
A7	1.89623	0.00406	0.00000	0.01405	0.01405	1.91029
A8	2.24543	-0.00166	0.00000	-0.00566	-0.00567	2.23977
A9	2.14152	-0.00240	0.00000	-0.00838	-0.00838	2.13313
A10	1.88971	-0.00331	0.00000	-0.00848	-0.00848	1.88123
A11	2.24697	-0.01844	0.00000	-0.10589	-0.10606	2.14090
A12	2.14520	0.02179	0.00000	0.11551	0.11545	2.26065
A13	1.90146	-0.00414	0.00000	-0.01111	-0.01112	1.89034
A14	2.22831	-0.02043	0.00000	-0.07674	-0.07692	2.15139
A15	2.15113	0.02462	0.00000	0.08947	0.08939	2.24052
A16	1.95878	0.00784	0.00000	0.03199	0.03064	1.98943
A17	1.86477	0.00317	0.00000	0.05593	0.05482	1.91959
A18	1.87525	-0.00736	0.00000	-0.06554	-0.06526	1.80999
A19	1.88706	-0.00252	0.00000	0.00964	0.00757	1.89462
A20	1.96601	-0.00252	0.00000	-0.03324	-0.03340	1.93261
A21	1.90904	0.00171	0.00000	0.00604	0.00707	1.91611
A22	1.92965	-0.00183	0.00000	-0.01230	-0.01215	1.91750
A23	1.89283	0.00124	0.00000	-0.00844	-0.00876	1.88407
A24	1.92654	-0.00523	0.00000	-0.02090	-0.02099	1.90555
A25	1.89508	-0.00115	0.00000	-0.00623	-0.00648	1.88860
A26	1.87659	0.00672	0.00000	0.05580	0.05583	1.93242
A27	1.94319	0.00026	0.00000	-0.00775	-0.00815	1.93504
A28	2.66802	0.02584	0.00000	0.09503	0.09503	2.76305
A29	2.17753	0.00003	0.00000	0.00012	0.00012	2.17765

A30	1.95760	-0.00021	0.00000	-0.00114	-0.00114	1.95647
A31	2.14805	0.00018	0.00000	0.00102	0.00102	2.14907
A32	2.07971	-0.00001	0.00000	-0.00008	-0.00008	2.07962
A33	2.15775	0.00001	0.00000	0.00004	0.00004	2.15779
A34	2.04573	0.00001	0.00000	0.00004	0.00004	2.04577
A35	1.91063	0.00376	0.00000	0.02874	0.02780	1.93843
A36	1.91063	0.00750	0.00000	0.04927	0.04835	1.95898
A37	1.91063	-0.00323	0.00000	-0.00169	-0.00334	1.90729
D1	0.00444	-0.00052	0.00000	-0.00864	-0.00818	-0.00375
D2	-3.13680	0.00010	0.00000	0.00108	0.00102	-3.13578
D3	3.14022	-0.00072	0.00000	-0.01001	-0.00950	3.13072
D4	-0.00102	-0.00009	0.00000	-0.00028	-0.00030	-0.00132
D5	-0.00643	0.00036	0.00000	0.00620	0.00589	-0.00055
D6	-3.07654	-0.00167	0.00000	-0.02348	-0.02256	-3.09910
D7	3.14037	0.00053	0.00000	0.00743	0.00709	-3.13573
D8	0.07026	-0.00149	0.00000	-0.02225	-0.02136	0.04890
D9	-0.00098	0.00054	0.00000	0.00823	0.00776	0.00678
D10	3.13888	0.00063	0.00000	0.01132	0.01074	-3.13356
D11	3.14029	-0.00003	0.00000	-0.00058	-0.00056	3.13973
D12	-0.00303	0.00007	0.00000	0.00252	0.00242	-0.00061
D13	-0.00302	-0.00032	0.00000	-0.00443	-0.00418	-0.00720
D14	3.08412	0.00126	0.00000	0.02384	0.02247	3.10659
D15	3.14018	-0.00040	0.00000	-0.00730	-0.00695	3.13324
D16	-0.05587	0.00117	0.00000	0.02097	0.01970	-0.03616
D17	0.05324	-0.00004	0.00000	-0.00146	-0.00138	0.05185
D18	-3.08570	-0.00006	0.00000	-0.00178	-0.00170	-3.08740
D19	-3.09031	0.00007	0.00000	0.00204	0.00196	-3.08835
D20	0.05395	0.00005	0.00000	0.00172	0.00164	0.05559
D21	0.00582	-0.00004	0.00000	-0.00110	-0.00106	0.00476
D22	3.07976	-0.00028	0.00000	0.01899	0.02069	3.10045
D23	-3.08518	-0.00004	0.00000	-0.01928	-0.02130	-3.10648
D24	-0.01124	-0.00028	0.00000	0.00081	0.00045	-0.01079
D25	-2.75347	0.00130	0.00000	0.05743	0.05740	-2.69607
D26	0.32652	0.00214	0.00000	0.08464	0.08468	0.41119
D27	1.68519	-0.00270	0.00000	-0.06307	-0.06362	1.62157
D28	-2.53248	0.00064	0.00000	0.00184	0.00308	-2.52940
D29	-0.48532	0.00054	0.00000	0.00442	0.00406	-0.48126
D30	-1.37554	-0.00357	0.00000	-0.09160	-0.09236	-1.46790
D31	0.68998	-0.00023	0.00000	-0.02668	-0.02566	0.66432
D32	2.73714	-0.00033	0.00000	-0.02410	-0.02469	2.71246
D33	-1.60211	0.00935	0.00000	0.21929	0.21934	-1.38277
D34	0.47379	0.00763	0.00000	0.19928	0.19933	0.67311
D35	2.60690	0.00547	0.00000	0.17106	0.17122	2.77812
D36	2.62877	0.00248	0.00000	0.12590	0.12575	2.75452

D37	-1.57851	0.00077	0.00000	0.10590	0.10573	-1.47278
D38	0.55460	-0.00139	0.00000	0.07768	0.07762	0.63223
D39	0.51717	0.00366	0.00000	0.13276	0.13277	0.64994
D40	2.59307	0.00194	0.00000	0.11275	0.11275	2.70582
D41	-1.55700	-0.00022	0.00000	0.08453	0.08464	-1.47236
D42	1.63719	0.00091	0.00000	0.06304	0.06248	1.69967
D43	-2.55160	0.00385	0.00000	0.10875	0.10904	-2.44257
D44	-0.46901	0.00205	0.00000	0.05574	0.05545	-0.41357
D45	1.62538	0.00499	0.00000	0.10144	0.10200	1.72739
D46	-2.54278	-0.00086	0.00000	0.03322	0.03279	-2.50999
D47	-0.44839	0.00208	0.00000	0.07892	0.07935	-0.36904
D48	-3.13556	-0.00001	0.00000	-0.00019	-0.00019	-3.13575
D49	0.00608	0.00002	0.00000	0.00028	0.00028	0.00637
D50	0.00309	0.00001	0.00000	0.00016	0.00016	0.00325
D51	-3.13845	0.00003	0.00000	0.00063	0.00063	-3.13782

Item	Value	Threshold	Converged?
Maximum Force	0.025836	0.000450	NO
RMS Force	0.005760	0.000300	NO
Maximum Displacement	1.406316	0.001800	NO
RMS Displacement	0.230894	0.001200	NO

Predicted change in Energy=-1.448524D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.756456	-1.937466	0.207214
2	6	0	-2.788868	-1.088670	-0.010105
3	7	0	-2.249119	0.188516	0.010220
4	6	0	-0.919483	0.111019	0.226286
5	7	0	-0.599453	-1.187247	0.353518
6	6	0	0.743721	-1.791002	0.554067
7	6	0	1.536029	-2.009855	-0.754896
8	1	0	-1.745653	-3.011504	0.276321
9	1	0	-3.834591	-1.281551	-0.165267
10	1	0	1.338485	-1.164210	1.218920
11	1	0	0.528789	-2.744303	1.039419
12	1	0	1.176839	-2.916464	-1.261697
13	1	0	1.348228	-1.158189	-1.407310
14	35	0	1.621115	2.221573	0.078548
15	1	0	-0.263781	1.005670	0.251657
16	6	0	-2.918204	1.431035	-0.159068

17	6	0	-4.228189	1.569644	-0.316270
18	1	0	-2.231619	2.268160	-0.148144
19	1	0	-4.641460	2.560542	-0.443370
20	1	0	-4.922264	0.738870	-0.325095
21	7	0	2.965680	-2.122473	-0.440284
22	1	0	3.250419	-3.092978	-0.382422
23	1	0	3.545357	-1.644203	-1.116958

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.354089	0.000000			
3	N	2.191192	1.386704	0.000000		
4	C	2.212957	2.233772	1.349305	0.000000	
5	N	1.386683	2.221593	2.175311	1.343169	0.000000
6	C	2.528368	3.645647	3.629236	2.547817	1.486222
7	C	3.430940	4.484197	4.443600	3.389744	2.542744
8	H	1.076314	2.206270	3.250295	3.230358	2.155840
9	H	2.210794	1.074623	2.169243	3.254293	3.277827
10	H	3.346660	4.307116	4.020165	2.776680	2.122512
11	H	2.562400	3.853501	4.168627	3.303262	2.041522
12	H	3.423500	4.542482	4.795400	3.971689	2.958770
13	H	3.585111	4.367216	4.094375	3.069534	2.625799
14	Br	5.359305	5.514845	4.372265	3.306191	4.077571
15	H	3.300319	3.291025	2.160463	1.109499	2.220797
16	C	3.581985	2.527416	1.421332	2.426072	3.534791
17	C	4.322421	3.038423	2.435329	3.656431	4.606169
18	H	4.247276	3.405568	2.085738	2.552480	3.854280
19	H	5.383176	4.115406	3.399345	4.505743	5.569451
20	H	4.179530	2.826748	2.749733	4.089068	4.780914
21	N	4.769911	5.862476	5.721692	4.530706	3.770271
22	H	5.172202	6.374077	6.416174	5.293790	4.358318
23	H	5.472537	6.454158	6.181047	4.981958	4.421601

		6	7	8	9	10
6	C	0.000000				
7	C	1.545650	0.000000			
8	H	2.786351	3.582757	0.000000		
9	H	4.662394	5.451756	2.747981	0.000000	
10	H	1.090249	2.156407	3.716571	5.356347	0.000000
11	H	1.091121	2.184837	2.413877	4.757099	1.784523
12	H	2.179738	1.099001	3.303860	5.384192	3.041379
13	H	2.147762	1.089150	3.980137	5.330994	2.626255
14	Br	4.134815	4.313566	6.225700	6.488147	3.583832
15	H	2.987957	3.653198	4.281851	4.260973	2.865525

16	C	4.929480	5.659940	4.615256	2.863202	5.172383
17	C	6.063936	6.799368	5.244146	2.882193	6.388945
18	H	5.081589	5.732777	5.318947	3.894902	5.137672
19	H	6.995069	7.690705	6.320709	3.935742	7.238559
20	H	6.267102	7.032053	4.951552	2.300148	6.723293
21	N	2.456768	1.468185	4.847737	6.857585	2.513760
22	H	2.975851	2.061802	5.039972	7.316132	3.152767
23	H	3.265431	2.074173	5.639639	7.449890	3.249155

		11	12	13	14	15
11	H	0.000000				
12	H	2.396820	0.000000			
13	H	3.028815	1.772599	0.000000		
14	Br	5.174589	5.328514	3.702031	0.000000	
15	H	3.912932	4.443958	3.167496	2.249715	0.000000
16	C	5.545410	6.073377	5.144378	4.613765	2.719484
17	C	6.563297	7.087547	6.303004	5.898750	4.044396
18	H	5.844223	6.303801	5.112795	3.859678	2.371942
19	H	7.554570	8.032426	7.115793	6.293421	4.697315
20	H	6.611231	7.172012	6.639962	6.721394	4.701627
21	N	2.917984	2.122520	2.116869	4.576875	4.549009
22	H	3.090385	2.259207	2.900369	5.577776	5.436044
23	H	3.867799	2.692485	2.268896	4.480644	4.837816

		16	17	18	19	20
16	C	0.000000				
17	C	1.326645	0.000000			
18	H	1.082727	2.121906	0.000000		
19	H	2.079959	1.081123	2.445400	0.000000	
20	H	2.126714	1.082591	3.099937	1.846978	0.000000
21	N	6.879432	8.086956	6.809914	8.933041	8.391676
22	H	7.653005	8.813286	7.671338	9.708129	9.026578
23	H	7.221652	8.449730	7.044050	9.228087	8.832140

		21	22	23
21	N	0.000000		
22	H	1.013067	0.000000	
23	H	1.011265	1.650904	0.000000

Stoichiometry C7H12BrN3
Framework group C1[X(C7H12BrN3)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Atomic Atomic Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-1.637778	2.159343	-0.258318
2	6	0	-2.676335	1.327150	-0.008493
3	7	0	-2.150017	0.044221	-0.002987
4	6	0	-0.822192	0.102286	-0.235646
5	7	0	-0.490288	1.393546	-0.398712
6	6	0	0.856663	1.977919	-0.629116
7	6	0	1.665982	2.220768	0.665125
8	1	0	-1.616712	3.231164	-0.354268
9	1	0	-3.718190	1.534856	0.153402
10	1	0	1.437366	1.328590	-1.284706
11	1	0	0.646055	2.921114	-1.135647
12	1	0	1.321911	3.143405	1.153141
13	1	0	1.476845	1.387568	1.340590
14	35	0	1.698074	-2.030682	-0.063568
15	1	0	-0.176057	-0.799597	-0.245996
16	6	0	-2.829884	-1.186581	0.204602
17	6	0	-4.139358	-1.307403	0.379723
18	1	0	-2.152115	-2.030927	0.206918
19	1	0	-4.561331	-2.290424	0.536035
20	1	0	-4.824705	-0.469379	0.375549
21	7	0	3.093054	2.310442	0.331974
22	1	0	3.387086	3.276152	0.246805
23	1	0	3.675422	1.842994	1.013881

Rotational constants (GHZ): 0.7052309 0.4890493 0.2975302
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 365 symmetry adapted cartesian basis functions of A symmetry.
There are 352 symmetry adapted basis functions of A symmetry.
352 basis functions, 562 primitive gaussians, 365 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 822.5646007602 Hartrees.
NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 352 RedAO= T EigKep= 4.28D-06 NBF= 352
NBsUse= 352 1.00D-06 EigRej= -1.00D+00 NBFU= 352
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999278 0.016830 -0.002035 0.033988 Ang= 4.35 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3012.45662646 A.U. after 15 cycles

NFock= 15 Conv=0.23D-08 -V/T= 2.0017

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000161671	-0.003506160	-0.000287235
2	6	0.000204294	0.000005544	0.000714355
3	7	-0.000262473	0.000620060	-0.000632683
4	6	-0.004521975	-0.001426711	0.000470926
5	7	-0.000209261	0.004074086	-0.002730994
6	6	-0.001540889	0.000924643	0.000637187
7	6	0.002113177	-0.001934367	0.001373624
8	1	0.000186047	-0.000136985	-0.000169609
9	1	0.000153583	-0.000114738	-0.000032860
10	1	-0.002977128	0.002351444	-0.001335065
11	1	0.004286484	0.000224098	0.003154698
12	1	-0.003670995	0.002786553	-0.000878851
13	1	0.003117954	0.002029588	-0.000568108
14	35	-0.003943423	-0.002162519	-0.000569902
15	1	0.010830624	-0.004951907	0.000946157
16	6	0.000189928	0.001503132	-0.000158042
17	6	0.000107653	-0.000464263	0.000051973
18	1	0.000463458	0.000279437	-0.000023552
19	1	0.000074063	0.000009018	0.000024962

20	1	-0.000153895	-0.000004245	-0.000013471
21	7	-0.006603934	-0.002790739	0.000168090
22	1	0.002224259	0.001553486	-0.001143151
23	1	0.000094120	0.001131547	0.001001552

Cartesian Forces: Max 0.010830624 RMS 0.002358223

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.011803741 RMS 0.002674747

Search for a local minimum.

Step number 2 out of a maximum of 121

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 1 2

DE= -6.37D-03 DEPred=-1.45D-02 R= 4.40D-01

Trust test= 4.40D-01 RLast= 5.69D-01 DXMaxT set to 3.00D-01

ITU= 0 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00230	0.00265	0.00665	0.00787	0.01402
Eigenvalues ---	0.01532	0.01866	0.01908	0.02144	0.02173
Eigenvalues ---	0.02315	0.02385	0.02430	0.03062	0.03062
Eigenvalues ---	0.03595	0.03749	0.04406	0.04481	0.05295
Eigenvalues ---	0.05555	0.08737	0.09578	0.12279	0.12916
Eigenvalues ---	0.15710	0.15999	0.16000	0.16000	0.16000
Eigenvalues ---	0.16000	0.16000	0.17743	0.21602	0.22000
Eigenvalues ---	0.22286	0.22929	0.23555	0.24062	0.24999
Eigenvalues ---	0.27438	0.29194	0.33125	0.34088	0.34405
Eigenvalues ---	0.34762	0.34920	0.35138	0.35687	0.35690
Eigenvalues ---	0.35858	0.36095	0.36436	0.36656	0.42176
Eigenvalues ---	0.43012	0.46393	0.47366	0.47698	0.49570
Eigenvalues ---	0.54374	0.57986	0.60352		

RFO step: Lambda=-2.66525463D-03 EMin= 2.29999493D-03

Quartic linear search produced a step of -0.24226.

Iteration 1 RMS(Cart)= 0.10476797 RMS(Int)= 0.00380722

Iteration 2 RMS(Cart)= 0.00467106 RMS(Int)= 0.00013428

Iteration 3 RMS(Cart)= 0.00001405 RMS(Int)= 0.00013394

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00013394

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55886	0.00219	0.00183	0.00196	0.00375	2.56261
R2	2.62045	0.00052	-0.00108	0.00193	0.00083	2.62128

R3	2.03394	0.00013	0.00003	0.00022	0.00026	2.03419
R4	2.62049	0.00276	0.00190	0.00295	0.00484	2.62533
R5	2.03074	-0.00012	-0.00002	-0.00023	-0.00024	2.03050
R6	2.54982	-0.00109	-0.00076	-0.00113	-0.00186	2.54795
R7	2.68593	0.00084	0.00028	0.00114	0.00142	2.68735
R8	2.53822	-0.01044	-0.00459	-0.00870	-0.01325	2.52497
R9	2.09665	-0.00166	-0.00181	-0.00158	-0.00338	2.09327
R10	2.80855	-0.00489	-0.00351	-0.00624	-0.00975	2.79880
R11	2.92086	-0.00175	0.00262	-0.00769	-0.00507	2.91578
R12	2.06027	-0.00109	-0.00060	-0.00159	-0.00218	2.05809
R13	2.06192	0.00036	-0.00032	0.00114	0.00082	2.06274
R14	2.07681	-0.00070	-0.00254	0.00148	-0.00106	2.07575
R15	2.05819	0.00139	0.00334	-0.00090	0.00244	2.06063
R16	2.77447	-0.00415	0.00083	-0.00951	-0.00868	2.76579
R17	4.25135	-0.00443	0.01584	-0.09329	-0.07745	4.17390
R18	2.50699	-0.00008	-0.00009	0.00001	-0.00008	2.50692
R19	2.04606	0.00051	-0.00007	0.00113	0.00106	2.04711
R20	2.04303	-0.00002	0.00000	-0.00005	-0.00005	2.04298
R21	2.04580	0.00011	-0.00002	0.00025	0.00022	2.04602
R22	1.91442	-0.00093	-0.00598	0.00566	-0.00032	1.91410
R23	1.91101	-0.00008	-0.00516	0.00600	0.00084	1.91186
A1	1.89016	-0.00360	-0.00359	-0.00558	-0.00921	1.88094
A2	2.26982	0.00196	0.00188	0.00339	0.00528	2.27510
A3	2.12319	0.00164	0.00171	0.00215	0.00387	2.12706
A4	1.85273	0.00010	0.00225	0.00220	0.00438	1.85711
A5	2.28181	-0.00019	-0.00109	-0.00171	-0.00282	2.27899
A6	2.14861	0.00009	-0.00115	-0.00036	-0.00154	2.14707
A7	1.91029	-0.00248	-0.00340	-0.00293	-0.00630	1.90399
A8	2.23977	0.00264	0.00137	0.00595	0.00730	2.24707
A9	2.13313	-0.00016	0.00203	-0.00302	-0.00101	2.13212
A10	1.88123	0.00248	0.00205	0.00189	0.00383	1.88507
A11	2.14090	0.00797	0.02569	0.01125	0.03666	2.17757
A12	2.26065	-0.01048	-0.02797	-0.01400	-0.04215	2.21849
A13	1.89034	0.00350	0.00269	0.00448	0.00719	1.89753
A14	2.15139	0.00830	0.01864	0.00400	0.02261	2.17400
A15	2.24052	-0.01180	-0.02166	-0.00892	-0.03063	2.20989
A16	1.98943	-0.00638	-0.00742	-0.01288	-0.02047	1.96896
A17	1.91959	-0.00002	-0.01328	-0.01158	-0.02518	1.89441
A18	1.80999	0.00382	0.01581	0.01838	0.03421	1.84420
A19	1.89462	0.00168	-0.00183	-0.00926	-0.01130	1.88332
A20	1.93261	0.00248	0.00809	0.01866	0.02683	1.95944
A21	1.91611	-0.00152	-0.00171	-0.00212	-0.00375	1.91236
A22	1.91750	-0.00006	0.00294	0.00090	0.00377	1.92127
A23	1.88407	0.00101	0.00212	-0.00405	-0.00199	1.88208

A24	1.90555	-0.00199	0.00509	-0.01210	-0.00709	1.89846
A25	1.88860	-0.00059	0.00157	-0.00463	-0.00292	1.88568
A26	1.93242	0.00281	-0.01352	0.03666	0.02315	1.95557
A27	1.93504	-0.00121	0.00197	-0.01763	-0.01560	1.91944
A28	2.76305	0.00035	-0.02302	0.02738	0.00436	2.76741
A29	2.17765	-0.00041	-0.00003	-0.00132	-0.00135	2.17630
A30	1.95647	0.00002	0.00028	-0.00044	-0.00017	1.95630
A31	2.14907	0.00038	-0.00025	0.00176	0.00152	2.15058
A32	2.07962	-0.00017	0.00002	-0.00081	-0.00079	2.07883
A33	2.15779	0.00020	-0.00001	0.00094	0.00093	2.15872
A34	2.04577	-0.00003	-0.00001	-0.00013	-0.00014	2.04563
A35	1.93843	0.00360	-0.00674	0.02543	0.01887	1.95730
A36	1.95898	-0.00025	-0.01171	0.01328	0.00174	1.96072
A37	1.90729	-0.00140	0.00081	-0.00485	-0.00374	1.90355
D1	-0.00375	0.00058	0.00198	0.01568	0.01773	0.01398
D2	-3.13578	0.00004	-0.00025	0.00113	0.00086	-3.13492
D3	3.13072	0.00037	0.00230	0.00894	0.01124	-3.14122
D4	-0.00132	-0.00017	0.00007	-0.00560	-0.00563	-0.00694
D5	-0.00055	-0.00055	-0.00143	-0.01448	-0.01597	-0.01652
D6	-3.09910	0.00005	0.00546	-0.00400	0.00132	-3.09778
D7	-3.13573	-0.00037	-0.00172	-0.00843	-0.01016	3.13729
D8	0.04890	0.00023	0.00517	0.00205	0.00713	0.05603
D9	0.00678	-0.00043	-0.00188	-0.01159	-0.01360	-0.00681
D10	-3.13356	-0.00058	-0.00260	-0.01734	-0.02015	3.12947
D11	3.13973	0.00006	0.00014	0.00156	0.00167	3.14140
D12	-0.00061	-0.00009	-0.00059	-0.00419	-0.00488	-0.00550
D13	-0.00720	0.00008	0.00101	0.00276	0.00382	-0.00338
D14	3.10659	-0.00100	-0.00544	-0.02719	-0.03322	3.07337
D15	3.13324	0.00023	0.00168	0.00809	0.00986	-3.14009
D16	-0.03616	-0.00086	-0.00477	-0.02185	-0.02717	-0.06334
D17	0.05185	0.00011	0.00034	0.00456	0.00495	0.05680
D18	-3.08740	0.00012	0.00041	0.00466	0.00512	-3.08228
D19	-3.08835	-0.00006	-0.00047	-0.00184	-0.00237	-3.09071
D20	0.05559	-0.00005	-0.00040	-0.00175	-0.00219	0.05339
D21	0.00476	0.00029	0.00026	0.00708	0.00739	0.01215
D22	3.10045	0.00033	-0.00501	-0.00365	-0.00861	3.09184
D23	-3.10648	0.00106	0.00516	0.03920	0.04384	-3.06264
D24	-0.01079	0.00110	-0.00011	0.02847	0.02784	0.01705
D25	-2.69607	0.00126	-0.01391	0.07405	0.06007	-2.63600
D26	0.41119	0.00024	-0.02051	0.03749	0.01705	0.42824
D27	1.62157	0.00219	0.01541	0.08732	0.10274	1.72430
D28	-2.52940	-0.00017	-0.00075	0.05737	0.05673	-2.47267
D29	-0.48126	0.00011	-0.00098	0.05939	0.05849	-0.42277
D30	-1.46790	0.00237	0.02238	0.09957	0.12182	-1.34608

D31	0.66432	0.00001	0.00622	0.06961	0.07581	0.74013
D32	2.71246	0.00029	0.00598	0.07164	0.07757	2.79003
D33	-1.38277	0.00039	-0.05314	0.10951	0.05645	-1.32632
D34	0.67311	0.00024	-0.04829	0.10211	0.05389	0.72700
D35	2.77812	-0.00178	-0.04148	0.07135	0.02993	2.80805
D36	2.75452	0.00356	-0.03046	0.14027	0.10972	2.86425
D37	-1.47278	0.00340	-0.02562	0.13287	0.10716	-1.36561
D38	0.63223	0.00139	-0.01881	0.10211	0.08321	0.71544
D39	0.64994	0.00284	-0.03216	0.13734	0.10521	0.75514
D40	2.70582	0.00268	-0.02732	0.12994	0.10265	2.80847
D41	-1.47236	0.00067	-0.02051	0.09918	0.07869	-1.39367
D42	1.69967	0.00098	-0.01514	0.05158	0.03652	1.73618
D43	-2.44257	0.00162	-0.02642	0.07347	0.04697	-2.39559
D44	-0.41357	0.00056	-0.01343	0.03510	0.02166	-0.39191
D45	1.72739	0.00121	-0.02471	0.05698	0.03211	1.75950
D46	-2.50999	0.00024	-0.00794	0.02832	0.02054	-2.48945
D47	-0.36904	0.00089	-0.01922	0.05021	0.03100	-0.33804
D48	-3.13575	-0.00001	0.00005	-0.00030	-0.00026	-3.13601
D49	0.00637	0.00000	-0.00007	0.00010	0.00003	0.00640
D50	0.00325	-0.00002	-0.00004	-0.00042	-0.00045	0.00280
D51	-3.13782	0.00000	-0.00015	-0.00001	-0.00016	-3.13798

Item	Value	Threshold	Converged?
Maximum Force	0.011804	0.000450	NO
RMS Force	0.002675	0.000300	NO
Maximum Displacement	0.481887	0.001800	NO
RMS Displacement	0.105453	0.001200	NO

Predicted change in Energy=-3.086627D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.800433	-1.980173	0.254366
2	6	0	-2.817410	-1.109051	0.040266
3	7	0	-2.250001	0.158880	0.018884
4	6	0	-0.921827	0.051159	0.224592
5	7	0	-0.631571	-1.243843	0.379635
6	6	0	0.714890	-1.830793	0.569563
7	6	0	1.522364	-1.912639	-0.742697
8	1	0	-1.808046	-3.053251	0.339145
9	1	0	-3.868362	-1.282641	-0.100808
10	1	0	1.270556	-1.204593	1.266148

11	1	0	0.547950	-2.813483	1.014475
12	1	0	1.155018	-2.743367	-1.360370
13	1	0	1.360293	-0.985280	-1.292967
14	35	0	1.703108	1.966570	-0.093385
15	1	0	-0.207708	0.897500	0.197075
16	6	0	-2.884942	1.414812	-0.185582
17	6	0	-4.191891	1.584338	-0.337314
18	1	0	-2.174074	2.231954	-0.206920
19	1	0	-4.578225	2.581963	-0.493066
20	1	0	-4.909272	0.773733	-0.314090
21	7	0	2.941255	-2.057778	-0.414395
22	1	0	3.251824	-3.019672	-0.479731
23	1	0	3.532027	-1.479428	-0.997541

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.356073	0.000000			
3	N	2.198434	1.389265	0.000000		
4	C	2.213401	2.230089	1.348319	0.000000	
5	N	1.387124	2.216130	2.171886	1.336158	0.000000
6	C	2.539392	3.643928	3.612841	2.517855	1.481060
7	C	3.469824	4.482458	4.370576	3.281192	2.519197
8	H	1.076449	2.210896	3.258171	3.230460	2.158632
9	H	2.211115	1.074493	2.170576	3.250689	3.272484
10	H	3.325087	4.268885	3.976059	2.732818	2.098936
11	H	2.605202	3.896129	4.201746	3.315167	2.063507
12	H	3.453191	4.518070	4.681830	3.825541	2.909998
13	H	3.657081	4.387030	4.008026	2.930061	2.613804
14	Br	5.288904	5.469221	4.348266	3.264995	3.997652
15	H	3.289538	3.295661	2.179054	1.107708	2.190512
16	C	3.591050	2.534848	1.422084	2.425204	3.530666
17	C	4.333001	3.047311	2.435107	3.655091	4.603097
18	H	4.253753	3.411348	2.086718	2.551508	3.847666
19	H	5.393317	4.124136	3.399125	4.504359	5.565472
20	H	4.191899	2.836605	2.749662	4.088032	4.780230
21	N	4.789245	5.853975	5.661310	4.447395	3.749408
22	H	5.210063	6.384080	6.373530	5.229287	4.355782
23	H	5.500286	6.444344	6.095000	4.865503	4.391772

		6	7	8	9	10
6	C	0.000000				
7	C	1.542965	0.000000			
8	H	2.812952	3.682800	0.000000		
9	H	4.664340	5.465240	2.752003	0.000000	

10	H	1.089093	2.144807	3.708728	5.318190	0.000000
11	H	1.091556	2.201967	2.462575	4.805325	1.781580
12	H	2.179712	1.098441	3.429888	5.380945	3.046272
13	H	2.144867	1.090440	4.120517	5.371080	2.570062
14	Br	3.979452	3.937326	6.141163	6.449705	3.477313
15	H	2.904052	3.431210	4.264939	4.271082	2.783339
16	C	4.905404	5.550375	4.625866	2.872378	5.122204
17	C	6.046656	6.711624	5.258093	2.894853	6.339365
18	H	5.045291	5.579280	5.325933	3.903108	5.083824
19	H	6.972708	7.581619	6.334201	3.948789	7.186173
20	H	6.260639	6.983283	4.968916	2.314661	6.678413
21	N	2.444667	1.463591	4.910667	6.860762	2.518608
22	H	2.991736	2.070194	5.125814	7.338795	3.204377
23	H	3.242767	2.071560	5.725385	7.457119	3.211553

		11	12	13	14	15
11	H	0.000000				
12	H	2.452211	0.000000			
13	H	3.053934	1.771313	0.000000		
14	Br	5.040897	4.908070	3.204674	0.000000	
15	H	3.874346	4.187908	2.867702	2.208731	0.000000
16	C	5.577039	5.915392	5.000876	4.622027	2.753475
17	C	6.605623	6.954503	6.192168	5.912411	4.078116
18	H	5.861541	6.096485	4.901208	3.887912	2.410514
19	H	7.593496	7.872829	6.973597	6.324048	4.734462
20	H	6.664419	7.088040	6.584813	6.722732	4.730889
21	N	2.888022	2.134371	2.102756	4.222727	4.361597
22	H	3.096143	2.290953	2.894477	5.235494	5.269788
23	H	3.838310	2.716497	2.246751	4.004665	4.589391

		16	17	18	19	20
16	C	0.000000				
17	C	1.326603	0.000000			
18	H	1.083286	2.123203	0.000000		
19	H	2.079421	1.081096	2.446288	0.000000	
20	H	2.127301	1.082708	3.101484	1.846976	0.000000
21	N	6.786443	8.009539	6.679180	8.836060	8.346154
22	H	7.577010	8.753633	7.556083	9.627469	9.001158
23	H	7.086141	8.335555	6.852666	9.084359	8.763525

		21	22	23
21	N	0.000000		
22	H	1.012899	0.000000	
23	H	1.011711	1.648937	0.000000

Stoichiometry C7H12BrN3

Framework group C1[X(C7H12BrN3)]

Deg. of freedom 63

Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.696604	2.141139	-0.209847
2	6	0	-2.720310	1.280317	0.013642
3	7	0	-2.172814	0.003797	-0.014648
4	6	0	-0.850020	0.096621	-0.258705
5	7	0	-0.544027	1.390634	-0.389912
6	6	0	0.805173	1.961790	-0.606660
7	6	0	1.653692	1.997562	0.681547
8	1	0	-1.689690	3.216036	-0.267207
9	1	0	-3.763541	1.466138	0.191619
10	1	0	1.329166	1.345378	-1.335762
11	1	0	0.640375	2.958029	-1.021201
12	1	0	1.318751	2.817586	1.331121
13	1	0	1.493786	1.058907	1.212974
14	35	0	1.752533	-1.865936	-0.070879
15	1	0	-0.148987	-0.760883	-0.274768
16	6	0	-2.821148	-1.247210	0.177631
17	6	0	-4.125370	-1.400743	0.365534
18	1	0	-2.123088	-2.075318	0.156234
19	1	0	-4.522616	-2.396074	0.507947
20	1	0	-4.830101	-0.579021	0.385085
21	7	0	3.063988	2.129568	0.313124
22	1	0	3.391721	3.084640	0.393071
23	1	0	3.663053	1.527501	0.862846

Rotational constants (GHZ): 0.7844732 0.4835611 0.3082103
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 365 symmetry adapted cartesian basis functions of A symmetry.
There are 352 symmetry adapted basis functions of A symmetry.
352 basis functions, 562 primitive gaussians, 365 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 833.5001773764 Hartrees.
NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.
NBasis= 352 RedAO= T EigKep= 4.31D-06 NBF= 352
NBsUse= 352 1.00D-06 EigRej= -1.00D+00 NBFU= 352
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999925 -0.008950 -0.000807 -0.008364 Ang= -1.41 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3012.46070248 A.U. after 12 cycles
NFock= 12 Conv=0.96D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000712998	-0.000027048	0.001297467
2	6	0.000025360	-0.000058946	-0.001031437
3	7	-0.000511398	-0.000078810	0.000066499
4	6	-0.004329998	-0.000415726	0.000014769
5	7	-0.001614034	-0.002539133	-0.002449096
6	6	0.000790698	0.004464481	-0.000290690
7	6	0.002069154	-0.001722994	0.000769346
8	1	0.000055622	0.000111453	0.000177244
9	1	-0.000075150	-0.000001872	-0.000066821
10	1	-0.000950387	0.000864126	-0.000184408
11	1	0.002201175	0.000409883	0.000913967
12	1	-0.002008207	0.001036714	-0.000287469
13	1	0.002168153	0.001676907	0.000844272

14	35	-0.001982255	-0.000540281	-0.000868029
15	1	0.007547541	-0.001719490	0.001429211
16	6	0.000047002	0.000279474	0.000121099
17	6	-0.000012513	-0.000065963	0.000035434
18	1	0.000100464	-0.000165555	-0.000047905
19	1	-0.000021311	0.000027013	-0.000024196
20	1	0.000031637	-0.000016078	0.000013779
21	7	-0.002946217	-0.004310942	-0.000921890
22	1	0.000793619	0.001155490	-0.000980703
23	1	-0.000665958	0.001637295	0.001469559

Cartesian Forces: Max 0.007547541 RMS 0.001661158

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.005974176 RMS 0.001300589
Search for a local minimum.
Step number 3 out of a maximum of 121
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 2 3
DE= -4.08D-03 DEPred=-3.09D-03 R= 1.32D+00
TightC=F SS= 1.41D+00 RLast= 3.76D-01 DXNew= 5.0454D-01 1.1279D+00
Trust test= 1.32D+00 RLast= 3.76D-01 DXMaxT set to 5.05D-01
ITU= 1 0 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00227	0.00265	0.00481	0.00788	0.01401
Eigenvalues ---	0.01535	0.01832	0.01875	0.02126	0.02207
Eigenvalues ---	0.02316	0.02375	0.02405	0.03062	0.03062
Eigenvalues ---	0.03600	0.03677	0.04404	0.04601	0.05342
Eigenvalues ---	0.05605	0.08678	0.09452	0.12391	0.12890
Eigenvalues ---	0.15172	0.15845	0.15998	0.15999	0.16000
Eigenvalues ---	0.16000	0.16000	0.16077	0.21719	0.22000
Eigenvalues ---	0.22368	0.23188	0.23464	0.23766	0.24243
Eigenvalues ---	0.25157	0.27472	0.33498	0.34064	0.34406
Eigenvalues ---	0.34758	0.34924	0.35482	0.35587	0.35689
Eigenvalues ---	0.35829	0.35865	0.36443	0.36661	0.42191
Eigenvalues ---	0.42931	0.46275	0.47247	0.47686	0.49414
Eigenvalues ---	0.54373	0.57167	0.60352		

RFO step: Lambda=-2.61375517D-03 EMin= 2.27384549D-03
Quartic linear search produced a step of 0.93645.
Iteration 1 RMS(Cart)= 0.15145497 RMS(Int)= 0.01547770

Iteration 2 RMS(Cart)= 0.01865246 RMS(Int)= 0.00071923
Iteration 3 RMS(Cart)= 0.00042838 RMS(Int)= 0.00065253
Iteration 4 RMS(Cart)= 0.00000023 RMS(Int)= 0.00065253

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56261	0.00083	0.00351	0.00065	0.00398	2.56659
R2	2.62128	0.00024	0.00078	-0.00037	0.00036	2.62164
R3	2.03419	-0.00010	0.00024	-0.00068	-0.00044	2.03375
R4	2.62533	0.00069	0.00453	-0.00046	0.00403	2.62936
R5	2.03050	0.00008	-0.00023	0.00060	0.00037	2.03087
R6	2.54795	0.00011	-0.00174	0.00147	-0.00014	2.54781
R7	2.68735	-0.00003	0.00133	-0.00130	0.00003	2.68739
R8	2.52497	-0.00372	-0.01241	-0.00133	-0.01359	2.51138
R9	2.09327	0.00185	-0.00317	0.01222	0.00905	2.10232
R10	2.79880	-0.00057	-0.00913	0.00490	-0.00424	2.79456
R11	2.91578	-0.00106	-0.00475	-0.00143	-0.00618	2.90960
R12	2.05809	-0.00010	-0.00205	0.00126	-0.00078	2.05731
R13	2.06274	-0.00033	0.00077	-0.00247	-0.00170	2.06104
R14	2.07575	0.00005	-0.00099	0.00054	-0.00046	2.07530
R15	2.06063	0.00068	0.00228	0.00213	0.00441	2.06504
R16	2.76579	-0.00267	-0.00813	-0.00512	-0.01325	2.75254
R17	4.17390	-0.00186	-0.07253	0.01329	-0.05923	4.11466
R18	2.50692	0.00000	-0.00007	0.00004	-0.00004	2.50688
R19	2.04711	-0.00006	0.00099	-0.00124	-0.00025	2.04687
R20	2.04298	0.00004	-0.00005	0.00022	0.00017	2.04315
R21	2.04602	-0.00001	0.00021	-0.00024	-0.00003	2.04599
R22	1.91410	-0.00079	-0.00030	-0.00399	-0.00429	1.90981
R23	1.91186	-0.00030	0.00079	-0.00303	-0.00224	1.90961
A1	1.88094	-0.00083	-0.00863	0.00222	-0.00654	1.87440
A2	2.27510	0.00050	0.00495	-0.00073	0.00425	2.27935
A3	2.12706	0.00033	0.00363	-0.00129	0.00237	2.12943
A4	1.85711	-0.00018	0.00410	-0.00108	0.00285	1.85996
A5	2.27899	0.00011	-0.00264	0.00138	-0.00126	2.27772
A6	2.14707	0.00008	-0.00144	-0.00012	-0.00157	2.14549
A7	1.90399	-0.00084	-0.00590	-0.00042	-0.00620	1.89779
A8	2.24707	0.00068	0.00684	-0.00184	0.00482	2.25188
A9	2.13212	0.00016	-0.00095	0.00221	0.00114	2.13327
A10	1.88507	0.00100	0.00359	0.00153	0.00474	1.88981
A11	2.17757	0.00405	0.03433	0.02079	0.05366	2.23122
A12	2.21849	-0.00510	-0.03947	-0.02382	-0.06366	2.15483
A13	1.89753	0.00086	0.00673	-0.00159	0.00524	1.90277
A14	2.17400	0.00513	0.02117	0.02192	0.04304	2.21703
A15	2.20989	-0.00597	-0.02868	-0.01880	-0.04768	2.16221
A16	1.96896	-0.00144	-0.01917	0.00581	-0.01386	1.95509

A17	1.89441	0.00081	-0.02358	0.02384	-0.00044	1.89397
A18	1.84420	0.00043	0.03203	-0.01734	0.01478	1.85898
A19	1.88332	-0.00013	-0.01059	0.00208	-0.00925	1.87407
A20	1.95944	0.00083	0.02513	-0.00947	0.01573	1.97517
A21	1.91236	-0.00047	-0.00351	-0.00411	-0.00727	1.90509
A22	1.92127	0.00027	0.00353	0.00770	0.01116	1.93243
A23	1.88208	-0.00073	-0.00186	-0.01503	-0.01713	1.86496
A24	1.89846	0.00000	-0.00664	0.00604	-0.00084	1.89762
A25	1.88568	0.00034	-0.00273	0.01192	0.00937	1.89505
A26	1.95557	0.00047	0.02168	-0.01193	0.00972	1.96529
A27	1.91944	-0.00039	-0.01461	0.00105	-0.01375	1.90569
A28	2.76741	0.00074	0.00408	-0.00519	-0.00111	2.76631
A29	2.17630	-0.00005	-0.00126	0.00081	-0.00045	2.17584
A30	1.95630	-0.00015	-0.00016	-0.00147	-0.00163	1.95467
A31	2.15058	0.00020	0.00142	0.00066	0.00207	2.15266
A32	2.07883	0.00004	-0.00074	0.00118	0.00044	2.07927
A33	2.15872	-0.00006	0.00087	-0.00148	-0.00060	2.15812
A34	2.04563	0.00002	-0.00013	0.00029	0.00016	2.04580
A35	1.95730	0.00151	0.01767	0.00065	0.01825	1.97555
A36	1.96072	-0.00075	0.00163	-0.00987	-0.00830	1.95242
A37	1.90355	-0.00001	-0.00350	0.00980	0.00620	1.90975
D1	0.01398	-0.00021	0.01660	-0.03950	-0.02232	-0.00834
D2	-3.13492	-0.00013	0.00081	-0.01122	-0.01034	3.13792
D3	-3.14122	-0.00010	0.01053	-0.02204	-0.01149	3.13047
D4	-0.00694	-0.00001	-0.00527	0.00624	0.00049	-0.00646
D5	-0.01652	0.00016	-0.01496	0.03624	0.02078	0.00427
D6	-3.09778	0.00025	0.00124	0.01102	0.01125	-3.08652
D7	3.13729	0.00005	-0.00951	0.02058	0.01106	-3.13484
D8	0.05603	0.00014	0.00668	-0.00465	0.00153	0.05756
D9	-0.00681	0.00018	-0.01273	0.02961	0.01642	0.00960
D10	3.12947	-0.00009	-0.01887	0.01750	-0.00233	3.12714
D11	3.14140	0.00010	0.00156	0.00398	0.00557	-3.13622
D12	-0.00550	-0.00016	-0.00457	-0.00813	-0.01318	-0.01867
D13	-0.00338	-0.00008	0.00358	-0.00739	-0.00367	-0.00705
D14	3.07337	-0.00105	-0.03111	-0.03214	-0.06643	3.00693
D15	-3.14009	0.00016	0.00924	0.00378	0.01353	-3.12656
D16	-0.06334	-0.00081	-0.02545	-0.02097	-0.04924	-0.11257
D17	0.05680	0.00017	0.00463	0.00784	0.01279	0.06959
D18	-3.08228	0.00021	0.00480	0.01071	0.01581	-3.06646
D19	-3.09071	-0.00013	-0.00222	-0.00569	-0.00821	-3.09893
D20	0.05339	-0.00008	-0.00205	-0.00282	-0.00519	0.04821
D21	0.01215	-0.00004	0.00692	-0.01751	-0.01037	0.00178
D22	3.09184	0.00036	-0.00806	0.01018	0.00267	3.09452
D23	-3.06264	0.00051	0.04106	0.00582	0.04359	-3.01905

D24	0.01705	0.00091	0.02607	0.03350	0.05664	0.07369
D25	-2.63600	0.00134	0.05626	0.15680	0.21286	-2.42314
D26	0.42824	0.00051	0.01597	0.12869	0.14485	0.57309
D27	1.72430	0.00133	0.09621	0.04920	0.14541	1.86971
D28	-2.47267	0.00081	0.05312	0.07148	0.12515	-2.34752
D29	-0.42277	0.00088	0.05478	0.06931	0.12424	-0.29853
D30	-1.34608	0.00109	0.11407	0.01846	0.13207	-1.21402
D31	0.74013	0.00057	0.07099	0.04074	0.11181	0.85194
D32	2.79003	0.00064	0.07264	0.03857	0.11090	2.90093
D33	-1.32632	0.00162	0.05286	0.15261	0.20564	-1.12068
D34	0.72700	0.00175	0.05046	0.16246	0.21299	0.93999
D35	2.80805	0.00087	0.02803	0.15852	0.18672	2.99477
D36	2.86425	0.00159	0.10275	0.11792	0.22053	3.08478
D37	-1.36561	0.00172	0.10035	0.12777	0.22788	-1.13773
D38	0.71544	0.00084	0.07792	0.12383	0.20161	0.91705
D39	0.75514	0.00176	0.09852	0.12754	0.22613	0.98127
D40	2.80847	0.00188	0.09612	0.13738	0.23348	3.04195
D41	-1.39367	0.00100	0.07369	0.13344	0.20721	-1.18646
D42	1.73618	0.00135	0.03420	0.08287	0.11699	1.85317
D43	-2.39559	0.00191	0.04399	0.08883	0.13280	-2.26280
D44	-0.39191	0.00070	0.02028	0.07678	0.09696	-0.29494
D45	1.75950	0.00127	0.03007	0.08275	0.11277	1.87227
D46	-2.48945	0.00023	0.01924	0.06885	0.08819	-2.40126
D47	-0.33804	0.00080	0.02903	0.07482	0.10400	-0.23404
D48	-3.13601	0.00005	-0.00024	0.00320	0.00296	-3.13305
D49	0.00640	0.00003	0.00003	0.00173	0.00176	0.00816
D50	0.00280	0.00000	-0.00042	0.00002	-0.00041	0.00239
D51	-3.13798	-0.00002	-0.00015	-0.00145	-0.00161	-3.13959

Item	Value	Threshold	Converged?
Maximum Force	0.005974	0.000450	NO
RMS Force	0.001301	0.000300	NO
Maximum Displacement	0.690747	0.001800	NO
RMS Displacement	0.158132	0.001200	NO

Predicted change in Energy=-4.773758D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.845214	-2.018626	0.323523
2	6	0	-2.847236	-1.133770	0.083439
3	7	0	-2.259604	0.126343	0.030650

4	6	0	-0.931821	-0.006614	0.223210
5	7	0	-0.663788	-1.295765	0.403193
6	6	0	0.700272	-1.836376	0.587536
7	6	0	1.535488	-1.748023	-0.702915
8	1	0	-1.869208	-3.087620	0.445637
9	1	0	-3.902154	-1.292328	-0.046825
10	1	0	1.208328	-1.241931	1.344990
11	1	0	0.582362	-2.857073	0.953331
12	1	0	1.101124	-2.377839	-1.490761
13	1	0	1.501560	-0.706401	-1.031589
14	35	0	1.764249	1.673384	-0.405252
15	1	0	-0.146607	0.775627	0.127354
16	6	0	-2.868306	1.388802	-0.210298
17	6	0	-4.172255	1.581508	-0.359981
18	1	0	-2.138472	2.187325	-0.264412
19	1	0	-4.538411	2.581247	-0.548171
20	1	0	-4.906268	0.787509	-0.305105
21	7	0	2.912701	-2.107968	-0.394120
22	1	0	3.170645	-3.023809	-0.734813
23	1	0	3.568137	-1.422685	-0.743336

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.358182	0.000000			
3	N	2.204175	1.391397	0.000000		
4	C	2.211909	2.226844	1.348245	0.000000	
5	N	1.387315	2.212675	2.169749	1.328965	0.000000
6	C	2.565622	3.651380	3.594892	2.478808	1.478817
7	C	3.543437	4.494878	4.295822	3.158770	2.502964
8	H	1.076214	2.214781	3.264075	3.228121	2.159996
9	H	2.212616	1.074692	2.171774	3.247901	3.269487
10	H	3.312215	4.248624	3.953001	2.713786	2.096353
11	H	2.644386	3.935559	4.222426	3.309221	2.072009
12	H	3.478731	4.428923	4.458712	3.562761	2.805862
13	H	3.841766	4.509763	3.996020	2.825875	2.663585
14	Br	5.214429	5.420768	4.332983	3.238233	3.919795
15	H	3.275912	3.307737	2.212618	1.112497	2.152726
16	C	3.597534	2.539704	1.422103	2.425921	3.527489
17	C	4.340883	3.053692	2.434816	3.655497	4.601139
18	H	4.256958	3.413652	2.085517	2.550912	3.840873
19	H	5.401110	4.130419	3.399198	4.505502	5.563185
20	H	4.199954	2.842867	2.748582	4.087295	4.779158
21	N	4.812562	5.861228	5.650249	4.424605	3.753220

22	H	5.223918	6.360556	6.324318	5.181843	4.357072
23	H	5.549568	6.474878	6.079565	4.815506	4.386323

		6	7	8	9	10
6	C	0.000000				
7	C	1.539694	0.000000			
8	H	2.861464	3.834795	0.000000		
9	H	4.677684	5.496005	2.756531	0.000000	
10	H	1.088679	2.134731	3.699545	5.296859	0.000000
11	H	1.090657	2.209433	2.514180	4.853826	1.775927
12	H	2.184761	1.098200	3.616117	5.319406	3.056675
13	H	2.130839	1.092774	4.383433	5.523876	2.453753
14	Br	3.799485	3.441941	6.049230	6.405626	3.445497
15	H	2.784157	3.144455	4.241856	4.290794	2.718276
16	C	4.875762	5.429157	4.633229	2.878198	5.094960
17	C	6.026710	6.616775	5.268188	2.903439	6.311054
18	H	4.997444	5.401595	5.329327	3.907161	5.054803
19	H	6.946151	7.460481	6.344159	3.957367	7.157217
20	H	6.254188	6.934219	4.980358	2.323935	6.650543
21	N	2.435623	1.456581	4.952936	6.872273	2.584456
22	H	3.043247	2.074219	5.176646	7.314086	3.369178
23	H	3.188576	2.058918	5.809509	7.503825	3.156339

		11	12	13	14	15
11	H	0.000000				
12	H	2.544084	0.000000			
13	H	3.067609	1.779014	0.000000		
14	Br	4.875208	4.246230	2.474809	0.000000	
15	H	3.796070	3.757589	2.501202	2.177385	0.000000
16	C	5.593622	5.619924	4.915296	4.645381	2.810274
17	C	6.635674	6.690562	6.154492	5.937388	4.134342
18	H	5.859333	5.730588	4.712966	3.938934	2.472630
19	H	7.619196	7.568710	6.893735	6.369315	4.796305
20	H	6.707585	6.893037	6.619654	6.729830	4.779282
21	N	2.794149	2.134775	2.088558	3.951922	4.236321
22	H	3.094648	2.296008	2.871288	4.914283	5.116953
23	H	3.721694	2.749021	2.206104	3.599161	4.403408

		16	17	18	19	20
16	C	0.000000				
17	C	1.326583	0.000000			
18	H	1.083155	2.124246	0.000000		
19	H	2.079744	1.081186	2.448551	0.000000	
20	H	2.126930	1.082692	3.101909	1.847132	0.000000
21	N	6.758790	7.988116	6.631796	8.805200	8.338344
22	H	7.497679	8.675692	7.454121	9.533155	8.941327
23	H	7.043891	8.311788	6.769559	9.043545	8.768840

		21	22	23
21	N	0.000000		
22	H	1.010629	0.000000	
23	H	1.010525	1.649748	0.000000

Stoichiometry C7H12BrN3
Framework group C1[X(C7H12BrN3)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.726852	2.142767	-0.116520
2	6	0	-2.743958	1.267324	0.092651
3	7	0	-2.202749	-0.007945	-0.036840
4	6	0	-0.886452	0.105490	-0.305652
5	7	0	-0.581769	1.397964	-0.358796
6	6	0	0.786832	1.914155	-0.576461
7	6	0	1.701378	1.653735	0.634507
8	1	0	-1.717948	3.218944	-0.116484
9	1	0	-3.781146	1.442137	0.313205
10	1	0	1.220699	1.394737	-1.429214
11	1	0	0.684169	2.973033	-0.816814
12	1	0	1.344346	2.202560	1.516188
13	1	0	1.649395	0.582950	0.846336
14	35	0	1.778977	-1.716780	-0.058723
15	1	0	-0.127118	-0.706195	-0.352878
16	6	0	-2.842066	-1.270461	0.103523
17	6	0	-4.139712	-1.439064	0.321493
18	1	0	-2.141327	-2.091862	0.016970
19	1	0	-4.530623	-2.442089	0.421955
20	1	0	-4.844841	-0.621940	0.407077
21	7	0	3.067973	2.004315	0.272375
22	1	0	3.382672	2.867016	0.694374
23	1	0	3.718331	1.263980	0.496198

Rotational constants (GHZ): 0.8800882 0.4773073 0.3179447
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 365 symmetry adapted cartesian basis functions of A symmetry.
There are 352 symmetry adapted basis functions of A symmetry.
352 basis functions, 562 primitive gaussians, 365 cartesian basis functions

55 alpha electrons 55 beta electrons
nuclear repulsion energy 846.6221527270 Hartrees.
NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 352 RedAO= T EigKep= 4.57D-06 NBF= 352
NBsUse= 352 1.00D-06 EigRej= -1.00D+00 NBFU= 352
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999931 -0.011519 -0.001185 -0.002122 Ang= -1.35 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3012.46265867 A.U. after 13 cycles
NFock= 13 Conv=0.35D-08 -V/T= 2.0016
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000750434	0.001044017	-0.000780432
2	6	0.000309610	0.000258755	0.001379183
3	7	0.000255776	0.000081065	-0.001547381
4	6	-0.001588347	0.002201054	-0.001593268
5	7	-0.001462136	-0.003222668	0.001112428
6	6	0.001791175	-0.000531392	-0.000817825

7	6	-0.000795716	-0.004005331	-0.001852780
8	1	-0.000054639	-0.000053779	-0.000169912
9	1	-0.000029623	0.000088777	0.000306005
10	1	-0.001212047	0.000233916	0.001372570
11	1	0.001530743	-0.000513941	-0.000164783
12	1	-0.001477711	-0.000526789	0.001042408
13	1	0.000755590	-0.001224982	-0.000686968
14	35	0.001120069	0.006843197	0.000147815
15	1	0.000076666	0.001138492	0.001597721
16	6	-0.000106034	-0.000708808	-0.000030615
17	6	-0.000059335	0.000314213	0.000031977
18	1	-0.000176764	-0.000085138	-0.000091274
19	1	-0.000035282	-0.000024513	0.000026886
20	1	0.000079580	-0.000038209	0.000015367
21	7	-0.000606113	-0.003316569	0.001050726
22	1	0.000574044	0.000095872	-0.000861997
23	1	0.000360062	0.001952764	0.000514149

Cartesian Forces: Max 0.006843197 RMS 0.001411110

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.023403093 RMS 0.004103744
Search for a local minimum.
Step number 4 out of a maximum of 121
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 3 4
DE= -1.96D-03 DEPred=-4.77D-03 R= 4.10D-01
Trust test= 4.10D-01 RLast= 8.23D-01 DXMaxT set to 5.05D-01
ITU= 0 1 0 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00225	0.00303	0.00676	0.00932	0.01401
Eigenvalues ---	0.01511	0.01868	0.01972	0.02193	0.02225
Eigenvalues ---	0.02318	0.02391	0.02570	0.03062	0.03062
Eigenvalues ---	0.03500	0.03689	0.04342	0.04602	0.05399
Eigenvalues ---	0.05635	0.08638	0.09349	0.12390	0.13274
Eigenvalues ---	0.15655	0.15939	0.16000	0.16000	0.16000
Eigenvalues ---	0.16000	0.16014	0.17514	0.21901	0.21999
Eigenvalues ---	0.22222	0.22721	0.23487	0.23584	0.25023
Eigenvalues ---	0.27462	0.32100	0.34016	0.34260	0.34448
Eigenvalues ---	0.34790	0.34932	0.35409	0.35689	0.35690

Eigenvalues --- 0.35859 0.36437 0.36657 0.38116 0.42190
Eigenvalues --- 0.43270 0.47193 0.47450 0.47712 0.50127
Eigenvalues --- 0.54382 0.60350 0.60697
RFO step: Lambda=-5.05364531D-03 EMin= 2.24711529D-03
Quartic linear search produced a step of -0.29062.
Iteration 1 RMS(Cart)= 0.11244585 RMS(Int)= 0.00409897
Iteration 2 RMS(Cart)= 0.00695939 RMS(Int)= 0.00009125
Iteration 3 RMS(Cart)= 0.00003661 RMS(Int)= 0.00008469
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00008469

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56659	-0.00243	-0.00116	-0.00070	-0.00190	2.56469
R2	2.62164	-0.00056	-0.00010	-0.00064	-0.00075	2.62089
R3	2.03375	0.00004	0.00013	-0.00004	0.00009	2.03384
R4	2.62936	-0.00229	-0.00117	-0.00057	-0.00176	2.62760
R5	2.03087	-0.00002	-0.00011	0.00005	-0.00006	2.03081
R6	2.54781	0.00099	0.00004	0.00071	0.00078	2.54859
R7	2.68739	-0.00035	-0.00001	-0.00011	-0.00012	2.68727
R8	2.51138	0.01248	0.00395	0.00416	0.00814	2.51952
R9	2.10232	0.00631	-0.00263	0.01178	0.00915	2.11147
R10	2.79456	0.00366	0.00123	0.00145	0.00268	2.79724
R11	2.90960	-0.00038	0.00180	-0.00241	-0.00061	2.90899
R12	2.05731	0.00052	0.00023	-0.00002	0.00021	2.05751
R13	2.06104	0.00026	0.00049	-0.00014	0.00035	2.06140
R14	2.07530	0.00014	0.00013	-0.00110	-0.00097	2.07432
R15	2.06504	-0.00098	-0.00128	0.00155	0.00026	2.06531
R16	2.75254	0.00077	0.00385	-0.00395	-0.00010	2.75244
R17	4.11466	0.00377	0.01721	0.01873	0.03594	4.15061
R18	2.50688	0.00004	0.00001	-0.00002	-0.00001	2.50687
R19	2.04687	-0.00018	0.00007	-0.00022	-0.00015	2.04672
R20	2.04315	-0.00002	-0.00005	0.00002	-0.00003	2.04312
R21	2.04599	-0.00002	0.00001	-0.00002	-0.00002	2.04598
R22	1.90981	0.00035	0.00125	-0.00342	-0.00217	1.90764
R23	1.90961	0.00138	0.00065	-0.00112	-0.00047	1.90915
A1	1.87440	0.00270	0.00190	-0.00012	0.00180	1.87620
A2	2.27935	-0.00143	-0.00124	0.00025	-0.00099	2.27836
A3	2.12943	-0.00127	-0.00069	-0.00012	-0.00081	2.12862
A4	1.85996	0.00060	-0.00083	0.00039	-0.00043	1.85953
A5	2.27772	-0.00025	0.00037	-0.00008	0.00029	2.27801
A6	2.14549	-0.00035	0.00046	-0.00035	0.00010	2.14559
A7	1.89779	0.00301	0.00180	0.00157	0.00342	1.90120
A8	2.25188	-0.00207	-0.00140	-0.00083	-0.00229	2.24959
A9	2.13327	-0.00092	-0.00033	-0.00051	-0.00090	2.13236
A10	1.88981	-0.00395	-0.00138	-0.00283	-0.00428	1.88553

A11	2.23122	-0.01308	-0.01559	-0.01217	-0.02802	2.20320
A12	2.15483	0.01734	0.01850	0.01843	0.03673	2.19155
A13	1.90277	-0.00236	-0.00152	0.00095	-0.00055	1.90222
A14	2.21703	-0.01215	-0.01251	-0.00203	-0.01465	2.20239
A15	2.16221	0.01454	0.01386	0.00218	0.01595	2.17816
A16	1.95509	0.00396	0.00403	0.00055	0.00452	1.95961
A17	1.89397	-0.00230	0.00013	-0.00474	-0.00473	1.88924
A18	1.85898	-0.00007	-0.00429	0.00769	0.00336	1.86234
A19	1.87407	0.00352	0.00269	0.02023	0.02295	1.89702
A20	1.97517	-0.00530	-0.00457	-0.01666	-0.02119	1.95398
A21	1.90509	0.00010	0.00211	-0.00748	-0.00527	1.89982
A22	1.93243	-0.00106	-0.00324	-0.00044	-0.00367	1.92876
A23	1.86496	0.00103	0.00498	-0.00092	0.00408	1.86904
A24	1.89762	-0.00074	0.00024	-0.00111	-0.00083	1.89679
A25	1.89505	-0.00005	-0.00272	0.00368	0.00093	1.89598
A26	1.96529	0.00097	-0.00282	0.00478	0.00197	1.96725
A27	1.90569	-0.00013	0.00400	-0.00638	-0.00235	1.90334
A28	2.76631	0.02340	0.00032	0.04084	0.04116	2.80746
A29	2.17584	0.00016	0.00013	0.00002	0.00016	2.17600
A30	1.95467	0.00001	0.00047	-0.00034	0.00014	1.95481
A31	2.15266	-0.00017	-0.00060	0.00031	-0.00029	2.15236
A32	2.07927	0.00011	-0.00013	0.00040	0.00027	2.07954
A33	2.15812	-0.00014	0.00018	-0.00053	-0.00035	2.15777
A34	2.04580	0.00003	-0.00005	0.00013	0.00008	2.04588
A35	1.97555	0.00059	-0.00530	0.00791	0.00261	1.97816
A36	1.95242	-0.00094	0.00241	-0.01006	-0.00764	1.94477
A37	1.90975	0.00030	-0.00180	0.00325	0.00146	1.91121
D1	-0.00834	-0.00049	0.00649	-0.00967	-0.00311	-0.01144
D2	3.13792	0.00014	0.00301	0.00011	0.00308	3.14100
D3	3.13047	-0.00026	0.00334	-0.00583	-0.00238	3.12809
D4	-0.00646	0.00037	-0.00014	0.00395	0.00381	-0.00265
D5	0.00427	0.00072	-0.00604	0.01464	0.00855	0.01282
D6	-3.08652	-0.00050	-0.00327	-0.00920	-0.01222	-3.09874
D7	-3.13484	0.00052	-0.00321	0.01120	0.00790	-3.12693
D8	0.05756	-0.00070	-0.00044	-0.01263	-0.01286	0.04470
D9	0.00960	0.00010	-0.00477	0.00160	-0.00329	0.00631
D10	3.12714	0.00108	0.00068	0.01291	0.01347	3.14061
D11	-3.13622	-0.00047	-0.00162	-0.00726	-0.00889	3.13807
D12	-0.01867	0.00051	0.00383	0.00405	0.00786	-0.01081
D13	-0.00705	0.00037	0.00107	0.00753	0.00865	0.00160
D14	3.00693	0.00449	0.01931	0.03882	0.05789	3.06482
D15	-3.12656	-0.00051	-0.00393	-0.00285	-0.00673	-3.13329
D16	-0.11257	0.00361	0.01431	0.02844	0.04251	-0.07006
D17	0.06959	-0.00046	-0.00372	-0.00218	-0.00589	0.06371

D18	-3.06646	-0.00049	-0.00460	-0.00154	-0.00613	-3.07259
D19	-3.09893	0.00068	0.00239	0.01051	0.01289	-3.08604
D20	0.04821	0.00066	0.00151	0.01114	0.01264	0.06085
D21	0.00178	-0.00068	0.00301	-0.01364	-0.01060	-0.00882
D22	3.09452	-0.00043	-0.00078	0.00913	0.00873	3.10325
D23	-3.01905	-0.00195	-0.01267	-0.04062	-0.05366	-3.07271
D24	0.07369	-0.00170	-0.01646	-0.01784	-0.03432	0.03936
D25	-2.42314	-0.00047	-0.06186	0.16262	0.10067	-2.32247
D26	0.57309	0.00236	-0.04210	0.19641	0.15439	0.72749
D27	1.86971	-0.00548	-0.04226	-0.04915	-0.09136	1.77835
D28	-2.34752	-0.00023	-0.03637	-0.02690	-0.06326	-2.41078
D29	-0.29853	-0.00132	-0.03611	-0.03397	-0.07004	-0.36857
D30	-1.21402	-0.00626	-0.03838	-0.07624	-0.11464	-1.32866
D31	0.85194	-0.00101	-0.03249	-0.05399	-0.08654	0.76540
D32	2.90093	-0.00210	-0.03223	-0.06106	-0.09332	2.80761
D33	-1.12068	0.00116	-0.05976	0.16776	0.10802	-1.01266
D34	0.93999	0.00113	-0.06190	0.17140	0.10954	1.04953
D35	2.99477	0.00116	-0.05426	0.16280	0.10856	3.10333
D36	3.08478	-0.00058	-0.06409	0.16038	0.09621	-3.10219
D37	-1.13773	-0.00060	-0.06623	0.16401	0.09773	-1.04000
D38	0.91705	-0.00058	-0.05859	0.15542	0.09675	1.01380
D39	0.98127	0.00016	-0.06572	0.16620	0.10051	1.08178
D40	3.04195	0.00014	-0.06785	0.16983	0.10203	-3.13921
D41	-1.18646	0.00016	-0.06022	0.16124	0.10105	-1.08541
D42	1.85317	-0.00003	-0.03400	0.08494	0.05095	1.90412
D43	-2.26280	0.00009	-0.03859	0.08748	0.04889	-2.21391
D44	-0.29494	0.00121	-0.02818	0.08308	0.05491	-0.24004
D45	1.87227	0.00133	-0.03277	0.08561	0.05285	1.92511
D46	-2.40126	0.00072	-0.02563	0.07971	0.05407	-2.34719
D47	-0.23404	0.00084	-0.03022	0.08225	0.05201	-0.18204
D48	-3.13305	-0.00004	-0.00086	0.00037	-0.00049	-3.13354
D49	0.00816	-0.00002	-0.00051	0.00034	-0.00018	0.00798
D50	0.00239	-0.00001	0.00012	-0.00034	-0.00022	0.00217
D51	-3.13959	0.00001	0.00047	-0.00037	0.00010	-3.13949

Item	Value	Threshold	Converged?
Maximum Force	0.023403	0.000450	NO
RMS Force	0.004104	0.000300	NO
Maximum Displacement	0.684050	0.001800	NO
RMS Displacement	0.116475	0.001200	NO

Predicted change in Energy=-3.396532D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.793426	-1.994268	0.286581
2	6	0	-2.813149	-1.131463	0.046447
3	7	0	-2.255511	0.141922	0.016082
4	6	0	-0.926942	0.042892	0.225791
5	7	0	-0.629219	-1.246942	0.384858
6	6	0	0.736391	-1.779511	0.591196
7	6	0	1.555703	-1.805419	-0.711771
8	1	0	-1.794192	-3.064865	0.396870
9	1	0	-3.863198	-1.312918	-0.092694
10	1	0	1.246016	-1.141267	1.311188
11	1	0	0.622831	-2.775474	1.021432
12	1	0	1.047059	-2.409790	-1.473959
13	1	0	1.621847	-0.775032	-1.070082
14	35	0	1.619500	2.035368	-0.279331
15	1	0	-0.188670	0.880894	0.191743
16	6	0	-2.896646	1.392426	-0.201599
17	6	0	-4.204678	1.553751	-0.352710
18	1	0	-2.188280	2.211009	-0.236216
19	1	0	-4.596749	2.547083	-0.521550
20	1	0	-4.917349	0.739478	-0.317157
21	7	0	2.895474	-2.291083	-0.410745
22	1	0	3.075289	-3.217178	-0.769998
23	1	0	3.603424	-1.654694	-0.749093

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357177	0.000000			
3	N	2.202272	1.390465	0.000000		
4	C	2.214613	2.229136	1.348658	0.000000	
5	N	1.386915	2.213009	2.170200	1.333272	0.000000
6	C	2.557125	3.649103	3.601963	2.494264	1.480235
7	C	3.499862	4.485083	4.341343	3.234008	2.507663
8	H	1.076263	2.213393	3.262100	3.231028	2.159201
9	H	2.211796	1.074658	2.170957	3.249808	3.269715
10	H	3.318981	4.251644	3.947729	2.702233	2.094220
11	H	2.643594	3.931834	4.219808	3.313311	2.075876
12	H	3.367568	4.341308	4.431526	3.577916	2.759949
13	H	3.871842	4.587250	4.129705	2.973990	2.721552
14	Br	5.310959	5.457410	4.322975	3.272534	4.033788
15	H	3.294054	3.310375	2.201991	1.117341	2.181528

16	C	3.595150	2.537423	1.422040	2.425620	3.528657
17	C	4.337196	3.050583	2.434855	3.655258	4.601282
18	H	4.256005	3.412108	2.085496	2.550520	3.843674
19	H	5.397736	4.127414	3.399300	4.505215	5.563946
20	H	4.194849	2.839065	2.748364	4.086975	4.777735
21	N	4.749753	5.843126	5.712648	4.523659	3.761206
22	H	5.129937	6.300038	6.349716	5.257139	4.351884
23	H	5.505808	6.486837	6.175794	4.935222	4.400837

		6	7	8	9	10
6	C	0.000000				
7	C	1.539372	0.000000			
8	H	2.844952	3.746610	0.000000		
9	H	4.673504	5.476340	2.754955	0.000000	
10	H	1.088789	2.151596	3.712017	5.301360	0.000000
11	H	1.090844	2.194368	2.513130	4.848175	1.772836
12	H	2.181428	1.097685	3.464366	5.217436	3.066884
13	H	2.133742	1.092913	4.366303	5.597350	2.438406
14	Br	4.011359	3.865581	6.174376	6.426962	3.572149
15	H	2.844830	3.327980	4.264832	4.289041	2.720407
16	C	4.887603	5.505442	4.630443	2.874886	5.086233
17	C	6.034547	6.677944	5.263452	2.898622	6.304105
18	H	5.016230	5.511375	5.328315	3.904358	5.042479
19	H	6.957011	7.538774	6.339698	3.952419	7.148478
20	H	6.255812	6.966536	4.973627	2.318177	6.646486
21	N	2.434590	1.456528	4.821198	6.836492	2.647233
22	H	3.064339	2.074993	5.009653	7.226863	3.462222
23	H	3.167306	2.053600	5.695267	7.503207	3.172654

		11	12	13	14	15
11	H	0.000000				
12	H	2.557473	0.000000			
13	H	3.061737	1.779306	0.000000		
14	Br	5.082276	4.638346	2.919528	0.000000	
15	H	3.836136	3.889754	2.759033	2.196406	0.000000
16	C	5.590519	5.623926	5.086149	4.562345	2.783795
17	C	6.628370	6.674398	6.315556	5.844518	4.108222
18	H	5.860804	5.775050	4.912112	3.812073	2.439425
19	H	7.612779	7.571673	7.071652	6.241977	4.766144
20	H	6.696289	6.843262	6.754385	6.664170	4.758086
21	N	2.729592	2.135686	2.086927	4.512600	4.465017
22	H	3.069019	2.293721	2.857730	5.472596	5.326590
23	H	3.643465	2.762354	2.191686	4.215826	4.657720

		16	17	18	19	20
16	C	0.000000				
17	C	1.326578	0.000000			

18	H	1.083078	2.124010	0.000000		
19	H	2.079892	1.081173	2.448486	0.000000	
20	H	2.126719	1.082684	3.101576	1.847159	0.000000
21	N	6.867360	8.074545	6.792926	8.919279	8.380529
22	H	7.565417	8.714001	7.579927	9.599406	8.929863
23	H	7.199694	8.450899	6.982158	9.216807	8.861275

		21	22	23
21	N	0.000000		
22	H	1.009479	0.000000	
23	H	1.010278	1.649460	0.000000

Stoichiometry C7H12BrN3
Framework group C1[X(C7H12BrN3)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.644098	2.196406	-0.172302
2	6	0	-2.674828	1.345125	0.061891
3	7	0	-2.152966	0.059025	-0.021782
4	6	0	-0.834199	0.138716	-0.292672
5	7	0	-0.508046	1.428509	-0.380276
6	6	0	0.860252	1.939430	-0.620726
7	6	0	1.743816	1.855770	0.637042
8	1	0	-1.619776	3.271713	-0.210564
9	1	0	-3.711037	1.542992	0.266850
10	1	0	1.314965	1.339200	-1.407123
11	1	0	0.753906	2.964968	-0.976962
12	1	0	1.291215	2.419313	1.463167
13	1	0	1.798260	0.801999	0.921754
14	35	0	1.676285	-1.946943	-0.053993
15	1	0	-0.119383	-0.717942	-0.352880
16	6	0	-2.817923	-1.186910	0.144576
17	6	0	-4.120884	-1.325250	0.351852
18	1	0	-2.132381	-2.023489	0.087777
19	1	0	-4.532274	-2.317620	0.473891
20	1	0	-4.810894	-0.492797	0.407652
21	7	0	3.080265	2.327021	0.300439
22	1	0	3.304117	3.221632	0.711061
23	1	0	3.785715	1.651439	0.558491

```
 ----------------------------------------------------------------------
 Rotational constants (GHZ):           0.7523626           0.4936738           0.3066171
 Standard basis: 6-311++G(d,p) (5D, 7F)
 There are     365 symmetry adapted cartesian basis functions of A      symmetry.
 There are     352 symmetry adapted basis functions of A      symmetry.
    352 basis functions,      562 primitive gaussians,      365 cartesian basis functions
     55 alpha electrons              55 beta electrons
          nuclear repulsion energy              832.7937283912 Hartrees.
 NAtoms=       23 NActive=       23 NUniq=       23 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      352 RedAO= T EigKep=    4.52D-06    NBF=      352
 NBsUse=      352 1.00D-06 EigRej= -1.00D+00 NBFU=      352
 Initial guess from the checkpoint file:    "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"
 B after Tr=          0.000000        0.000000        0.000000
             Rot=        0.999878        0.009413        0.000532        0.012489 Ang=      1.79 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn=                5 AccDes=
0.00D+00
 Harris functional with IExCor=    402 and IRadAn=             5 diagonalized for initial guess.
 HarFok:    IExCor=    402 AccDes= 0.00D+00 IRadAn=                5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=    3500011 ScaDFX=    1.000000    1.000000    1.000000    1.000000
 FoFCou: FMM=F IPFlag=                  0 FMFlag=           100000 FMFlg1=                  0
             NFxFlg=                    0 DoJE=T BraDBF=F KetDBF=T FulRan=T
             wScrn=      0.000000  ICntrl=             500  IOpCl=      0  I1Cent=        200000004  NGrid=
0
             NMat0=        1 NMatS0=            1 NMatT0=        0 NMatD0=        1 NMtDS0=        0
NMtDT0=        0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                       energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3012.46481693          A.U. after      13 cycles
                   NFock= 13    Conv=0.24D-08         -V/T= 2.0017
 Calling FoFJK, ICntrl=             2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 ----------------------------------------------------------------------
 Center         Atomic                             Forces (Hartrees/Bohr)
 Number          Number                       X                       Y                       Z
 ----------------------------------------------------------------------
```

1	6	0.000474595	0.000318887	-0.001599908
2	6	0.000030268	0.000242221	0.001203216
3	7	0.000531525	0.000081421	-0.000544676
4	6	-0.001100999	0.002303926	-0.000738821
5	7	-0.000062176	-0.000664120	0.002194525
6	6	-0.000312734	-0.000293097	-0.000607670
7	6	-0.000082227	0.002205850	0.000180262
8	1	0.000001367	-0.000071972	-0.000343476
9	1	0.000003116	0.000033919	0.000062900
10	1	-0.000296472	0.000461008	0.000283945
11	1	0.000863006	-0.000221001	-0.000109640
12	1	-0.000865080	0.000387268	0.000822527
13	1	-0.001587524	0.000435538	-0.001147997
14	35	-0.001348812	-0.000834673	-0.000020787
15	1	0.001442133	-0.002464268	-0.000126914
16	6	-0.000123892	0.000132580	-0.000148087
17	6	-0.000015478	-0.000050065	0.000069842
18	1	0.000176974	0.000024726	-0.000109523
19	1	0.000022878	-0.000015981	0.000021153
20	1	-0.000038246	-0.000019573	-0.000009002
21	7	-0.000016893	-0.001236784	0.001191988
22	1	0.000840923	-0.000718724	-0.000983111
23	1	0.001463748	-0.000037087	0.000459252

Cartesian Forces: Max 0.002464268 RMS 0.000833820

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.002912135 RMS 0.000769216
Search for a local minimum.
Step number 5 out of a maximum of 121
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Update second derivatives using D2CorX and points 4 5
DE= -2.16D-03 DEPred=-3.40D-03 R= 6.35D-01
TightC=F SS= 1.41D+00 RLast= 4.57D-01 DXNew= 8.4853D-01 1.3717D+00
Trust test= 6.35D-01 RLast= 4.57D-01 DXMaxT set to 8.49D-01
ITU= 1 0 1 0 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00226	0.00327	0.00660	0.00971	0.01401
Eigenvalues ---	0.01525	0.01867	0.01978	0.02195	0.02216
Eigenvalues ---	0.02318	0.02391	0.02654	0.03062	0.03062

Eigenvalues ---	0.03527	0.03711	0.04387	0.04658	0.05336
Eigenvalues ---	0.05636	0.08608	0.09401	0.12396	0.13224
Eigenvalues ---	0.15657	0.15846	0.15999	0.16000	0.16000
Eigenvalues ---	0.16000	0.16011	0.17883	0.21846	0.21999
Eigenvalues ---	0.22080	0.22673	0.23496	0.23617	0.25037
Eigenvalues ---	0.27454	0.31441	0.34007	0.34402	0.34623
Eigenvalues ---	0.34782	0.34965	0.35419	0.35688	0.35690
Eigenvalues ---	0.35859	0.36437	0.36658	0.39425	0.42191
Eigenvalues ---	0.43392	0.47156	0.47583	0.47772	0.50710
Eigenvalues ---	0.54365	0.60351	0.61052		

RFO step: Lambda=-4.46377218D-04 EMin= 2.25510301D-03

Quartic linear search produced a step of -0.12694.

Iteration 1 RMS(Cart)= 0.03032831 RMS(Int)= 0.00039487

Iteration 2 RMS(Cart)= 0.00055500 RMS(Int)= 0.00004276

Iteration 3 RMS(Cart)= 0.00000018 RMS(Int)= 0.00004276

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56469	0.00042	0.00024	-0.00026	-0.00003	2.56466
R2	2.62089	-0.00048	0.00010	-0.00079	-0.00070	2.62019
R3	2.03384	0.00004	-0.00001	0.00010	0.00009	2.03393
R4	2.62760	0.00010	0.00022	-0.00085	-0.00063	2.62697
R5	2.03081	-0.00002	0.00001	-0.00005	-0.00004	2.03077
R6	2.54859	-0.00084	-0.00010	-0.00095	-0.00104	2.54755
R7	2.68727	0.00008	0.00002	0.00004	0.00006	2.68732
R8	2.51952	-0.00089	-0.00103	0.00249	0.00147	2.52099
R9	2.11147	-0.00241	-0.00116	-0.00238	-0.00354	2.10793
R10	2.79724	-0.00033	-0.00034	0.00104	0.00070	2.79793
R11	2.90899	-0.00061	0.00008	-0.00290	-0.00282	2.90617
R12	2.05751	0.00032	-0.00003	0.00103	0.00100	2.05852
R13	2.06140	0.00007	-0.00004	0.00034	0.00029	2.06169
R14	2.07432	-0.00039	0.00012	-0.00067	-0.00055	2.07378
R15	2.06531	0.00069	-0.00003	0.00108	0.00104	2.06635
R16	2.75244	0.00291	0.00001	0.00664	0.00665	2.75909
R17	4.15061	-0.00155	-0.00456	-0.02556	-0.03013	4.12048
R18	2.50687	0.00001	0.00000	0.00004	0.00004	2.50691
R19	2.04672	0.00014	0.00002	0.00029	0.00031	2.04703
R20	2.04312	-0.00003	0.00000	-0.00007	-0.00006	2.04306
R21	2.04598	0.00004	0.00000	0.00009	0.00010	2.04607
R22	1.90764	0.00116	0.00028	0.00281	0.00308	1.91072
R23	1.90915	0.00085	0.00006	0.00267	0.00273	1.91188
A1	1.87620	-0.00030	-0.00023	0.00094	0.00058	1.87678
A2	2.27836	0.00010	0.00013	-0.00081	-0.00066	2.27770
A3	2.12862	0.00020	0.00010	-0.00016	-0.00003	2.12858
A4	1.85953	0.00015	0.00005	0.00051	0.00039	1.85993

A5	2.27801	-0.00004	-0.00004	0.00002	-0.00003	2.27797
A6	2.14559	-0.00010	-0.00001	-0.00033	-0.00037	2.14522
A7	1.90120	-0.00064	-0.00043	-0.00028	-0.00079	1.90042
A8	2.24959	0.00038	0.00029	0.00022	0.00055	2.25015
A9	2.13236	0.00025	0.00011	0.00008	0.00024	2.13260
A10	1.88553	0.00088	0.00054	0.00075	0.00127	1.88680
A11	2.20320	0.00167	0.00356	-0.00594	-0.00230	2.20090
A12	2.19155	-0.00258	-0.00466	0.00516	0.00055	2.19210
A13	1.90222	-0.00008	0.00007	-0.00148	-0.00159	1.90062
A14	2.20239	0.00236	0.00186	-0.00130	0.00049	2.20288
A15	2.17816	-0.00229	-0.00203	0.00210	0.00001	2.17818
A16	1.95961	-0.00128	-0.00057	-0.00206	-0.00263	1.95698
A17	1.88924	0.00002	0.00060	-0.00294	-0.00232	1.88693
A18	1.86234	0.00101	-0.00043	0.00658	0.00616	1.86849
A19	1.89702	0.00032	-0.00291	0.00619	0.00327	1.90029
A20	1.95398	0.00010	0.00269	-0.00698	-0.00429	1.94969
A21	1.89982	-0.00015	0.00067	-0.00080	-0.00014	1.89968
A22	1.92876	-0.00062	0.00047	-0.01312	-0.01267	1.91609
A23	1.86904	-0.00015	-0.00052	0.00181	0.00126	1.87031
A24	1.89679	-0.00063	0.00011	-0.00330	-0.00322	1.89357
A25	1.89598	-0.00048	-0.00012	-0.00551	-0.00570	1.89028
A26	1.96725	0.00041	-0.00025	0.00322	0.00291	1.97016
A27	1.90334	0.00148	0.00030	0.01730	0.01757	1.92091
A28	2.80746	-0.00071	-0.00522	0.01795	0.01273	2.82019
A29	2.17600	-0.00004	-0.00002	-0.00011	-0.00013	2.17588
A30	1.95481	-0.00008	-0.00002	-0.00052	-0.00054	1.95427
A31	2.15236	0.00012	0.00004	0.00063	0.00066	2.15303
A32	2.07954	-0.00003	-0.00003	-0.00008	-0.00011	2.07943
A33	2.15777	0.00004	0.00004	0.00005	0.00009	2.15786
A34	2.04588	0.00000	-0.00001	0.00003	0.00002	2.04590
A35	1.97816	0.00017	-0.00033	0.00464	0.00427	1.98244
A36	1.94477	0.00177	0.00097	0.01055	0.01149	1.95626
A37	1.91121	-0.00098	-0.00019	-0.00334	-0.00358	1.90762
D1	-0.01144	0.00081	0.00039	0.03133	0.03172	0.02028
D2	3.14100	0.00021	-0.00039	0.00941	0.00903	-3.13316
D3	3.12809	0.00043	0.00030	0.01687	0.01718	-3.13791
D4	-0.00265	-0.00017	-0.00048	-0.00505	-0.00551	-0.00816
D5	0.01282	-0.00080	-0.00109	-0.03027	-0.03132	-0.01850
D6	-3.09874	-0.00020	0.00155	-0.00592	-0.00435	-3.10310
D7	-3.12693	-0.00046	-0.00100	-0.01732	-0.01829	3.13797
D8	0.04470	0.00015	0.00163	0.00703	0.00867	0.05337
D9	0.00631	-0.00055	0.00042	-0.02207	-0.02162	-0.01531
D10	3.14061	-0.00058	-0.00171	-0.01935	-0.02102	3.11959
D11	3.13807	-0.00001	0.00113	-0.00221	-0.00107	3.13701

D12	-0.01081	-0.00004	-0.00100	0.00050	-0.00047	-0.01128
D13	0.00160	0.00006	-0.00110	0.00346	0.00235	0.00395
D14	3.06482	-0.00046	-0.00735	0.00331	-0.00392	3.06091
D15	-3.13329	0.00009	0.00085	0.00097	0.00180	-3.13149
D16	-0.07006	-0.00043	-0.00540	0.00081	-0.00447	-0.07453
D17	0.06371	0.00009	0.00075	0.00403	0.00477	0.06848
D18	-3.07259	0.00011	0.00078	0.00472	0.00549	-3.06710
D19	-3.08604	0.00005	-0.00164	0.00707	0.00544	-3.08060
D20	0.06085	0.00007	-0.00160	0.00776	0.00616	0.06701
D21	-0.00882	0.00045	0.00135	0.01634	0.01767	0.00885
D22	3.10325	-0.00004	-0.00111	-0.00766	-0.00881	3.09445
D23	-3.07271	0.00073	0.00681	0.01712	0.02407	-3.04864
D24	0.03936	0.00023	0.00436	-0.00688	-0.00241	0.03695
D25	-2.32247	0.00042	-0.01278	0.03449	0.02172	-2.30075
D26	0.72749	0.00001	-0.01960	0.03399	0.01438	0.74187
D27	1.77835	0.00022	0.01160	0.00412	0.01570	1.79405
D28	-2.41078	-0.00016	0.00803	0.00860	0.01662	-2.39416
D29	-0.36857	0.00020	0.00889	0.00962	0.01850	-0.35007
D30	-1.32866	0.00086	0.01455	0.03223	0.04679	-1.28187
D31	0.76540	0.00048	0.01099	0.03671	0.04771	0.81311
D32	2.80761	0.00084	0.01185	0.03773	0.04959	2.85720
D33	-1.01266	0.00004	-0.01371	-0.01446	-0.02817	-1.04083
D34	1.04953	-0.00096	-0.01391	-0.02721	-0.04111	1.00842
D35	3.10333	0.00036	-0.01378	-0.00757	-0.02138	3.08195
D36	-3.10219	0.00060	-0.01221	-0.01362	-0.02581	-3.12800
D37	-1.04000	-0.00040	-0.01241	-0.02637	-0.03875	-1.07875
D38	1.01380	0.00093	-0.01228	-0.00673	-0.01902	0.99478
D39	1.08178	0.00051	-0.01276	-0.01235	-0.02511	1.05668
D40	-3.13921	-0.00049	-0.01295	-0.02511	-0.03805	3.10593
D41	-1.08541	0.00084	-0.01283	-0.00547	-0.01832	-1.10372
D42	1.90412	-0.00018	-0.00647	0.03111	0.02461	1.92873
D43	-2.21391	0.00004	-0.00621	0.03850	0.03229	-2.18162
D44	-0.24004	0.00079	-0.00697	0.04803	0.04108	-0.19896
D45	1.92511	0.00101	-0.00671	0.05543	0.04876	1.97388
D46	-2.34719	0.00011	-0.00686	0.04093	0.03405	-2.31314
D47	-0.18204	0.00033	-0.00660	0.04833	0.04173	-0.14030
D48	-3.13354	0.00000	0.00006	-0.00002	0.00005	-3.13350
D49	0.00798	0.00000	0.00002	0.00006	0.00008	0.00806
D50	0.00217	-0.00002	0.00003	-0.00079	-0.00076	0.00141
D51	-3.13949	-0.00002	-0.00001	-0.00071	-0.00072	-3.14021

Item	Value	Threshold	Converged?
Maximum Force	0.002912	0.000450	NO
RMS Force	0.000769	0.000300	NO
Maximum Displacement	0.098475	0.001800	NO

RMS Displacement 0.030288 0.001200 NO
Predicted change in Energy=-2.223001D-04
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.802998	-2.001305	0.289874
2	6	0	-2.819882	-1.129893	0.069712
3	7	0	-2.251565	0.137743	0.018858
4	6	0	-0.923612	0.029145	0.224138
5	7	0	-0.635090	-1.261753	0.397417
6	6	0	0.728644	-1.803852	0.593745
7	6	0	1.549409	-1.792161	-0.706748
8	1	0	-1.810303	-3.072729	0.392045
9	1	0	-3.872247	-1.303681	-0.061333
10	1	0	1.234701	-1.187121	1.335477
11	1	0	0.617413	-2.813580	0.991684
12	1	0	1.045081	-2.398616	-1.469729
13	1	0	1.583046	-0.757104	-1.057736
14	35	0	1.604595	2.009419	-0.324284
15	1	0	-0.180309	0.859187	0.171202
16	6	0	-2.882288	1.391024	-0.213009
17	6	0	-4.190040	1.562887	-0.354808
18	1	0	-2.165600	2.201437	-0.267779
19	1	0	-4.573798	2.557249	-0.536014
20	1	0	-4.910391	0.756432	-0.299679
21	7	0	2.898436	-2.263513	-0.407257
22	1	0	3.106180	-3.171717	-0.800133
23	1	0	3.606142	-1.602583	-0.700358

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357161	0.000000			
3	N	2.202315	1.390134	0.000000		
4	C	2.213678	2.227792	1.348107	0.000000	
5	N	1.386546	2.213164	2.171380	1.334050	0.000000
6	C	2.557447	3.649777	3.603045	2.495283	1.480603
7	C	3.503660	4.486892	4.324169	3.209289	2.504506
8	H	1.076309	2.213089	3.262072	3.230485	2.158885
9	H	2.211746	1.074638	2.170425	3.248441	3.269770

10	H	3.314181	4.247950	3.955098	2.715270	2.093238
11	H	2.647776	3.936983	4.229389	3.323398	2.080885
12	H	3.371292	4.349423	4.417792	3.555132	2.757112
13	H	3.850893	4.560251	4.082162	2.923135	2.700420
14	Br	5.298564	5.439348	4.300103	3.257926	4.029591
15	H	3.290838	3.306673	2.198589	1.115469	2.180914
16	C	3.595226	2.537488	1.422071	2.425329	3.529836
17	C	4.337863	3.051002	2.434820	3.654736	4.602403
18	H	4.255056	3.411707	2.085278	2.550171	3.844299
19	H	5.398133	4.127728	3.399214	4.504775	5.565024
20	H	4.196257	2.839876	2.748381	4.086286	4.778830
21	N	4.760065	5.849082	5.698256	4.501443	3.759897
22	H	5.163139	6.328024	6.350489	5.247273	4.367973
23	H	5.513468	6.489239	6.152945	4.902642	4.394237

		6	7	8	9	10
6	C	0.000000				
7	C	1.537880	0.000000			
8	H	2.845519	3.759636	0.000000		
9	H	4.674131	5.481746	2.754396	0.000000	
10	H	1.089320	2.153090	3.703732	5.295808	0.000000
11	H	1.090999	2.190110	2.514067	4.852391	1.773304
12	H	2.170669	1.097395	3.474744	5.230925	3.061512
13	H	2.133793	1.093465	4.356466	5.572413	2.456364
14	Br	4.018843	3.821169	6.164647	6.406370	3.620703
15	H	2.845437	3.285173	4.262113	4.285146	2.746846
16	C	4.888447	5.478721	4.630370	2.874797	5.098454
17	C	6.035573	6.657439	5.264017	2.899022	6.312482
18	H	5.016095	5.472003	5.327141	3.903987	5.061107
19	H	6.957833	7.512668	6.339941	3.952755	7.159710
20	H	6.257153	6.956296	4.975088	2.319184	6.649307
21	N	2.433370	1.460048	4.844165	6.847123	2.638893
22	H	3.076789	2.082170	5.059930	7.261806	3.464374
23	H	3.161519	2.065461	5.717739	7.511591	3.152929

		11	12	13	14	15
11	H	0.000000				
12	H	2.532519	0.000000			
13	H	3.059683	1.775868	0.000000		
14	Br	5.095842	4.588668	2.862178	0.000000	
15	H	3.846916	3.848053	2.689257	2.180463	0.000000
16	C	5.601597	5.600441	5.026651	4.530664	2.780497
17	C	6.639135	6.659058	6.261389	5.811895	4.104855
18	H	5.872121	5.737042	4.840387	3.775505	2.436334
19	H	7.624194	7.550114	7.011694	6.206246	4.763016
20	H	6.705909	6.840394	6.710452	6.634427	4.754573

21	N	2.731789	2.140567	2.103008	4.465294	4.423182
22	H	3.087528	2.300907	2.866470	5.415289	5.290811
23	H	3.641705	2.790095	2.221592	4.146586	4.599688

		16	17	18	19	20
16	C	0.000000				
17	C	1.326597	0.000000			
18	H	1.083241	2.124542	0.000000		
19	H	2.079812	1.081138	2.449075	0.000000	
20	H	2.126833	1.082735	3.102085	1.847185	0.000000
21	N	6.841794	8.055469	6.752755	8.893290	8.373136
22	H	7.551494	8.709169	7.546248	9.585033	8.941265
23	H	7.162326	8.421405	6.926089	9.178378	8.846288

		21	22	23
21	N	0.000000		
22	H	1.011110	0.000000	
23	H	1.011723	1.649878	0.000000

Stoichiometry C7H12BrN3
Framework group C1[X(C7H12BrN3)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.644150	2.203419	-0.148136
2	6	0	-2.674761	1.345149	0.059467
3	7	0	-2.145426	0.062482	-0.024443
4	6	0	-0.828008	0.151031	-0.296401
5	7	0	-0.508249	1.443378	-0.381750
6	6	0	0.859264	1.962087	-0.612042
7	6	0	1.749662	1.821256	0.633924
8	1	0	-1.622732	3.279408	-0.163331
9	1	0	-3.712192	1.536446	0.264380
10	1	0	1.303644	1.394588	-1.428797
11	1	0	0.758690	3.003718	-0.920534
12	1	0	1.307849	2.376727	1.470900
13	1	0	1.769401	0.760372	0.898125
14	35	0	1.661813	-1.936236	-0.055182
15	1	0	-0.109902	-0.700658	-0.353160
16	6	0	-2.802254	-1.187792	0.141918
17	6	0	-4.105039	-1.334719	0.344464

```
      18           1           0       -2.109980      -2.019346       0.090093
      19           1           0       -4.509899      -2.329674       0.466997
      20           1           0       -4.801115      -0.506979       0.395825
      21           7           0        3.094545       2.278347       0.296138
      22           1           0        3.352628       3.145226       0.748085
      23           1           0        3.795782       1.576420       0.494001
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.7593978           0.4967119           0.3087908
 Standard basis: 6-311++G(d,p) (5D, 7F)
 There are     365 symmetry adapted cartesian basis functions of A      symmetry.
 There are     352 symmetry adapted basis functions of A      symmetry.
   352 basis functions,      562 primitive gaussians,      365 cartesian basis functions
    55 alpha electrons              55 beta electrons
         nuclear repulsion energy              834.6366422834 Hartrees.
 NAtoms=       23 NActive=       23 NUniq=       23 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      352 RedAO= T EigKep=    4.38D-06    NBF=      352
 NBsUse=      352 1.00D-06 EigRej= -1.00D+00 NBFU=      352
 Initial guess from the checkpoint file:    "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"
 B after Tr=          0.000000        0.000000        0.000000
             Rot=        0.999997      -0.002139      -0.000334        0.001267 Ang=    -0.29 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn=                5 AccDes=
0.00D+00
 Harris functional with IExCor=    402 and IRadAn=             5 diagonalized for initial guess.
 HarFok:    IExCor=    402 AccDes= 0.00D+00 IRadAn=                5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=    3500011 ScaDFX=    1.000000    1.000000    1.000000    1.000000
 FoFCou: FMM=F IPFlag=                  0 FMFlag=           100000 FMFlg1=                  0
             NFxFlg=                    0 DoJE=T BraDBF=F KetDBF=T FulRan=T
             wScrn=      0.000000  ICntrl=             500  IOpCl=      0  I1Cent=        200000004  NGrid=
0
             NMat0=         1 NMatS0=             1 NMatT0=         0 NMatD0=         1 NMtDS0=         0
NMtDT0=         0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                      energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3012.46505845          A.U. after      11 cycles
                  NFock= 11    Conv=0.68D-08         -V/T= 2.0017
 Calling FoFJK, ICntrl=             2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
```

NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000239988	0.000209448	0.001726381
2	6	0.000030522	-0.000262850	-0.001783058
3	7	0.000325234	-0.000169365	0.000859703
4	6	-0.001332110	0.001142400	0.000066883
5	7	-0.000292955	-0.000992691	-0.000966249
6	6	-0.000052121	0.000762052	0.000245547
7	6	0.000561173	0.000890968	0.000185072
8	1	-0.000096722	0.000006794	0.000249385
9	1	0.000022407	-0.000046068	-0.000186834
10	1	-0.000309395	0.000159547	0.000078388
11	1	0.000159393	0.000219491	0.000192806
12	1	0.000373646	-0.000167954	0.000209689
13	1	0.000453644	0.000082853	-0.000738629
14	35	-0.000635580	-0.000036844	-0.000181480
15	1	0.002018004	-0.001479173	0.000395745
16	6	-0.000048639	0.000224870	0.000064490
17	6	0.000014300	-0.000094090	0.000051842
18	1	0.000101570	-0.000004946	-0.000062249
19	1	0.000013152	0.000003024	-0.000010425
20	1	-0.000013704	-0.000000900	0.000024851
21	7	-0.000543517	-0.001296900	-0.000176102
22	1	-0.000117481	0.000710794	-0.000690463
23	1	-0.000390832	0.000139541	0.000444707

Cartesian Forces: Max 0.002018004 RMS 0.000610430

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.002024194 RMS 0.000442692

Search for a local minimum.

Step number 6 out of a maximum of 121

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 4 5 6

DE= -2.42D-04 DEPred=-2.22D-04 R= 1.09D+00

TightC=F SS= 1.41D+00 RLast= 1.78D-01 DXNew= 1.4270D+00 5.3478D-01
Trust test= 1.09D+00 RLast= 1.78D-01 DXMaxT set to 8.49D-01
ITU= 1 1 0 1 0 0

Eigenvalues ---	0.00215	0.00315	0.00481	0.00910	0.01396
Eigenvalues ---	0.01529	0.01871	0.01963	0.02194	0.02318
Eigenvalues ---	0.02390	0.02595	0.03025	0.03062	0.03065
Eigenvalues ---	0.03511	0.03785	0.04190	0.04710	0.05344
Eigenvalues ---	0.05704	0.09177	0.09648	0.12324	0.13259
Eigenvalues ---	0.15656	0.15979	0.15998	0.15999	0.16000
Eigenvalues ---	0.16007	0.16337	0.17764	0.21422	0.21980
Eigenvalues ---	0.22016	0.22717	0.23579	0.23908	0.25034
Eigenvalues ---	0.27788	0.31929	0.33993	0.34385	0.34523
Eigenvalues ---	0.34792	0.34944	0.35682	0.35689	0.35859
Eigenvalues ---	0.36436	0.36657	0.37287	0.38251	0.42190
Eigenvalues ---	0.43280	0.47357	0.47708	0.47893	0.50184
Eigenvalues ---	0.54322	0.60346	0.60561		

En-DIIS/RFO-DIIS IScMMF= 0 using points: 6 5
RFO step: Lambda=-7.28005100D-05.
DidBck=F Rises=F RFO-DIIS coefs: 0.98493 0.01507
Iteration 1 RMS(Cart)= 0.03481118 RMS(Int)= 0.00191480
Iteration 2 RMS(Cart)= 0.00231625 RMS(Int)= 0.00002057
Iteration 3 RMS(Cart)= 0.00001210 RMS(Int)= 0.00001622
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001622

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56466	0.00021	0.00000	0.00072	0.00071	2.56538
R2	2.62019	-0.00001	0.00001	-0.00089	-0.00088	2.61932
R3	2.03393	0.00002	0.00000	0.00010	0.00010	2.03403
R4	2.62697	0.00036	0.00001	0.00067	0.00068	2.62765
R5	2.03077	0.00001	0.00000	0.00002	0.00002	2.03079
R6	2.54755	-0.00042	0.00002	-0.00156	-0.00154	2.54601
R7	2.68732	0.00007	0.00000	0.00023	0.00023	2.68756
R8	2.52099	-0.00096	-0.00002	-0.00068	-0.00070	2.52029
R9	2.10793	-0.00022	0.00005	-0.00005	0.00001	2.10794
R10	2.79793	-0.00045	-0.00001	-0.00104	-0.00105	2.79689
R11	2.90617	0.00083	0.00004	0.00000	0.00004	2.90621
R12	2.05852	0.00000	-0.00002	0.00067	0.00065	2.05917
R13	2.06169	-0.00015	0.00000	-0.00032	-0.00032	2.06136
R14	2.07378	-0.00023	0.00001	-0.00171	-0.00170	2.07207
R15	2.06635	0.00033	-0.00002	0.00281	0.00279	2.06914
R16	2.75909	-0.00091	-0.00010	0.00110	0.00099	2.76009
R17	4.12048	-0.00050	0.00045	-0.02960	-0.02914	4.09134
R18	2.50691	-0.00003	0.00000	-0.00004	-0.00004	2.50687
R19	2.04703	0.00007	0.00000	0.00037	0.00036	2.04739

R20	2.04306	0.00000	0.00000	-0.00004	-0.00004	2.04301
R21	2.04607	0.00001	0.00000	0.00011	0.00010	2.04618
R22	1.91072	-0.00040	-0.00005	-0.00013	-0.00018	1.91054
R23	1.91188	-0.00031	-0.00004	0.00061	0.00057	1.91245
A1	1.87678	-0.00032	-0.00001	-0.00132	-0.00136	1.87542
A2	2.27770	0.00010	0.00001	0.00023	0.00022	2.27792
A3	2.12858	0.00022	0.00000	0.00127	0.00125	2.12984
A4	1.85993	-0.00012	-0.00001	0.00102	0.00100	1.86093
A5	2.27797	0.00003	0.00000	-0.00049	-0.00049	2.27748
A6	2.14522	0.00009	0.00001	-0.00048	-0.00047	2.14476
A7	1.90042	-0.00010	0.00001	-0.00113	-0.00114	1.89928
A8	2.25015	0.00016	-0.00001	0.00116	0.00115	2.25129
A9	2.13260	-0.00006	0.00000	-0.00007	-0.00008	2.13252
A10	1.88680	0.00020	-0.00002	0.00090	0.00087	1.88767
A11	2.20090	0.00128	0.00003	0.00784	0.00787	2.20877
A12	2.19210	-0.00150	-0.00001	-0.00938	-0.00940	2.18270
A13	1.90062	0.00035	0.00002	0.00082	0.00083	1.90145
A14	2.20288	0.00168	-0.00001	0.01070	0.01068	2.21356
A15	2.17818	-0.00202	0.00000	-0.01192	-0.01192	2.16626
A16	1.95698	-0.00031	0.00004	-0.00513	-0.00509	1.95190
A17	1.88693	0.00003	0.00003	-0.00571	-0.00566	1.88127
A18	1.86849	-0.00004	-0.00009	0.00915	0.00906	1.87755
A19	1.90029	0.00005	-0.00005	0.00807	0.00801	1.90830
A20	1.94969	0.00036	0.00006	-0.00329	-0.00322	1.94648
A21	1.89968	-0.00012	0.00000	-0.00333	-0.00331	1.89637
A22	1.91609	0.00022	0.00019	-0.00860	-0.00844	1.90765
A23	1.87031	0.00026	-0.00002	0.00630	0.00624	1.87654
A24	1.89357	0.00031	0.00005	-0.00099	-0.00100	1.89257
A25	1.89028	-0.00003	0.00009	-0.00360	-0.00347	1.88681
A26	1.97016	-0.00065	-0.00004	-0.00580	-0.00588	1.96428
A27	1.92091	-0.00007	-0.00026	0.01332	0.01303	1.93394
A28	2.82019	0.00042	-0.00019	0.02100	0.02081	2.84100
A29	2.17588	-0.00010	0.00000	-0.00060	-0.00059	2.17528
A30	1.95427	-0.00002	0.00001	-0.00077	-0.00076	1.95351
A31	2.15303	0.00012	-0.00001	0.00136	0.00135	2.15437
A32	2.07943	-0.00002	0.00000	-0.00008	-0.00008	2.07935
A33	2.15786	0.00001	0.00000	0.00000	0.00000	2.15786
A34	2.04590	0.00000	0.00000	0.00008	0.00008	2.04598
A35	1.98244	-0.00053	-0.00006	0.00056	0.00050	1.98294
A36	1.95626	-0.00027	-0.00017	0.00104	0.00087	1.95713
A37	1.90762	0.00023	0.00005	-0.00369	-0.00363	1.90399
D1	0.02028	-0.00073	-0.00048	-0.01286	-0.01333	0.00695
D2	-3.13316	-0.00033	-0.00014	-0.00787	-0.00801	-3.14117
D3	-3.13791	-0.00024	-0.00026	-0.00052	-0.00076	-3.13867

D4	-0.00816	0.00017	0.00008	0.00447	0.00455	-0.00360
D5	-0.01850	0.00064	0.00047	0.01095	0.01141	-0.00709
D6	-3.10310	0.00061	0.00007	0.01899	0.01909	-3.08400
D7	3.13797	0.00020	0.00028	-0.00011	0.00015	3.13812
D8	0.05337	0.00017	-0.00013	0.00793	0.00784	0.06120
D9	-0.01531	0.00057	0.00033	0.01049	0.01080	-0.00451
D10	3.11959	0.00031	0.00032	0.00256	0.00286	3.12245
D11	3.13701	0.00021	0.00002	0.00597	0.00599	-3.14019
D12	-0.01128	-0.00005	0.00001	-0.00196	-0.00195	-0.01324
D13	0.00395	-0.00017	-0.00004	-0.00379	-0.00381	0.00014
D14	3.06091	-0.00052	0.00006	-0.01231	-0.01228	3.04863
D15	-3.13149	0.00006	-0.00003	0.00350	0.00347	-3.12801
D16	-0.07453	-0.00028	0.00007	-0.00502	-0.00499	-0.07952
D17	0.06848	0.00021	-0.00007	0.01429	0.01422	0.08270
D18	-3.06710	0.00022	-0.00008	0.01565	0.01557	-3.05152
D19	-3.08060	-0.00008	-0.00008	0.00542	0.00534	-3.07526
D20	0.06701	-0.00007	-0.00009	0.00678	0.00669	0.07370
D21	0.00885	-0.00028	-0.00027	-0.00433	-0.00460	0.00425
D22	3.09445	-0.00010	0.00013	-0.01132	-0.01113	3.08331
D23	-3.04864	-0.00011	-0.00036	0.00309	0.00267	-3.04598
D24	0.03695	0.00007	0.00004	-0.00391	-0.00387	0.03308
D25	-2.30075	0.00042	-0.00033	0.16973	0.16939	-2.13136
D26	0.74187	0.00013	-0.00022	0.16045	0.16024	0.90211
D27	1.79405	0.00039	-0.00024	0.00368	0.00343	1.79748
D28	-2.39416	0.00030	-0.00025	0.00679	0.00655	-2.38761
D29	-0.35007	0.00016	-0.00028	0.00477	0.00449	-0.34558
D30	-1.28187	0.00026	-0.00071	0.01239	0.01167	-1.27020
D31	0.81311	0.00016	-0.00072	0.01550	0.01478	0.82789
D32	2.85720	0.00002	-0.00075	0.01347	0.01272	2.86992
D33	-1.04083	-0.00005	0.00042	0.03993	0.04036	-1.00046
D34	1.00842	0.00018	0.00062	0.03462	0.03522	1.04364
D35	3.08195	0.00041	0.00032	0.05332	0.05363	3.13558
D36	-3.12800	0.00006	0.00039	0.04492	0.04532	-3.08268
D37	-1.07875	0.00029	0.00058	0.03960	0.04018	-1.03857
D38	0.99478	0.00052	0.00029	0.05830	0.05859	1.05337
D39	1.05668	-0.00006	0.00038	0.04581	0.04620	1.10288
D40	3.10593	0.00018	0.00057	0.04049	0.04106	-3.13620
D41	-1.10372	0.00040	0.00028	0.05919	0.05946	-1.04426
D42	1.92873	0.00042	-0.00037	0.08869	0.08831	2.01704
D43	-2.18162	0.00010	-0.00049	0.08500	0.08451	-2.09711
D44	-0.19896	0.00035	-0.00062	0.10411	0.10347	-0.09549
D45	1.97388	0.00003	-0.00074	0.10042	0.09967	2.07355
D46	-2.31314	0.00088	-0.00051	0.10316	0.10267	-2.21047
D47	-0.14030	0.00056	-0.00063	0.09947	0.09887	-0.04143

D48	-3.13350	0.00002	0.00000	0.00085	0.00085	-3.13265
D49	0.00806	0.00003	0.00000	0.00110	0.00110	0.00916
D50	0.00141	0.00000	0.00001	-0.00067	-0.00066	0.00075
D51	-3.14021	0.00001	0.00001	-0.00042	-0.00041	-3.14062

Item	Value	Threshold	Converged?
Maximum Force	0.002024	0.000450	NO
RMS Force	0.000443	0.000300	NO
Maximum Displacement	0.214960	0.001800	NO
RMS Displacement	0.035278	0.001200	NO

Predicted change in Energy=-2.926776D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.804807	-2.008907	0.307490
2	6	0	-2.816400	-1.135902	0.067799
3	7	0	-2.245950	0.131400	0.023086
4	6	0	-0.920564	0.019264	0.237504
5	7	0	-0.636090	-1.271539	0.415264
6	6	0	0.732552	-1.801206	0.607141
7	6	0	1.545512	-1.771707	-0.697990
8	1	0	-1.815781	-3.080035	0.412928
9	1	0	-3.867319	-1.308146	-0.076306
10	1	0	1.227482	-1.181770	1.354612
11	1	0	0.641431	-2.815104	0.999074
12	1	0	1.016159	-2.345779	-1.467745
13	1	0	1.600534	-0.729294	-1.028520
14	35	0	1.553168	2.034614	-0.366000
15	1	0	-0.166959	0.839849	0.182732
16	6	0	-2.870612	1.385815	-0.219553
17	6	0	-4.177406	1.561722	-0.364995
18	1	0	-2.149306	2.191941	-0.280397
19	1	0	-4.556757	2.556048	-0.555315
20	1	0	-4.901155	0.758667	-0.303963
21	7	0	2.879225	-2.300025	-0.423458
22	1	0	3.082883	-3.160348	-0.913885
23	1	0	3.605684	-1.624641	-0.624216

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				

2	C	1.357538	0.000000			
3	N	2.203725	1.390491	0.000000		
4	C	2.213653	2.226522	1.347292	0.000000	
5	N	1.386083	2.211986	2.171103	1.333678	0.000000
6	C	2.563420	3.650833	3.598272	2.486672	1.480049
7	C	3.505979	4.474031	4.303132	3.188143	2.499778
8	H	1.076361	2.213596	3.263485	3.230765	2.159244
9	H	2.211859	1.074647	2.170486	3.247131	3.268612
10	H	3.312914	4.243934	3.944883	2.702687	2.088859
11	H	2.666894	3.955198	4.239269	3.324675	2.086980
12	H	3.350043	4.302349	4.358938	3.500314	2.725737
13	H	3.875395	4.569087	4.079474	2.918749	2.716806
14	Br	5.299023	5.416038	4.266955	3.247338	4.041519
15	H	3.288392	3.307013	2.202178	1.115473	2.175343
16	C	3.596922	2.538614	1.422193	2.424675	3.529534
17	C	4.339453	3.052347	2.434533	3.653656	4.601858
18	H	4.255751	3.411861	2.085012	2.549226	3.843106
19	H	5.399673	4.128875	3.399014	4.503969	5.564538
20	H	4.197703	2.841444	2.747825	4.084729	4.778055
21	N	4.749651	5.834094	5.690223	4.500485	3.757483
22	H	5.167890	6.313765	6.333243	5.240536	4.377784
23	H	5.503558	6.477725	6.143639	4.892025	4.381535

		6	7	8	9	10
6	C	0.000000				
7	C	1.537901	0.000000			
8	H	2.857817	3.774142	0.000000		
9	H	4.676433	5.468100	2.754587	0.000000	
10	H	1.089665	2.159246	3.708319	5.293439	0.000000
11	H	1.090827	2.187708	2.540009	4.874032	1.771340
12	H	2.163826	1.096493	3.477922	5.182773	3.060274
13	H	2.139574	1.094944	4.390326	5.580251	2.454225
14	Br	4.041526	3.820779	6.173830	6.374923	3.662198
15	H	2.822130	3.244757	4.258767	4.286449	2.721160
16	C	4.880913	5.449862	4.632118	2.875999	5.085751
17	C	6.030093	6.631321	5.265771	2.900972	6.300525
18	H	5.003805	5.434756	5.327821	3.904335	5.045580
19	H	6.950810	7.482480	6.341599	3.954335	7.146784
20	H	6.254736	6.936682	4.976857	2.322146	6.639003
21	N	2.432932	1.460575	4.832290	6.827898	2.672130
22	H	3.112048	2.082893	5.075804	7.241374	3.536009
23	H	3.130863	2.066732	5.708425	7.499744	3.125339

		11	12	13	14	15
11	H	0.000000				
12	H	2.538875	0.000000			

13	H	3.062944	1.774102	0.000000		
14	Br	5.120005	4.548633	2.842598	0.000000	
15	H	3.831265	3.777839	2.655819	2.165042	0.000000
16	C	5.609565	5.530801	5.011912	4.473502	2.787410
17	C	6.651201	6.592248	6.250889	5.750053	4.111544
18	H	5.873309	5.658699	4.811924	3.706804	2.443838
19	H	7.634563	7.477822	6.994972	6.135056	4.770784
20	H	6.722351	6.782815	6.709022	6.579527	4.759840
21	N	2.701227	2.136269	2.113846	4.533301	4.416504
22	H	3.120785	2.289461	2.849653	5.443145	5.269309
23	H	3.583165	2.817308	2.232876	4.203528	4.577960

		16	17	18	19	20
16	C	0.000000				
17	C	1.326577	0.000000			
18	H	1.083432	2.125446	0.000000		
19	H	2.079728	1.081117	2.450300	0.000000	
20	H	2.126862	1.082790	3.102822	1.847259	0.000000
21	N	6.832833	8.044411	6.744209	8.882154	8.360872
22	H	7.522885	8.678192	7.511598	9.548290	8.914906
23	H	7.153252	8.414072	6.914075	9.171061	8.840194

		21	22	23
21	N	0.000000		
22	H	1.011015	0.000000	
23	H	1.012023	1.647915	0.000000

Stoichiometry C7H12BrN3
Framework group C1[X(C7H12BrN3)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.618200	2.229775	-0.144908
2	6	0	-2.646949	1.372458	0.077786
3	7	0	-2.124615	0.088190	-0.028458
4	6	0	-0.810982	0.175552	-0.314698
5	7	0	-0.487560	1.467092	-0.392286
6	6	0	0.886815	1.966418	-0.621005
7	6	0	1.774247	1.788835	0.622405
8	1	0	-1.593724	3.305835	-0.151953
9	1	0	-3.679925	1.565478	0.302662

10	1	0	1.311890	1.402910	-1.451149
11	1	0	0.812065	3.014790	-0.912948
12	1	0	1.314396	2.306278	1.472751
13	1	0	1.808224	0.718989	0.853005
14	35	0	1.613953	-1.968365	-0.052949
15	1	0	-0.087969	-0.671210	-0.381975
16	6	0	-2.782086	-1.161834	0.138287
17	6	0	-4.083762	-1.306873	0.349025
18	1	0	-2.090366	-1.993697	0.080385
19	1	0	-4.489532	-2.301388	0.471923
20	1	0	-4.778050	-0.477969	0.406615
21	7	0	3.108809	2.295654	0.313608
22	1	0	3.374632	3.099475	0.866203
23	1	0	3.819087	1.580738	0.406290

Rotational constants (GHZ): 0.7472404 0.5049521 0.3100846

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 365 symmetry adapted cartesian basis functions of A symmetry.

There are 352 symmetry adapted basis functions of A symmetry.

352 basis functions, 562 primitive gaussians, 365 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 835.3268288519 Hartrees.

NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 352 RedAO= T EigKep= 4.50D-06 NBF= 352

NBsUse= 352 1.00D-06 EigRej= -1.00D+00 NBFU= 352

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999983 -0.000742 -0.000182 0.005718 Ang= -0.66 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3012.46544779 A.U. after 12 cycles
NFock= 12 Conv=0.70D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000081773	-0.000078974	0.000155295
2	6	-0.000231172	-0.000198918	-0.000469600
3	7	0.000298561	-0.000328013	-0.000049563
4	6	-0.000691433	0.000148955	0.000440980
5	7	-0.000202440	-0.000373291	0.000050534
6	6	-0.000299683	0.000748473	0.000688941
7	6	0.000353308	0.000543245	0.000160419
8	1	-0.000096326	0.000019632	0.000177656
9	1	-0.000019981	-0.000020313	0.000043601
10	1	0.000140313	-0.000112373	-0.000033015
11	1	-0.000394772	0.000208288	-0.000183286
12	1	0.000850945	-0.000558186	-0.000116784
13	1	0.000387035	-0.000589852	-0.000358627
14	35	-0.000042019	0.000351789	-0.000148661
15	1	0.000911593	-0.000067343	0.000112114
16	6	-0.000016490	0.000238391	-0.000037105
17	6	0.000001149	-0.000095946	0.000089428
18	1	0.000060377	-0.000024291	-0.000029269
19	1	0.000003143	0.000016530	-0.000035742
20	1	0.000002435	0.000011498	0.000049927
21	7	0.000016308	-0.000734911	-0.000112038
22	1	-0.000343277	0.000804939	-0.000586972
23	1	-0.000605802	0.000090671	0.000191764

Cartesian Forces: Max 0.000911593 RMS 0.000343457

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.001035458 RMS 0.000307235
Search for a local minimum.
Step number 7 out of a maximum of 121
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 5 6 7
DE= -3.89D-04 DEPred=-2.93D-04 R= 1.33D+00
TightC=F SS= 1.41D+00 RLast= 3.68D-01 DXNew= 1.4270D+00 1.1032D+00
Trust test= 1.33D+00 RLast= 3.68D-01 DXMaxT set to 1.10D+00
ITU= 1 1 1 0 1 0 0

Eigenvalues ---	0.00131	0.00332	0.00375	0.00935	0.01392
Eigenvalues ---	0.01538	0.01874	0.01959	0.02209	0.02320
Eigenvalues ---	0.02390	0.02608	0.03062	0.03062	0.03218
Eigenvalues ---	0.03457	0.03800	0.04251	0.04736	0.05342
Eigenvalues ---	0.05704	0.09283	0.09953	0.12279	0.13372
Eigenvalues ---	0.15714	0.15978	0.16000	0.16000	0.16000
Eigenvalues ---	0.16007	0.16863	0.17673	0.21580	0.21972
Eigenvalues ---	0.22031	0.22704	0.23567	0.23998	0.25039
Eigenvalues ---	0.27786	0.31871	0.34004	0.34393	0.34727
Eigenvalues ---	0.34789	0.34966	0.35684	0.35689	0.35858
Eigenvalues ---	0.36436	0.36657	0.37436	0.41088	0.42190
Eigenvalues ---	0.43645	0.47510	0.47703	0.48389	0.51316
Eigenvalues ---	0.54323	0.60353	0.61811		

En-DIIS/RFO-DIIS IScMMF= 0 using points: 7 6 5
RFO step: Lambda=-3.28383085D-05.
DidBck=F Rises=F RFO-DIIS coefs: 1.56527 -0.38563 -0.17964
Iteration 1 RMS(Cart)= 0.04329999 RMS(Int)= 0.00274155
Iteration 2 RMS(Cart)= 0.00309789 RMS(Int)= 0.00004488
Iteration 3 RMS(Cart)= 0.00001360 RMS(Int)= 0.00004253
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00004253

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56538	-0.00003	0.00040	0.00023	0.00061	2.56598
R2	2.61932	0.00024	-0.00062	0.00044	-0.00018	2.61914
R3	2.03403	0.00000	0.00007	0.00006	0.00013	2.03416
R4	2.62765	0.00019	0.00027	0.00071	0.00096	2.62861
R5	2.03079	0.00002	0.00000	0.00003	0.00003	2.03082
R6	2.54601	-0.00009	-0.00106	-0.00080	-0.00185	2.54416
R7	2.68756	0.00010	0.00014	0.00049	0.00064	2.68819
R8	2.52029	0.00005	-0.00013	-0.00024	-0.00035	2.51994
R9	2.10794	0.00080	-0.00063	0.00210	0.00147	2.10941
R10	2.79689	-0.00009	-0.00047	-0.00094	-0.00140	2.79548
R11	2.90621	0.00104	-0.00048	0.00342	0.00294	2.90915

R12	2.05917	-0.00002	0.00055	0.00012	0.00067	2.05984
R13	2.06136	-0.00023	-0.00013	-0.00070	-0.00083	2.06053
R14	2.07207	-0.00004	-0.00106	-0.00059	-0.00166	2.07042
R15	2.06914	-0.00043	0.00177	-0.00106	0.00071	2.06985
R16	2.76009	-0.00100	0.00176	-0.00180	-0.00004	2.76004
R17	4.09134	0.00020	-0.02189	-0.01077	-0.03265	4.05868
R18	2.50687	-0.00003	-0.00001	-0.00005	-0.00007	2.50680
R19	2.04739	0.00002	0.00026	0.00031	0.00057	2.04796
R20	2.04301	0.00002	-0.00003	0.00005	0.00001	2.04303
R21	2.04618	-0.00001	0.00008	0.00004	0.00011	2.04629
R22	1.91054	-0.00047	0.00045	-0.00036	0.00009	1.91063
R23	1.91245	-0.00041	0.00081	-0.00010	0.00071	1.91316
A1	1.87542	-0.00002	-0.00067	-0.00068	-0.00135	1.87406
A2	2.27792	-0.00006	0.00001	-0.00034	-0.00034	2.27758
A3	2.12984	0.00008	0.00070	0.00100	0.00169	2.13152
A4	1.86093	-0.00016	0.00064	-0.00031	0.00029	1.86121
A5	2.27748	0.00005	-0.00028	-0.00004	-0.00032	2.27716
A6	2.14476	0.00010	-0.00033	0.00033	-0.00001	2.14475
A7	1.89928	0.00027	-0.00078	0.00070	-0.00009	1.89918
A8	2.25129	-0.00003	0.00075	0.00068	0.00142	2.25271
A9	2.13252	-0.00024	0.00000	-0.00134	-0.00135	2.13117
A10	1.88767	-0.00022	0.00072	-0.00067	0.00004	1.88772
A11	2.20877	-0.00009	0.00403	0.00014	0.00411	2.21288
A12	2.18270	0.00030	-0.00521	-0.00024	-0.00551	2.17719
A13	1.90145	0.00013	0.00018	0.00090	0.00103	1.90249
A14	2.21356	0.00005	0.00613	0.00230	0.00832	2.22188
A15	2.16626	-0.00018	-0.00673	-0.00366	-0.01047	2.15579
A16	1.95190	0.00062	-0.00335	0.00088	-0.00246	1.94944
A17	1.88127	-0.00001	-0.00362	-0.00094	-0.00453	1.87673
A18	1.87755	-0.00050	0.00623	-0.00029	0.00594	1.88349
A19	1.90830	-0.00025	0.00512	0.00151	0.00662	1.91492
A20	1.94648	0.00000	-0.00259	-0.00123	-0.00381	1.94267
A21	1.89637	0.00013	-0.00190	0.00002	-0.00186	1.89451
A22	1.90765	0.00050	-0.00705	0.00349	-0.00361	1.90404
A23	1.87654	0.00002	0.00375	0.00439	0.00803	1.88457
A24	1.89257	0.00077	-0.00114	0.00316	0.00190	1.89447
A25	1.88681	0.00012	-0.00299	-0.00211	-0.00505	1.88176
A26	1.96428	-0.00096	-0.00280	-0.00892	-0.01177	1.95251
A27	1.93394	-0.00039	0.01052	0.00064	0.01109	1.94503
A28	2.84100	0.00069	0.01405	0.01138	0.02543	2.86643
A29	2.17528	-0.00010	-0.00036	-0.00078	-0.00114	2.17415
A30	1.95351	-0.00001	-0.00053	-0.00044	-0.00097	1.95253
A31	2.15437	0.00011	0.00088	0.00123	0.00210	2.15648
A32	2.07935	-0.00001	-0.00007	-0.00017	-0.00023	2.07912

A33	2.15786	0.00000	0.00002	0.00011	0.00013	2.15799
A34	2.04598	0.00001	0.00005	0.00006	0.00011	2.04608
A35	1.98294	-0.00084	0.00105	-0.00743	-0.00642	1.97651
A36	1.95713	-0.00055	0.00256	-0.00436	-0.00184	1.95529
A37	1.90399	0.00044	-0.00270	-0.00483	-0.00759	1.89640
D1	0.00695	-0.00015	-0.00183	0.00909	0.00729	0.01424
D2	-3.14117	-0.00002	-0.00291	0.00469	0.00177	-3.13940
D3	-3.13867	-0.00011	0.00266	0.00203	0.00475	-3.13393
D4	-0.00360	0.00002	0.00158	-0.00237	-0.00077	-0.00437
D5	-0.00709	0.00016	0.00082	-0.00643	-0.00562	-0.01271
D6	-3.08400	0.00012	0.01001	0.00153	0.01169	-3.07231
D7	3.13812	0.00013	-0.00320	-0.00010	-0.00334	3.13478
D8	0.06120	0.00009	0.00599	0.00786	0.01398	0.07518
D9	-0.00451	0.00008	0.00222	-0.00872	-0.00653	-0.01104
D10	3.12245	0.00009	-0.00216	-0.00588	-0.00807	3.11438
D11	-3.14019	-0.00004	0.00319	-0.00473	-0.00153	3.14146
D12	-0.01324	-0.00003	-0.00119	-0.00189	-0.00307	-0.01630
D13	0.00014	0.00002	-0.00173	0.00480	0.00309	0.00322
D14	3.04863	-0.00005	-0.00764	-0.00404	-0.01171	3.03692
D15	-3.12801	0.00001	0.00229	0.00217	0.00447	-3.12354
D16	-0.07952	-0.00006	-0.00362	-0.00667	-0.01033	-0.08985
D17	0.08270	0.00009	0.00890	0.00990	0.01879	0.10149
D18	-3.05152	0.00007	0.00979	0.00936	0.01914	-3.03238
D19	-3.07526	0.00010	0.00399	0.01309	0.01709	-3.05818
D20	0.07370	0.00009	0.00489	0.01255	0.01744	0.09114
D21	0.00425	-0.00011	0.00058	0.00095	0.00153	0.00578
D22	3.08331	-0.00006	-0.00787	-0.00648	-0.01416	3.06915
D23	-3.04598	-0.00002	0.00583	0.00960	0.01531	-3.03066
D24	0.03308	0.00003	-0.00262	0.00217	-0.00038	0.03271
D25	-2.13136	0.00022	0.09965	0.11605	0.21568	-1.91568
D26	0.90211	0.00012	0.09316	0.10577	0.19896	1.10106
D27	1.79748	0.00003	0.00476	0.00592	0.01067	1.80815
D28	-2.38761	0.00010	0.00669	0.00771	0.01442	-2.37319
D29	-0.34558	-0.00002	0.00586	0.00709	0.01297	-0.33261
D30	-1.27020	-0.00003	0.01500	0.01481	0.02978	-1.24042
D31	0.82789	0.00004	0.01693	0.01660	0.03353	0.86142
D32	2.86992	-0.00008	0.01610	0.01598	0.03208	2.90200
D33	-1.00046	-0.00016	0.01776	-0.03139	-0.01362	-1.01409
D34	1.04364	0.00025	0.01252	-0.02960	-0.01711	1.02654
D35	3.13558	0.00022	0.02647	-0.02460	0.00186	3.13745
D36	-3.08268	-0.00038	0.02098	-0.03177	-0.01076	-3.09344
D37	-1.03857	0.00004	0.01575	-0.02998	-0.01424	-1.05281
D38	1.05337	0.00001	0.02970	-0.02498	0.00473	1.05810
D39	1.10288	-0.00038	0.02161	-0.03200	-0.01037	1.09251

D40	-3.13620	0.00004	0.01637	-0.03022	-0.01386	3.13313
D41	-1.04426	0.00001	0.03032	-0.02521	0.00511	-1.03915
D42	2.01704	0.00064	0.05434	0.08043	0.13473	2.15177
D43	-2.09711	0.00013	0.05357	0.06454	0.11811	-1.97901
D44	-0.09549	0.00010	0.06587	0.07958	0.14541	0.04992
D45	2.07355	-0.00041	0.06510	0.06369	0.12878	2.20233
D46	-2.21047	0.00090	0.06415	0.08805	0.15224	-2.05823
D47	-0.04143	0.00039	0.06338	0.07216	0.13561	0.09418
D48	-3.13265	0.00002	0.00049	0.00083	0.00132	-3.13133
D49	0.00916	0.00003	0.00064	0.00142	0.00206	0.01122
D50	0.00075	0.00004	-0.00051	0.00143	0.00092	0.00167
D51	-3.14062	0.00005	-0.00036	0.00202	0.00166	-3.13897

Item	Value	Threshold	Converged?
Maximum Force	0.001035	0.000450	NO
RMS Force	0.000307	0.000300	NO
Maximum Displacement	0.220205	0.001800	NO
RMS Displacement	0.044400	0.001200	NO

Predicted change in Energy=-1.854204D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.818618	-2.021298	0.323290
2	6	0	-2.821331	-1.138887	0.078954
3	7	0	-2.237509	0.122509	0.024959
4	6	0	-0.915314	-0.001147	0.246474
5	7	0	-0.644400	-1.293317	0.433836
6	6	0	0.724723	-1.822655	0.617273
7	6	0	1.536193	-1.767088	-0.689766
8	1	0	-1.840747	-3.091994	0.432043
9	1	0	-3.873517	-1.301590	-0.067085
10	1	0	1.212498	-1.214509	1.379097
11	1	0	0.642310	-2.844286	0.989327
12	1	0	1.011737	-2.340817	-1.461878
13	1	0	1.577325	-0.722926	-1.018024
14	35	0	1.491929	2.053856	-0.428472
15	1	0	-0.147716	0.806436	0.178479
16	6	0	-2.846229	1.381885	-0.233929
17	6	0	-4.151947	1.573227	-0.368850
18	1	0	-2.112768	2.175372	-0.316934
19	1	0	-4.519366	2.569000	-0.574436

20	1	0	-4.886185	0.781877	-0.283869
21	7	0	2.871782	-2.298200	-0.430283
22	1	0	3.116117	-3.074341	-1.030413
23	1	0	3.586554	-1.586189	-0.514509

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357860	0.000000			
3	N	2.204628	1.391001	0.000000		
4	C	2.214243	2.226076	1.346314	0.000000	
5	N	1.385989	2.211067	2.170195	1.333493	0.000000
6	C	2.567970	3.651277	3.592955	2.478932	1.479306
7	C	3.513639	4.469181	4.280448	3.163064	2.498384
8	H	1.076432	2.213784	3.264379	3.231748	2.160205
9	H	2.212009	1.074661	2.170957	3.246605	3.267750
10	H	3.309577	4.238852	3.940033	2.698641	2.085137
11	H	2.679008	3.966608	4.245615	3.325878	2.090382
12	H	3.361522	4.302466	4.340077	3.479375	2.726496
13	H	3.875219	4.552423	4.044197	2.886723	2.714646
14	Br	5.303938	5.390297	4.224264	3.236265	4.063379
15	H	3.287699	3.307930	2.204214	1.116252	2.172755
16	C	3.598352	2.540238	1.422529	2.423221	3.528551
17	C	4.340978	3.053953	2.434078	3.651448	4.600464
18	H	4.255402	3.412198	2.084873	2.547265	3.840777
19	H	5.400999	4.130214	3.398744	4.502082	5.563225
20	H	4.199571	2.843342	2.746930	4.081937	4.776429
21	N	4.758613	5.832226	5.672031	4.480686	3.757662
22	H	5.224272	6.342710	6.324158	5.227561	4.411072
23	H	5.486995	6.450835	6.093471	4.833039	4.345814

		6	7	8	9	10
6	C	0.000000				
7	C	1.539455	0.000000			
8	H	2.868304	3.797046	0.000000		
9	H	4.677999	5.465289	2.754420	0.000000	
10	H	1.090019	2.165713	3.707312	5.288344	0.000000
11	H	1.090388	2.186032	2.556854	4.887599	1.770087
12	H	2.161883	1.095617	3.505407	5.185668	3.062681
13	H	2.147214	1.095317	4.404361	5.563346	2.474053
14	Br	4.087729	3.830124	6.190880	6.338583	3.745344
15	H	2.804605	3.195688	4.257746	4.287852	2.715858
16	C	4.872917	5.415666	4.633584	2.878229	5.080982
17	C	6.023817	6.604212	5.267576	2.903990	6.293175
18	H	4.990823	5.384877	5.327297	3.905372	5.042341

19	H	6.943146	7.448808	6.343094	3.956765	7.140413
20	H	6.251235	6.921626	4.979366	2.326655	6.629098
21	N	2.435852	1.460551	4.856094	6.828192	2.683554
22	H	3.162333	2.078729	5.168133	7.275001	3.590052
23	H	3.086571	2.065774	5.711306	7.478894	3.059417

		11	12	13	14	15
11	H	0.000000				
12	H	2.529499	0.000000			
13	H	3.066575	1.770443	0.000000		
14	Br	5.169508	4.540007	2.839962	0.000000	
15	H	3.822223	3.733671	2.597370	2.147762	0.000000
16	C	5.614872	5.500025	4.961135	4.394201	2.789838
17	C	6.659127	6.571003	6.206311	5.664617	4.113563
18	H	5.873137	5.609758	4.744306	3.608468	2.445577
19	H	7.641461	7.448957	6.942851	6.035093	4.773347
20	H	6.733078	6.776755	6.676853	6.505319	4.761035
21	N	2.698897	2.127386	2.121921	4.565566	4.373410
22	H	3.201873	2.269941	2.810193	5.412830	5.212912
23	H	3.537358	2.845462	2.244049	4.200570	4.488837

		16	17	18	19	20
16	C	0.000000				
17	C	1.326542	0.000000			
18	H	1.083732	2.126858	0.000000		
19	H	2.079561	1.081123	2.452135	0.000000	
20	H	2.126952	1.082850	3.103992	1.847375	0.000000
21	N	6.802737	8.020255	6.698614	8.850959	8.348315
22	H	7.486114	8.652300	7.443774	9.505567	8.914291
23	H	7.090056	8.359876	6.831592	9.109069	8.800468

		21	22	23
21	N	0.000000		
22	H	1.011064	0.000000	
23	H	1.012400	1.643796	0.000000

Stoichiometry C7H12BrN3
Framework group C1[X(C7H12BrN3)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.602385	2.259646	-0.126092

2	6	0	-2.625912	1.394738	0.093241
3	7	0	-2.098121	0.113642	-0.029689
4	6	0	-0.789353	0.210219	-0.330290
5	7	0	-0.472684	1.503837	-0.397191
6	6	0	0.903957	1.997363	-0.619982
7	6	0	1.797318	1.767543	0.612499
8	1	0	-1.582696	3.335867	-0.117857
9	1	0	-3.657481	1.580541	0.330393
10	1	0	1.311548	1.458381	-1.475266
11	1	0	0.843770	3.056084	-0.873820
12	1	0	1.352277	2.272614	1.476916
13	1	0	1.812410	0.692834	0.823433
14	35	0	1.560955	-1.997062	-0.052130
15	1	0	-0.056688	-0.628712	-0.403887
16	6	0	-2.745224	-1.142341	0.135705
17	6	0	-4.046434	-1.297260	0.342018
18	1	0	-2.044939	-1.967615	0.080932
19	1	0	-4.444517	-2.294804	0.465563
20	1	0	-4.747723	-0.473861	0.394658
21	7	0	3.135549	2.272468	0.316869
22	1	0	3.454586	2.968064	0.977636
23	1	0	3.821016	1.528697	0.273351

Rotational constants (GHZ): 0.7364246 0.5148880 0.3118910

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 365 symmetry adapted cartesian basis functions of A symmetry.

There are 352 symmetry adapted basis functions of A symmetry.

352 basis functions, 562 primitive gaussians, 365 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 836.2658328008 Hartrees.

NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 352 RedAO= T EigKep= 4.57D-06 NBF= 352

NBsUse= 352 1.00D-06 EigRej= -1.00D+00 NBFU= 352

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999982 -0.001892 -0.000624 0.005662 Ang= -0.69 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3012.46571223 A.U. after 12 cycles
NFock= 12 Conv=0.35D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000249312	-0.000030215	0.000801399
2	6	0.000044947	-0.000167185	-0.001064591
3	7	-0.000187734	-0.000055322	0.000425643
4	6	-0.000055127	-0.000960831	0.000368126
5	7	0.000183056	-0.000432153	-0.000722641
6	6	-0.000051625	0.000570951	0.000352876
7	6	-0.000208877	0.000728280	-0.000032959
8	1	-0.000046719	0.000067694	0.000291831
9	1	-0.000010128	0.000012154	-0.000032716
10	1	0.000517958	-0.000302308	-0.000206062
11	1	-0.000617961	0.000102136	-0.000168548
12	1	0.000895108	-0.000907678	0.000094150
13	1	0.000139490	-0.000323628	0.000010520
14	35	0.000600042	0.000766391	-0.000248608
15	1	-0.000297070	0.001044290	0.000195188
16	6	-0.000077597	0.000207611	0.000073740
17	6	-0.000009263	-0.000032737	0.000083997
18	1	0.000017847	-0.000051418	-0.000026521
19	1	-0.000014060	0.000015929	-0.000051200
20	1	0.000025410	0.000007285	0.000041266
21	7	0.000482556	-0.001395098	-0.000017329
22	1	-0.000383024	0.000753952	-0.000356513

```
      23        1             -0.000697919      0.000381900      0.000188954
 ---------------------------------------------------------------------
 Cartesian Forces:  Max        0.001395098 RMS      0.000443689

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 Internal  Forces:  Max        0.001727202 RMS      0.000451968
 Search for a local minimum.
 Step number   8 out of a maximum of   121
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swapping is turned off.
 Update second derivatives using D2CorX and points      7      8
 DE= -2.64D-04 DEPred=-1.85D-04 R= 1.43D+00
 TightC=F SS=  1.41D+00  RLast= 4.55D-01 DXNew= 1.8553D+00 1.3661D+00
 Trust test= 1.43D+00 RLast= 4.55D-01 DXMaxT set to 1.37D+00
 ITU=  1  1  1  1  0  1  0  0
      Eigenvalues ---      0.00056     0.00313     0.00378     0.00943     0.01390
      Eigenvalues ---      0.01551     0.01875     0.02006     0.02220     0.02321
      Eigenvalues ---      0.02391     0.02609     0.03061     0.03062     0.03282
      Eigenvalues ---      0.03477     0.03999     0.04288     0.04759     0.05336
      Eigenvalues ---      0.05827     0.09250     0.09878     0.12266     0.13448
      Eigenvalues ---      0.15675     0.15985     0.15999     0.16000     0.16001
      Eigenvalues ---      0.16007     0.16845     0.18335     0.21825     0.22014
      Eigenvalues ---      0.22026     0.22663     0.23517     0.23932     0.25037
      Eigenvalues ---      0.28090     0.31947     0.34097     0.34395     0.34725
      Eigenvalues ---      0.34821     0.35006     0.35686     0.35689     0.35858
      Eigenvalues ---      0.36436     0.36658     0.37993     0.40911     0.42191
      Eigenvalues ---      0.43742     0.47640     0.47962     0.48206     0.51645
      Eigenvalues ---      0.54361     0.60352     0.64204
 En-DIIS/RFO-DIIS IScMMF=        0 using points:      8      7      6      5
 RFO step:  Lambda=-5.02926812D-05.
 DidBck=F Rises=F RFO-DIIS coefs:      1.64848     -0.33067     -0.39161      0.07380
 Iteration  1 RMS(Cart)=  0.06425389 RMS(Int)=  0.01823724
 Iteration  2 RMS(Cart)=  0.01367754 RMS(Int)=  0.00035489
 Iteration  3 RMS(Cart)=  0.00051204 RMS(Int)=  0.00007676
 Iteration  4 RMS(Cart)=  0.00000048 RMS(Int)=  0.00007675
 Variable          Old X       -DE/DX      Delta X      Delta X      Delta X          New X
                                           (Linear)       (Quad)     (Total)
     R1            2.56598    -0.00016     0.00062      0.00036      0.00096      2.56695
     R2            2.61914     0.00027    -0.00034      0.00033      0.00000      2.61914
     R3            2.03416    -0.00004     0.00011      0.00001      0.00012      2.03428
```

R4	2.62861	-0.00012	0.00089	0.00025	0.00112	2.62973
R5	2.03082	0.00001	0.00003	-0.00004	-0.00001	2.03080
R6	2.54416	0.00032	-0.00161	-0.00074	-0.00234	2.54182
R7	2.68819	0.00013	0.00048	0.00101	0.00149	2.68969
R8	2.51994	0.00100	-0.00056	0.00087	0.00033	2.52027
R9	2.10941	0.00152	0.00122	0.00227	0.00348	2.11290
R10	2.79548	0.00020	-0.00129	-0.00123	-0.00252	2.79296
R11	2.90915	0.00019	0.00212	-0.00094	0.00119	2.91034
R12	2.05984	-0.00008	0.00057	0.00012	0.00069	2.06053
R13	2.06053	-0.00011	-0.00066	-0.00023	-0.00089	2.05964
R14	2.07042	-0.00002	-0.00158	-0.00137	-0.00294	2.06747
R15	2.06985	-0.00030	0.00127	0.00023	0.00150	2.07135
R16	2.76004	-0.00048	-0.00020	0.00287	0.00267	2.76271
R17	4.05868	0.00097	-0.02821	-0.00554	-0.03375	4.02493
R18	2.50680	-0.00001	-0.00006	-0.00003	-0.00009	2.50672
R19	2.04796	-0.00003	0.00046	0.00049	0.00095	2.04891
R20	2.04303	0.00003	0.00000	0.00006	0.00006	2.04308
R21	2.04629	-0.00002	0.00010	0.00007	0.00017	2.04646
R22	1.91063	-0.00046	-0.00022	0.00060	0.00037	1.91101
R23	1.91316	-0.00024	0.00044	0.00123	0.00167	1.91483
A1	1.87406	0.00027	-0.00135	-0.00040	-0.00175	1.87232
A2	2.27758	-0.00013	-0.00010	-0.00018	-0.00030	2.27728
A3	2.13152	-0.00013	0.00150	0.00057	0.00206	2.13358
A4	1.86121	-0.00001	0.00047	0.00050	0.00097	1.86219
A5	2.27716	0.00003	-0.00036	-0.00008	-0.00044	2.27672
A6	2.14475	-0.00001	-0.00013	-0.00037	-0.00049	2.14426
A7	1.89918	0.00034	-0.00036	-0.00024	-0.00060	1.89858
A8	2.25271	-0.00017	0.00125	0.00121	0.00243	2.25515
A9	2.13117	-0.00017	-0.00092	-0.00102	-0.00196	2.12921
A10	1.88772	-0.00038	0.00021	0.00040	0.00060	1.88831
A11	2.21288	-0.00133	0.00534	-0.00534	-0.00010	2.21278
A12	2.17719	0.00173	-0.00660	0.00451	-0.00218	2.17501
A13	1.90249	-0.00021	0.00105	-0.00020	0.00085	1.90333
A14	2.22188	-0.00114	0.00875	0.00065	0.00929	2.23117
A15	2.15579	0.00137	-0.01058	-0.00079	-0.01142	2.14436
A16	1.94944	0.00096	-0.00302	0.00003	-0.00299	1.94645
A17	1.87673	0.00017	-0.00457	0.00033	-0.00422	1.87251
A18	1.88349	-0.00073	0.00628	0.00205	0.00833	1.89182
A19	1.91492	-0.00050	0.00660	-0.00159	0.00500	1.91993
A20	1.94267	-0.00010	-0.00317	-0.00093	-0.00409	1.93857
A21	1.89451	0.00020	-0.00225	0.00021	-0.00201	1.89249
A22	1.90404	0.00053	-0.00409	-0.00161	-0.00586	1.89818
A23	1.88457	-0.00025	0.00709	0.00228	0.00912	1.89370
A24	1.89447	0.00047	0.00115	-0.00055	0.00033	1.89480

A25	1.88176	0.00030	-0.00396	-0.00040	-0.00416	1.87760
A26	1.95251	-0.00090	-0.00972	-0.01161	-0.02135	1.93116
A27	1.94503	-0.00012	0.01003	0.01214	0.02204	1.96707
A28	2.86643	0.00069	0.02216	0.01345	0.03561	2.90204
A29	2.17415	-0.00006	-0.00092	-0.00103	-0.00195	2.17220
A30	1.95253	-0.00001	-0.00083	-0.00080	-0.00163	1.95091
A31	2.15648	0.00007	0.00174	0.00182	0.00356	2.16004
A32	2.07912	0.00003	-0.00017	-0.00006	-0.00023	2.07889
A33	2.15799	-0.00004	0.00007	-0.00001	0.00006	2.15805
A34	2.04608	0.00001	0.00009	0.00007	0.00016	2.04625
A35	1.97651	-0.00069	-0.00432	-0.00732	-0.01179	1.96472
A36	1.95529	-0.00098	-0.00177	-0.00449	-0.00641	1.94888
A37	1.89640	0.00063	-0.00581	-0.00619	-0.01227	1.88413
D1	0.01424	-0.00052	-0.00185	-0.00431	-0.00612	0.00812
D2	-3.13940	-0.00010	-0.00206	0.00075	-0.00133	-3.14073
D3	-3.13393	-0.00033	0.00157	-0.00537	-0.00373	-3.13766
D4	-0.00437	0.00009	0.00135	-0.00031	0.00106	-0.00332
D5	-0.01271	0.00045	0.00229	0.00083	0.00309	-0.00962
D6	-3.07231	0.00012	0.01397	0.00545	0.01962	-3.05269
D7	3.13478	0.00029	-0.00077	0.00178	0.00096	3.13574
D8	0.07518	-0.00005	0.01092	0.00641	0.01748	0.09266
D9	-0.01104	0.00042	0.00079	0.00633	0.00709	-0.00395
D10	3.11438	0.00038	-0.00277	0.00244	-0.00038	3.11400
D11	3.14146	0.00004	0.00099	0.00175	0.00275	-3.13898
D12	-0.01630	0.00000	-0.00258	-0.00214	-0.00472	-0.02102
D13	0.00322	-0.00014	0.00062	-0.00588	-0.00523	-0.00201
D14	3.03692	0.00014	-0.01121	-0.00981	-0.02104	3.01588
D15	-3.12354	-0.00011	0.00387	-0.00233	0.00154	-3.12200
D16	-0.08985	0.00017	-0.00795	-0.00627	-0.01427	-0.10412
D17	0.10149	0.00009	0.01635	0.01818	0.03454	0.13603
D18	-3.03238	0.00009	0.01696	0.01892	0.03587	-2.99651
D19	-3.05818	0.00005	0.01238	0.01384	0.02622	-3.03195
D20	0.09114	0.00005	0.01298	0.01458	0.02756	0.11869
D21	0.00578	-0.00019	-0.00178	0.00315	0.00137	0.00715
D22	3.06915	-0.00001	-0.01207	-0.00118	-0.01302	3.05613
D23	-3.03066	-0.00023	0.00900	0.00774	0.01660	-3.01406
D24	0.03271	-0.00005	-0.00129	0.00340	0.00221	0.03492
D25	-1.91568	0.00002	0.19210	0.13929	0.33135	-1.58432
D26	1.10106	0.00018	0.17888	0.13436	0.31328	1.41434
D27	1.80815	-0.00003	0.00686	0.01759	0.02445	1.83260
D28	-2.37319	0.00003	0.01021	0.01587	0.02610	-2.34709
D29	-0.33261	-0.00002	0.00847	0.01735	0.02583	-0.30678
D30	-1.24042	-0.00032	0.01957	0.02280	0.04234	-1.19807
D31	0.86142	-0.00026	0.02292	0.02107	0.04400	0.90542

D32	2.90200	-0.00031	0.02118	0.02256	0.04373	2.94573
D33	-1.01409	-0.00018	0.00607	-0.06303	-0.05694	-1.07103
D34	1.02654	0.00033	0.00314	-0.06312	-0.06003	0.96650
D35	3.13745	0.00030	0.01983	-0.04750	-0.02766	3.10979
D36	-3.09344	-0.00067	0.00933	-0.06241	-0.05305	3.13669
D37	-1.05281	-0.00016	0.00639	-0.06250	-0.05615	-1.10896
D38	1.05810	-0.00019	0.02309	-0.04688	-0.02377	1.03433
D39	1.09251	-0.00052	0.00981	-0.06103	-0.05120	1.04131
D40	3.13313	-0.00002	0.00687	-0.06112	-0.05429	3.07884
D41	-1.03915	-0.00004	0.02357	-0.04550	-0.02191	-1.06106
D42	2.15177	0.00066	0.11362	0.12216	0.23569	2.38746
D43	-1.97901	0.00021	0.10106	0.10481	0.20592	-1.77309
D44	0.04992	0.00025	0.12415	0.13179	0.25574	0.30566
D45	2.20233	-0.00020	0.11159	0.11444	0.22597	2.42830
D46	-2.05823	0.00057	0.12884	0.13188	0.26080	-1.79744
D47	0.09418	0.00012	0.11628	0.11453	0.23102	0.32520
D48	-3.13133	0.00004	0.00112	0.00248	0.00360	-3.12772
D49	0.01122	0.00003	0.00168	0.00222	0.00390	0.01512
D50	0.00167	0.00004	0.00044	0.00164	0.00208	0.00375
D51	-3.13897	0.00003	0.00100	0.00138	0.00238	-3.13659

Item	Value	Threshold	Converged?
Maximum Force	0.001727	0.000450	NO
RMS Force	0.000452	0.000300	NO
Maximum Displacement	0.357753	0.001800	NO
RMS Displacement	0.073297	0.001200	NO

Predicted change in Energy=-2.590848D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.841453	-2.037648	0.348953
2	6	0	-2.828265	-1.141242	0.088521
3	7	0	-2.224118	0.110665	0.023188
4	6	0	-0.905207	-0.032893	0.244760
5	7	0	-0.655835	-1.326921	0.449645
6	6	0	0.710791	-1.862995	0.620981
7	6	0	1.518920	-1.778749	-0.687333
8	1	0	-1.882849	-3.106194	0.472821
9	1	0	-3.882717	-1.288126	-0.057904
10	1	0	1.195917	-1.271289	1.397817
11	1	0	0.635035	-2.893022	0.969152

12	1	0	1.017846	-2.382447	-1.449856
13	1	0	1.514094	-0.738501	-1.032760
14	35	0	1.404039	2.092735	-0.505295
15	1	0	-0.120593	0.758151	0.151112
16	6	0	-2.808648	1.378460	-0.254051
17	6	0	-4.112687	1.596204	-0.362046
18	1	0	-2.056760	2.149974	-0.376504
19	1	0	-4.462420	2.593949	-0.588061
20	1	0	-4.862336	0.825082	-0.234952
21	7	0	2.867637	-2.283164	-0.434612
22	1	0	3.200285	-2.888668	-1.173098
23	1	0	3.534847	-1.528446	-0.325194

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.358370	0.000000			
3	N	2.206310	1.391593	0.000000		
4	C	2.215053	2.225084	1.345076	0.000000	
5	N	1.385988	2.210054	2.169800	1.333670	0.000000
6	C	2.572635	3.650940	3.586974	2.470277	1.477971
7	C	3.526050	4.461657	4.252653	3.129410	2.495281
8	H	1.076497	2.214167	3.266009	3.233106	2.161460
9	H	2.212255	1.074655	2.171207	3.245424	3.266784
10	H	3.303490	4.233818	3.936501	2.697756	2.081133
11	H	2.692453	3.979785	4.253438	3.328277	2.094971
12	H	3.395614	4.324323	4.346929	3.477105	2.742890
13	H	3.854428	4.502839	3.976221	2.825413	2.693020
14	Br	5.321938	5.359442	4.167903	3.226994	4.104758
15	H	3.288920	3.308035	2.204636	1.118096	2.173277
16	C	3.601233	2.542958	1.423321	2.421532	3.528297
17	C	4.343836	3.057182	2.433501	3.648301	4.599275
18	H	4.255446	3.412267	2.084836	2.544985	3.838478
19	H	5.403624	4.132780	3.398576	4.499739	5.562387
20	H	4.202607	2.847545	2.745401	4.077391	4.774353
21	N	4.780144	5.832748	5.644994	4.445179	3.756483
22	H	5.334791	6.402233	6.312784	5.198157	4.465647
23	H	5.442276	6.388293	5.997811	4.719704	4.266475

		6	7	8	9	10
6	C	0.000000				
7	C	1.540083	0.000000			
8	H	2.880011	3.831462	0.000000		
9	H	4.678854	5.460272	2.754362	0.000000	
10	H	1.090385	2.170184	3.701526	5.283175	0.000000

11	H	1.089916	2.183300	2.575175	4.903123	1.768718
12	H	2.156960	1.094060	3.554508	5.210622	3.061964
13	H	2.155143	1.096111	4.405901	5.511624	2.508546
14	Br	4.170958	3.877464	6.228098	6.291276	3.870633
15	H	2.789692	3.134782	4.259366	4.287716	2.721415
16	C	4.864069	5.374342	4.636547	2.881454	5.078029
17	C	6.016506	6.573517	5.270837	2.909424	6.284975
18	H	4.975765	5.321369	5.327184	3.905912	5.043130
19	H	6.934569	7.409910	6.345966	3.960761	7.134462
20	H	6.246449	6.906882	4.983294	2.335947	6.615372
21	N	2.437786	1.461964	4.905907	6.833687	2.678868
22	H	3.235475	2.072407	5.347393	7.346720	3.639094
23	H	2.997076	2.063433	5.698908	7.426268	2.916417

		11	12	13	14	15
11	H	0.000000				
12	H	2.501765	0.000000			
13	H	3.069586	1.767142	0.000000		
14	Br	5.255771	4.590054	2.882053	0.000000	
15	H	3.817227	3.704389	2.512712	2.129903	0.000000
16	C	5.621453	5.496947	4.875860	4.280192	2.788293
17	C	6.668291	6.582960	6.128734	5.540878	4.111263
18	H	5.872678	5.581050	4.639500	3.463667	2.442190
19	H	7.649562	7.452551	6.857237	5.888412	4.771581
20	H	6.745017	6.807406	6.613634	6.399022	4.757904
21	N	2.706841	2.112417	2.139122	4.614716	4.303741
22	H	3.342119	2.257409	2.736083	5.337306	5.106961
23	H	3.456343	2.886084	2.282127	4.205441	4.337930

		16	17	18	19	20
16	C	0.000000				
17	C	1.326497	0.000000			
18	H	1.084234	2.129250	0.000000		
19	H	2.079408	1.081152	2.455416	0.000000	
20	H	2.127023	1.082938	3.105903	1.847568	0.000000
21	N	6.757241	7.986218	6.626143	8.805652	8.333879
22	H	7.426998	8.616927	7.325229	9.440254	8.926248
23	H	6.978187	8.261330	6.693241	9.001084	8.721234

		21	22	23
21	N	0.000000		
22	H	1.011262	0.000000	
23	H	1.013283	1.637399	0.000000

Stoichiometry C7H12BrN3

Framework group C1[X(C7H12BrN3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.581844	2.304772	-0.109364
2	6	0	-2.594784	1.428149	0.115697
3	7	0	-2.058356	0.152095	-0.027354
4	6	0	-0.753935	0.262831	-0.336308
5	7	0	-0.448770	1.559753	-0.395815
6	6	0	0.928881	2.050511	-0.609430
7	6	0	1.827324	1.759573	0.607127
8	1	0	-1.572663	3.381112	-0.093444
9	1	0	-3.625340	1.602769	0.365387
10	1	0	1.320255	1.543547	-1.491899
11	1	0	0.884798	3.119511	-0.817306
12	1	0	1.419664	2.281009	1.478268
13	1	0	1.790403	0.684493	0.817601
14	35	0	1.482829	-2.045811	-0.052495
15	1	0	-0.009942	-0.568724	-0.407932
16	6	0	-2.690282	-1.112946	0.134452
17	6	0	-3.992602	-1.283033	0.320534
18	1	0	-1.975608	-1.927416	0.096454
19	1	0	-4.379531	-2.284676	0.446581
20	1	0	-4.705418	-0.468449	0.353712
21	7	0	3.179243	2.230403	0.310523
22	1	0	3.599917	2.718626	1.089832
23	1	0	3.793079	1.466665	0.052355

Rotational constants (GHZ): 0.7179759 0.5294961 0.3135897
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 365 symmetry adapted cartesian basis functions of A symmetry.
There are 352 symmetry adapted basis functions of A symmetry.
352 basis functions, 562 primitive gaussians, 365 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 836.8865688611 Hartrees.
NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.

NBasis= 352 RedAO= T EigKep= 4.85D-06 NBF= 352
NBsUse= 352 1.00D-06 EigRej= -1.00D+00 NBFU= 352
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999960 -0.002482 -0.000943 0.008583 Ang= -1.03 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3012.46603922 A.U. after 12 cycles
NFock= 12 Conv=0.91D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000364765	0.000093459	0.000358685
2	6	0.000004613	0.000011701	-0.000038616
3	7	-0.000366803	-0.000230439	-0.000178769
4	6	0.001072876	-0.001847398	0.000341757
5	7	0.000257808	-0.000366736	-0.001199232
6	6	0.000769127	0.000613306	0.000271521
7	6	-0.000509407	0.000231179	-0.000195677
8	1	0.000046095	0.000089592	0.000154824
9	1	-0.000054736	0.000037919	0.000027192
10	1	0.000794240	-0.000407023	-0.000152073
11	1	-0.000938727	0.000064540	-0.000109699
12	1	0.000858959	-0.001335725	-0.000033241
13	1	0.000578054	0.000060419	0.000370290
14	35	0.001198423	0.001021309	-0.000495632

15	1	-0.001907772	0.001945769	0.000779898
16	6	-0.000103392	0.000077496	-0.000135709
17	6	0.000014815	-0.000015685	0.000051645
18	1	-0.000020898	-0.000030778	0.000070858
19	1	-0.000021759	0.000023679	-0.000001383
20	1	0.000050778	-0.000011700	0.000035864
21	7	-0.000087272	-0.001346437	0.000374794
22	1	-0.000515506	0.000572120	-0.000512270
23	1	-0.000754753	0.000749431	0.000214971

Cartesian Forces: Max 0.001945769 RMS 0.000634297

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.002850896 RMS 0.000682439
Search for a local minimum.
Step number 9 out of a maximum of 121
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 8 9
DE= -3.27D-04 DEPred=-2.59D-04 R= 1.26D+00
TightC=F SS= 1.41D+00 RLast= 7.63D-01 DXNew= 2.2975D+00 2.2881D+00
Trust test= 1.26D+00 RLast= 7.63D-01 DXMaxT set to 2.29D+00
ITU= 1 1 1 1 1 0 1 0 0
Eigenvalues --- 0.00035 0.00302 0.00379 0.00937 0.01395
Eigenvalues --- 0.01582 0.01875 0.02010 0.02218 0.02325
Eigenvalues --- 0.02391 0.02643 0.03061 0.03062 0.03540
Eigenvalues --- 0.03627 0.03950 0.04308 0.04767 0.05340
Eigenvalues --- 0.05883 0.09203 0.09806 0.12300 0.13321
Eigenvalues --- 0.15670 0.15987 0.15999 0.16000 0.16002
Eigenvalues --- 0.16009 0.16705 0.18406 0.21798 0.22004
Eigenvalues --- 0.22226 0.23016 0.23490 0.23976 0.25029
Eigenvalues --- 0.28442 0.32166 0.34159 0.34441 0.34695
Eigenvalues --- 0.34822 0.34996 0.35685 0.35689 0.35858
Eigenvalues --- 0.36436 0.36658 0.38009 0.40483 0.42189
Eigenvalues --- 0.43678 0.47641 0.47945 0.48280 0.51523
Eigenvalues --- 0.54368 0.60353 0.63698
En-DIIS/RFO-DIIS IScMMF= 0 using points: 9 8 7 6 5
RFO step: Lambda=-9.88396986D-05.
DidBck=F Rises=F RFO-DIIS coefs: 1.71082 -0.29749 -0.66157 -0.10640 0.35464

Iteration 1 RMS(Cart)= 0.06982395 RMS(Int)= 0.04594330
Iteration 2 RMS(Cart)= 0.03871488 RMS(Int)= 0.00297294
Iteration 3 RMS(Cart)= 0.00308196 RMS(Int)= 0.00022302
Iteration 4 RMS(Cart)= 0.00001550 RMS(Int)= 0.00022271
Iteration 5 RMS(Cart)= 0.00000002 RMS(Int)= 0.00022271

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56695	-0.00044	0.00077	-0.00003	0.00074	2.56769
R2	2.61914	0.00036	0.00039	0.00034	0.00071	2.61985
R3	2.03428	-0.00007	0.00009	-0.00011	-0.00003	2.03426
R4	2.62973	-0.00050	0.00125	-0.00055	0.00071	2.63044
R5	2.03080	0.00005	0.00001	0.00010	0.00011	2.03092
R6	2.54182	0.00065	-0.00168	-0.00051	-0.00218	2.53965
R7	2.68969	0.00007	0.00125	0.00114	0.00238	2.69207
R8	2.52027	0.00148	-0.00025	0.00097	0.00071	2.52098
R9	2.11290	0.00158	0.00434	0.00082	0.00516	2.11805
R10	2.79296	0.00050	-0.00236	-0.00119	-0.00355	2.78941
R11	2.91034	-0.00048	0.00305	-0.00452	-0.00147	2.90886
R12	2.06053	0.00002	0.00025	0.00078	0.00103	2.06155
R13	2.05964	-0.00003	-0.00100	-0.00002	-0.00102	2.05863
R14	2.06747	0.00037	-0.00216	-0.00057	-0.00273	2.06474
R15	2.07135	-0.00006	0.00029	0.00286	0.00316	2.07451
R16	2.76271	-0.00123	-0.00073	0.00100	0.00027	2.76298
R17	4.02493	0.00165	-0.01957	0.01202	-0.00755	4.01739
R18	2.50672	-0.00005	-0.00009	-0.00018	-0.00027	2.50644
R19	2.04891	-0.00004	0.00071	0.00065	0.00136	2.05027
R20	2.04308	0.00003	0.00008	0.00006	0.00014	2.04322
R21	2.04646	-0.00002	0.00011	0.00009	0.00020	2.04666
R22	1.91101	-0.00014	-0.00074	0.00141	0.00066	1.91167
R23	1.91483	0.00009	0.00037	0.00222	0.00259	1.91741
A1	1.87232	0.00058	-0.00167	0.00025	-0.00143	1.87088
A2	2.27728	-0.00022	-0.00017	-0.00004	-0.00022	2.27706
A3	2.13358	-0.00036	0.00186	-0.00024	0.00161	2.13519
A4	1.86219	-0.00006	0.00042	0.00010	0.00055	1.86274
A5	2.27672	0.00007	-0.00031	0.00034	0.00004	2.27676
A6	2.14426	-0.00001	-0.00010	-0.00049	-0.00058	2.14367
A7	1.89858	0.00057	0.00009	0.00006	0.00017	1.89875
A8	2.25515	-0.00040	0.00184	0.00081	0.00264	2.25779
A9	2.12921	-0.00017	-0.00201	-0.00073	-0.00276	2.12646
A10	1.88831	-0.00062	-0.00022	0.00039	0.00011	1.88843
A11	2.21278	-0.00220	0.00049	-0.00740	-0.00696	2.20582
A12	2.17501	0.00285	-0.00169	0.00672	0.00496	2.17997
A13	1.90333	-0.00046	0.00139	-0.00088	0.00059	1.90393
A14	2.23117	-0.00220	0.00722	0.00066	0.00799	2.23916

A15	2.14436	0.00269	-0.00949	0.00061	-0.00879	2.13558
A16	1.94645	0.00129	-0.00095	-0.00015	-0.00110	1.94534
A17	1.87251	0.00033	-0.00265	0.00404	0.00138	1.87389
A18	1.89182	-0.00113	0.00395	-0.00175	0.00219	1.89402
A19	1.91993	-0.00060	0.00314	-0.00048	0.00267	1.92260
A20	1.93857	-0.00012	-0.00216	-0.00080	-0.00298	1.93559
A21	1.89249	0.00023	-0.00133	-0.00073	-0.00207	1.89043
A22	1.89818	0.00074	0.00093	-0.00105	-0.00051	1.89767
A23	1.89370	-0.00011	0.00781	0.00395	0.01154	1.90524
A24	1.89480	-0.00016	0.00241	-0.00737	-0.00524	1.88956
A25	1.87760	0.00049	-0.00216	0.00699	0.00506	1.88266
A26	1.93116	-0.00071	-0.01961	-0.01678	-0.03632	1.89484
A27	1.96707	-0.00020	0.01078	0.01430	0.02503	1.99210
A28	2.90204	0.00005	0.02615	0.00882	0.03496	2.93700
A29	2.17220	-0.00009	-0.00166	-0.00171	-0.00337	2.16882
A30	1.95091	0.00003	-0.00118	-0.00073	-0.00191	1.94900
A31	2.16004	0.00006	0.00283	0.00247	0.00530	2.16534
A32	2.07889	0.00005	-0.00020	0.00008	-0.00012	2.07877
A33	2.15805	-0.00008	0.00006	-0.00036	-0.00030	2.15775
A34	2.04625	0.00003	0.00013	0.00028	0.00041	2.04666
A35	1.96472	-0.00095	-0.01268	-0.01487	-0.02834	1.93638
A36	1.94888	-0.00144	-0.00961	-0.01134	-0.02176	1.92712
A37	1.88413	0.00092	-0.00969	-0.00770	-0.01896	1.86517
D1	0.00812	-0.00025	-0.00928	0.01137	0.00207	0.01019
D2	-3.14073	0.00000	-0.00143	0.00444	0.00302	-3.13770
D3	-3.13766	-0.00023	-0.00660	0.00254	-0.00409	3.14143
D4	-0.00332	0.00001	0.00126	-0.00439	-0.00314	-0.00646
D5	-0.00962	0.00030	0.00815	-0.00700	0.00115	-0.00847
D6	-3.05269	-0.00026	0.01558	-0.01141	0.00411	-3.04858
D7	3.13574	0.00029	0.00575	0.00095	0.00671	-3.14074
D8	0.09266	-0.00027	0.01318	-0.00346	0.00967	0.10233
D9	-0.00395	0.00012	0.00732	-0.01195	-0.00459	-0.00854
D10	3.11400	0.00028	0.00314	-0.00536	-0.00219	3.11181
D11	-3.13898	-0.00010	0.00021	-0.00567	-0.00545	3.13876
D12	-0.02102	0.00006	-0.00397	0.00092	-0.00306	-0.02408
D13	-0.00201	0.00007	-0.00233	0.00769	0.00534	0.00334
D14	3.01588	0.00059	-0.01536	0.00573	-0.00958	3.00630
D15	-3.12200	-0.00008	0.00144	0.00165	0.00308	-3.11893
D16	-0.10412	0.00045	-0.01159	-0.00031	-0.01184	-0.11596
D17	0.13603	-0.00004	0.02709	0.01474	0.04183	0.17786
D18	-2.99651	-0.00011	0.02760	0.01118	0.03878	-2.95773
D19	-3.03195	0.00015	0.02245	0.02210	0.04455	-2.98740
D20	0.11869	0.00008	0.02295	0.01855	0.04150	0.16020
D21	0.00715	-0.00023	-0.00352	-0.00050	-0.00403	0.00312

D22	3.05613	-0.00002	-0.00922	0.00365	-0.00568	3.05045
D23	-3.01406	-0.00030	0.00893	0.00263	0.01166	-3.00241
D24	0.03492	-0.00010	0.00323	0.00679	0.01001	0.04492
D25	-1.58432	-0.00016	0.27493	0.13642	0.41136	-1.17296
D26	1.41434	0.00014	0.26004	0.13351	0.39354	1.80788
D27	1.83260	-0.00018	0.01537	0.01957	0.03495	1.86755
D28	-2.34709	0.00006	0.01699	0.02148	0.03846	-2.30863
D29	-0.30678	-0.00009	0.01605	0.02187	0.03791	-0.26887
D30	-1.19807	-0.00060	0.02292	0.01468	0.03762	-1.16046
D31	0.90542	-0.00036	0.02454	0.01659	0.04113	0.94655
D32	2.94573	-0.00051	0.02359	0.01698	0.04058	2.98630
D33	-1.07103	-0.00012	-0.04614	-0.04446	-0.09064	-1.16167
D34	0.96650	0.00080	-0.04391	-0.03455	-0.07847	0.88803
D35	3.10979	0.00039	-0.02462	-0.01920	-0.04375	3.06604
D36	3.13669	-0.00096	-0.04426	-0.04910	-0.09340	3.04329
D37	-1.10896	-0.00004	-0.04203	-0.03919	-0.08124	-1.19019
D38	1.03433	-0.00044	-0.02274	-0.02383	-0.04651	0.98782
D39	1.04131	-0.00077	-0.04325	-0.04736	-0.09065	0.95066
D40	3.07884	0.00016	-0.04102	-0.03745	-0.07849	3.00036
D41	-1.06106	-0.00025	-0.02173	-0.02209	-0.04376	-1.10482
D42	2.38746	0.00078	0.19257	0.17482	0.36710	2.75456
D43	-1.77309	0.00023	0.16276	0.14575	0.30906	-1.46403
D44	0.30566	0.00040	0.20163	0.19068	0.39161	0.69728
D45	2.42830	-0.00015	0.17182	0.16161	0.33357	2.76187
D46	-1.79744	0.00041	0.21074	0.18381	0.39428	-1.40315
D47	0.32520	-0.00014	0.18092	0.15474	0.33624	0.66144
D48	-3.12772	-0.00004	0.00288	-0.00196	0.00091	-3.12681
D49	0.01512	-0.00001	0.00332	-0.00021	0.00311	0.01823
D50	0.00375	0.00003	0.00229	0.00199	0.00429	0.00804
D51	-3.13659	0.00006	0.00273	0.00374	0.00648	-3.13011

Item	Value	Threshold	Converged?
Maximum Force	0.002851	0.000450	NO
RMS Force	0.000682	0.000300	NO
Maximum Displacement	0.604984	0.001800	NO
RMS Displacement	0.101373	0.001200	NO

Predicted change in Energy=-2.865013D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.865453	-2.052910	0.373875

2	6	0	-2.837044	-1.140913	0.108346
3	7	0	-2.208370	0.097106	0.010063
4	6	0	-0.891686	-0.067915	0.222769
5	7	0	-0.665045	-1.363247	0.447337
6	6	0	0.696289	-1.910982	0.607332
7	6	0	1.501216	-1.810206	-0.700869
8	1	0	-1.928127	-3.117196	0.522813
9	1	0	-3.896360	-1.268221	-0.020697
10	1	0	1.187037	-1.338499	1.395719
11	1	0	0.616191	-2.946640	0.935571
12	1	0	1.046914	-2.469868	-1.444014
13	1	0	1.442265	-0.782382	-1.081955
14	35	0	1.316487	2.153570	-0.571511
15	1	0	-0.094809	0.709686	0.094019
16	6	0	-2.767431	1.373244	-0.287183
17	6	0	-4.068699	1.624467	-0.340095
18	1	0	-1.997313	2.114958	-0.471324
19	1	0	-4.401941	2.622863	-0.587482
20	1	0	-4.831573	0.880893	-0.144891
21	7	0	2.862908	-2.273213	-0.437853
22	1	0	3.315942	-2.568524	-1.292788
23	1	0	3.424124	-1.521154	-0.051898

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.358762	0.000000			
3	N	2.207378	1.391970	0.000000		
4	C	2.216137	2.224598	1.343924	0.000000	
5	N	1.386366	2.209507	2.169260	1.334047	0.000000
6	C	2.576270	3.650539	3.581367	2.463016	1.476091
7	C	3.542378	4.463550	4.231346	3.100753	2.492156
8	H	1.076483	2.214409	3.266984	3.234557	2.162732
9	H	2.212693	1.074714	2.171261	3.244700	3.266417
10	H	3.297308	4.229609	3.938247	2.703938	2.080925
11	H	2.696815	3.983690	4.254303	3.326986	2.094534
12	H	3.458389	4.388744	4.393241	3.507950	2.780760
13	H	3.830755	4.456214	3.910644	2.767688	2.667751
14	Br	5.358449	5.344871	4.122122	3.231394	4.163235
15	H	3.293241	3.308288	2.202145	1.120826	2.178773
16	C	3.604038	2.546030	1.424582	2.419795	3.528162
17	C	4.345935	3.060294	2.432338	3.643403	4.596884
18	H	4.254747	3.412017	2.085187	2.543444	3.836246
19	H	5.405630	4.135105	3.398274	4.496519	5.560964

20	H	4.204068	2.851311	2.742176	4.069167	4.769365
21	N	4.802586	5.836942	5.615772	4.404173	3.749407
22	H	5.467218	6.469967	6.270647	5.123875	4.508768
23	H	5.333261	6.274750	5.860682	4.562188	4.122557

		6	7	8	9	10
6	C	0.000000				
7	C	1.539304	0.000000			
8	H	2.889577	3.868594	0.000000		
9	H	4.679742	5.467194	2.754642	0.000000	
10	H	1.090928	2.171842	3.691880	5.277508	0.000000
11	H	1.089378	2.180067	2.583218	4.908631	1.767404
12	H	2.154835	1.092616	3.624681	5.282589	3.060018
13	H	2.164234	1.097781	4.402975	5.464726	2.552112
14	Br	4.277254	3.970186	6.285384	6.259859	4.010149
15	H	2.785179	3.086907	4.264967	4.286848	2.744560
16	C	4.856300	5.341052	4.639459	2.884932	5.081685
17	C	6.008505	6.553708	5.273522	2.915366	6.278135
18	H	4.962578	5.263013	5.326212	3.905809	5.054928
19	H	6.926419	7.383240	6.348291	3.964517	7.131771
20	H	6.238402	6.903285	4.986035	2.347070	6.597184
21	N	2.432666	1.462107	4.958751	6.846294	2.654095
22	H	3.302332	2.053933	5.576532	7.438165	3.643249
23	H	2.833308	2.049949	5.614645	7.324919	2.670864

		11	12	13	14	15
11	H	0.000000				
12	H	2.464804	0.000000			
13	H	3.071941	1.770592	0.000000		
14	Br	5.364127	4.712760	2.982648	0.000000	
15	H	3.818697	3.711959	2.443722	2.125909	0.000000
16	C	5.621870	5.536876	4.795824	4.167511	2.780024
17	C	6.668623	6.644676	6.059209	5.416063	4.100864
18	H	5.867668	5.588745	4.538518	3.315539	2.431856
19	H	7.649883	7.507302	6.781958	5.737676	4.761941
20	H	6.745038	6.889987	6.557867	6.292881	4.745874
21	N	2.718002	2.085394	2.157700	4.691022	4.234225
22	H	3.520967	2.276201	2.597194	5.178439	4.929818
23	H	3.300241	2.913619	2.352566	4.267989	4.169032

		16	17	18	19	20
16	C	0.000000				
17	C	1.326353	0.000000			
18	H	1.084956	2.132708	0.000000		
19	H	2.079267	1.081224	2.460427	0.000000	
20	H	2.126813	1.083043	3.108457	1.847953	0.000000
21	N	6.709700	7.952902	6.548199	8.761963	8.321012

22	H	7.318210	8.545275	7.130251	9.328112	8.921779
23	H	6.838732	8.131445	6.541346	8.871699	8.598547

		21	22	23
21	N	0.000000		
22	H	1.011613	0.000000	
23	H	1.014651	1.627420	0.000000

Stoichiometry C7H12BrN3
Framework group C1[X(C7H12BrN3)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.565089	2.352083	-0.101219
2	6	0	-2.568333	1.463045	0.120919
3	7	0	-2.015404	0.192850	-0.014929
4	6	0	-0.713117	0.318234	-0.322272
5	7	0	-0.422333	1.618861	-0.381403
6	6	0	0.953611	2.112249	-0.586809
7	6	0	1.856581	1.779005	0.614460
8	1	0	-1.570700	3.428511	-0.091866
9	1	0	-3.602683	1.625242	0.363454
10	1	0	1.338673	1.636587	-1.489913
11	1	0	0.913862	3.187573	-0.756636
12	1	0	1.509650	2.345508	1.481940
13	1	0	1.762976	0.710942	0.850263
14	35	0	1.404621	-2.107936	-0.056213
15	1	0	0.039521	-0.510396	-0.378481
16	6	0	-2.629440	-1.082096	0.149101
17	6	0	-3.935323	-1.270031	0.285338
18	1	0	-1.896459	-1.881993	0.155020
19	1	0	-4.310920	-2.275109	0.418720
20	1	0	-4.661900	-0.467055	0.268112
21	7	0	3.218785	2.203769	0.295502
22	1	0	3.759761	2.346576	1.138302
23	1	0	3.695817	1.488082	-0.242782

Rotational constants (GHZ): 0.6940590 0.5444655 0.3136823
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 365 symmetry adapted cartesian basis functions of A symmetry.

```
 There are      352 symmetry adapted basis functions of A      symmetry.
    352 basis functions,      562 primitive gaussians,      365 cartesian basis functions
     55 alpha electrons             55 beta electrons
          nuclear repulsion energy             836.3626352120 Hartrees.
 NAtoms=       23 NActive=       23 NUniq=       23 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      352 RedAO= T EigKep=    5.08D-06    NBF=      352
 NBsUse=      352 1.00D-06 EigRej= -1.00D+00 NBFU=      352
 Initial guess from the checkpoint file:    "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"
 B after Tr=          0.000000        0.000000        0.000000
             Rot=        0.999961      -0.002181      -0.001077        0.008474 Ang=    -1.01 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn=                5 AccDes=
0.00D+00
 Harris functional with IExCor=    402 and IRadAn=             5 diagonalized for initial guess.
 HarFok:    IExCor=    402 AccDes= 0.00D+00 IRadAn=                5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=    3500011 ScaDFX=    1.000000    1.000000    1.000000    1.000000
 FoFCou: FMM=F IPFlag=                  0 FMFlag=           100000 FMFlg1=                  0
             NFxFlg=                    0 DoJE=T BraDBF=F KetDBF=T FulRan=T
             wScrn=      0.000000  ICntrl=             500  IOpCl=      0  I1Cent=        200000004  NGrid=
0
             NMat0=         1 NMatS0=            1 NMatT0=         0 NMatD0=         1 NMtDS0=         0
NMtDT0=        0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                    energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3012.46625078          A.U. after      13 cycles
                  NFock= 13    Conv=0.17D-08         -V/T= 2.0017
 Calling FoFJK, ICntrl=             2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center         Atomic                             Forces (Hartrees/Bohr)
 Number         Number                       X                      Y                      Z
 -------------------------------------------------------------------
        1              6               -0.000285086        0.000274075        0.000857608
        2              6                0.000247703        0.000196140        0.000006961
        3              7               -0.000574242       -0.000048856        0.000496497
        4              6                0.002327410       -0.002027667       -0.001479467
```

5	7	0.000373237	0.000310136	-0.001256677
6	6	0.001294780	-0.000035330	-0.000751079
7	6	-0.000971118	-0.001483712	-0.000022837
8	1	0.000150074	0.000040877	-0.000040882
9	1	-0.000012358	-0.000001278	-0.000132582
10	1	0.000420683	-0.000073312	0.000006020
11	1	-0.000780486	-0.000097651	0.000066675
12	1	-0.000720058	-0.000818552	-0.000644427
13	1	0.000994719	0.000213838	0.001031798
14	35	0.000871658	0.000481800	-0.000501780
15	1	-0.003040288	0.002206143	0.001620638
16	6	-0.000188999	-0.000107716	-0.000078927
17	6	0.000023215	0.000067887	-0.000037333
18	1	-0.000090462	0.000055257	0.000214011
19	1	-0.000025496	-0.000001101	-0.000001306
20	1	0.000056027	-0.000023432	-0.000014108
21	7	-0.000818078	0.000312129	0.001615814
22	1	0.000369733	-0.000367576	-0.001188006
23	1	0.000377431	0.000927902	0.000233388

Cartesian Forces: Max 0.003040288 RMS 0.000844957

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.003809326 RMS 0.000779629
Search for a local minimum.
Step number 10 out of a maximum of 121
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 9 10
DE= -2.12D-04 DEPred=-2.87D-04 R= 7.38D-01
TightC=F SS= 1.41D+00 RLast= 1.08D+00 DXNew= 3.8482D+00 3.2308D+00
Trust test= 7.38D-01 RLast= 1.08D+00 DXMaxT set to 3.00D+00
ITU= 1 1 1 1 1 1 0 1 0 0

Eigenvalues ---	0.00081	0.00300	0.00379	0.00924	0.01401
Eigenvalues ---	0.01551	0.01875	0.02031	0.02206	0.02328
Eigenvalues ---	0.02389	0.02635	0.03061	0.03062	0.03506
Eigenvalues ---	0.03782	0.03930	0.04376	0.04744	0.05337
Eigenvalues ---	0.05730	0.09164	0.09662	0.12409	0.12982
Eigenvalues ---	0.15414	0.15988	0.15999	0.16000	0.16000
Eigenvalues ---	0.16005	0.16211	0.17908	0.21633	0.21990

Eigenvalues --- 0.22105 0.22876 0.23490 0.24000 0.25030
Eigenvalues --- 0.28339 0.32254 0.34089 0.34464 0.34663
Eigenvalues --- 0.34803 0.34988 0.35680 0.35689 0.35858
Eigenvalues --- 0.36437 0.36658 0.38121 0.38670 0.42187
Eigenvalues --- 0.43301 0.47460 0.47726 0.48651 0.50333
Eigenvalues --- 0.54335 0.60348 0.60924
En-DIIS/RFO-DIIS IScMMF= 0 using points: 10 9 8 7 6
RFO step: Lambda=-1.39908655D-04.
DidBck=F Rises=F RFO-DIIS coefs: 0.83332 -0.89132 0.00316 1.22840 -0.17355
Iteration 1 RMS(Cart)= 0.09333082 RMS(Int)= 0.07525140
Iteration 2 RMS(Cart)= 0.04688373 RMS(Int)= 0.02866329
Iteration 3 RMS(Cart)= 0.02053031 RMS(Int)= 0.00109045
Iteration 4 RMS(Cart)= 0.00189380 RMS(Int)= 0.00024734
Iteration 5 RMS(Cart)= 0.00001898 RMS(Int)= 0.00024697
Iteration 6 RMS(Cart)= 0.00000000 RMS(Int)= 0.00024697

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56769	-0.00060	-0.00166	-0.00015	-0.00180	2.56588
R2	2.61985	0.00010	-0.00008	0.00015	0.00008	2.61993
R3	2.03426	-0.00006	-0.00025	0.00004	-0.00021	2.03405
R4	2.63044	-0.00082	-0.00220	-0.00001	-0.00221	2.62823
R5	2.03092	0.00003	-0.00003	0.00001	-0.00003	2.03089
R6	2.53965	0.00076	0.00452	-0.00012	0.00440	2.54405
R7	2.69207	0.00007	-0.00261	0.00042	-0.00219	2.68988
R8	2.52098	0.00154	-0.00022	-0.00010	-0.00032	2.52066
R9	2.11805	0.00019	-0.00610	-0.00105	-0.00715	2.11090
R10	2.78941	0.00072	0.00456	-0.00011	0.00445	2.79386
R11	2.90886	-0.00136	-0.00410	0.00105	-0.00305	2.90581
R12	2.06155	0.00015	-0.00149	0.00023	-0.00126	2.06029
R13	2.05863	0.00017	0.00193	-0.00023	0.00170	2.06033
R14	2.06474	0.00123	0.00502	0.00182	0.00684	2.07158
R15	2.07451	-0.00021	-0.00237	-0.00178	-0.00415	2.07036
R16	2.76298	-0.00022	-0.00265	0.00001	-0.00264	2.76034
R17	4.01739	0.00106	0.06635	-0.00883	0.05753	4.07491
R18	2.50644	-0.00005	0.00020	-0.00005	0.00015	2.50660
R19	2.05027	-0.00006	-0.00177	0.00011	-0.00166	2.04861
R20	2.04322	0.00001	-0.00010	0.00002	-0.00008	2.04314
R21	2.04666	-0.00003	-0.00031	-0.00002	-0.00034	2.04632
R22	1.91167	0.00128	-0.00064	0.00149	0.00086	1.91253
R23	1.91741	0.00098	-0.00285	0.00074	-0.00211	1.91530
A1	1.87088	0.00072	0.00328	0.00014	0.00342	1.87430
A2	2.27706	-0.00022	0.00075	-0.00019	0.00056	2.27763
A3	2.13519	-0.00050	-0.00401	0.00005	-0.00396	2.13124

A4	1.86274	0.00001	-0.00125	-0.00036	-0.00162	1.86112
A5	2.27676	0.00002	0.00072	-0.00003	0.00069	2.27745
A6	2.14367	-0.00003	0.00054	0.00041	0.00095	2.14462
A7	1.89875	0.00047	0.00051	0.00051	0.00100	1.89975
A8	2.25779	-0.00052	-0.00432	-0.00021	-0.00452	2.25327
A9	2.12646	0.00005	0.00394	-0.00033	0.00362	2.13007
A10	1.88843	-0.00057	-0.00054	-0.00036	-0.00089	1.88753
A11	2.20582	-0.00246	-0.00171	-0.00111	-0.00280	2.20301
A12	2.17997	0.00311	0.00566	0.00247	0.00819	2.18816
A13	1.90393	-0.00063	-0.00194	0.00010	-0.00187	1.90206
A14	2.23916	-0.00314	-0.01808	-0.00209	-0.02018	2.21897
A15	2.13558	0.00381	0.02253	0.00225	0.02475	2.16032
A16	1.94534	0.00169	0.00506	0.00407	0.00913	1.95447
A17	1.87389	-0.00009	0.00804	-0.00143	0.00661	1.88051
A18	1.89402	-0.00120	-0.01387	-0.00390	-0.01777	1.87624
A19	1.92260	-0.00037	-0.01133	0.00073	-0.01063	1.91197
A20	1.93559	-0.00034	0.00829	-0.00042	0.00787	1.94347
A21	1.89043	0.00027	0.00386	0.00080	0.00465	1.89508
A22	1.89767	0.00005	0.00862	0.00331	0.01235	1.91002
A23	1.90524	0.00013	-0.01896	0.00025	-0.01835	1.88688
A24	1.88956	-0.00058	-0.00165	0.00233	0.00112	1.89067
A25	1.88266	0.00037	0.00828	-0.00051	0.00747	1.89013
A26	1.89484	0.00063	0.04004	0.00238	0.04244	1.93728
A27	1.99210	-0.00057	-0.03692	-0.00731	-0.04407	1.94803
A28	2.93700	-0.00056	-0.06672	0.00020	-0.06652	2.87049
A29	2.16882	-0.00002	0.00372	-0.00034	0.00338	2.17220
A30	1.94900	0.00008	0.00293	0.00009	0.00302	1.95202
A31	2.16534	-0.00006	-0.00664	0.00025	-0.00639	2.15895
A32	2.07877	0.00006	0.00049	-0.00001	0.00048	2.07925
A33	2.15775	-0.00008	-0.00015	-0.00001	-0.00016	2.15759
A34	2.04666	0.00002	-0.00034	0.00003	-0.00031	2.04635
A35	1.93638	-0.00031	0.02406	-0.00456	0.02043	1.95680
A36	1.92712	-0.00038	0.01250	0.00013	0.01356	1.94068
A37	1.86517	0.00022	0.02352	-0.00416	0.02105	1.88622
D1	0.01019	-0.00039	-0.00387	-0.00338	-0.00723	0.00297
D2	-3.13770	-0.00007	-0.00235	-0.00002	-0.00236	-3.14006
D3	3.14143	-0.00027	-0.00051	-0.00304	-0.00357	3.13786
D4	-0.00646	0.00005	0.00101	0.00032	0.00130	-0.00516
D5	-0.00847	0.00029	0.00445	-0.00069	0.00374	-0.00473
D6	-3.04858	-0.00042	-0.03046	-0.00373	-0.03429	-3.08287
D7	-3.14074	0.00018	0.00142	-0.00099	0.00043	-3.14031
D8	0.10233	-0.00053	-0.03349	-0.00403	-0.03760	0.06474
D9	-0.00854	0.00036	0.00203	0.00629	0.00831	-0.00024
D10	3.11181	0.00044	0.00977	0.00493	0.01467	3.12648

D11	3.13876	0.00007	0.00066	0.00325	0.00390	-3.14053
D12	-0.02408	0.00014	0.00840	0.00189	0.01026	-0.01381
D13	0.00334	-0.00019	0.00073	-0.00677	-0.00604	-0.00271
D14	3.00630	0.00072	0.03408	0.00115	0.03505	3.04135
D15	-3.11893	-0.00024	-0.00626	-0.00553	-0.01175	-3.13068
D16	-0.11596	0.00066	0.02710	0.00238	0.02934	-0.08662
D17	0.17786	-0.00014	-0.06087	0.00033	-0.06051	0.11734
D18	-2.95773	-0.00022	-0.06191	-0.00073	-0.06263	-3.02035
D19	-2.98740	-0.00006	-0.05227	-0.00117	-0.05345	-3.04086
D20	0.16020	-0.00013	-0.05331	-0.00224	-0.05557	0.10463
D21	0.00312	-0.00007	-0.00319	0.00464	0.00146	0.00458
D22	3.05045	0.00013	0.02773	0.00717	0.03487	3.08532
D23	-3.00241	-0.00040	-0.03520	-0.00278	-0.03812	-3.04052
D24	0.04492	-0.00021	-0.00428	-0.00025	-0.00471	0.04021
D25	-1.17296	-0.00046	-0.61725	0.03610	-0.58114	-1.75410
D26	1.80788	0.00021	-0.57910	0.04500	-0.53412	1.27376
D27	1.86755	-0.00031	-0.04236	0.00048	-0.04188	1.82567
D28	-2.30863	0.00019	-0.04810	0.00288	-0.04519	-2.35382
D29	-0.26887	-0.00017	-0.04655	0.00103	-0.04550	-0.31437
D30	-1.16046	-0.00081	-0.08046	-0.00277	-0.08326	-1.24372
D31	0.94655	-0.00031	-0.08621	-0.00037	-0.08657	0.85997
D32	2.98630	-0.00066	-0.08465	-0.00222	-0.08688	2.89942
D33	-1.16167	0.00040	0.09673	0.00515	0.10188	-1.05979
D34	0.88803	0.00094	0.10075	0.00655	0.10735	0.99539
D35	3.06604	-0.00005	0.04389	-0.00082	0.04301	3.10905
D36	3.04329	-0.00033	0.09092	0.00386	0.09480	3.13809
D37	-1.19019	0.00021	0.09494	0.00527	0.10027	-1.08992
D38	0.98782	-0.00078	0.03808	-0.00210	0.03593	1.02374
D39	0.95066	-0.00020	0.08824	0.00266	0.09091	1.04156
D40	3.00036	0.00034	0.09226	0.00407	0.09638	3.09674
D41	-1.10482	-0.00066	0.03540	-0.00330	0.03204	-1.07278
D42	2.75456	0.00027	-0.43735	0.02416	-0.41282	2.34175
D43	-1.46403	0.00010	-0.37930	0.01621	-0.36359	-1.82762
D44	0.69728	0.00018	-0.47128	0.01761	-0.45294	0.24434
D45	2.76187	0.00002	-0.41323	0.00966	-0.40372	2.35815
D46	-1.40315	-0.00037	-0.48441	0.02133	-0.46287	-1.86602
D47	0.66144	-0.00054	-0.42636	0.01337	-0.41365	0.24779
D48	-3.12681	-0.00004	-0.00521	0.00076	-0.00444	-3.13125
D49	0.01823	-0.00006	-0.00662	-0.00006	-0.00668	0.01155
D50	0.00804	0.00004	-0.00400	0.00196	-0.00205	0.00599
D51	-3.13011	0.00002	-0.00542	0.00114	-0.00428	-3.13439

Item	Value	Threshold	Converged?
Maximum Force	0.003809	0.000450	NO
RMS Force	0.000780	0.000300	NO

Maximum Displacement 0.772979 0.001800 NO
RMS Displacement 0.129348 0.001200 NO
Predicted change in Energy=-1.861700D-04
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.827538	-2.022395	0.320371
2	6	0	-2.824713	-1.134771	0.072574
3	7	0	-2.233137	0.122597	0.014395
4	6	0	-0.909742	-0.009315	0.223246
5	7	0	-0.646182	-1.302873	0.414221
6	6	0	0.715939	-1.844516	0.606700
7	6	0	1.539556	-1.805674	-0.691236
8	1	0	-1.857548	-3.091446	0.442051
9	1	0	-3.879186	-1.290321	-0.064805
10	1	0	1.208671	-1.241298	1.369597
11	1	0	0.613754	-2.863170	0.981679
12	1	0	1.044434	-2.415578	-1.455829
13	1	0	1.569725	-0.769058	-1.044543
14	35	0	1.425496	2.122938	-0.511129
15	1	0	-0.145765	0.802312	0.149883
16	6	0	-2.835782	1.387582	-0.236135
17	6	0	-4.142758	1.588954	-0.339526
18	1	0	-2.096218	2.173721	-0.337389
19	1	0	-4.507267	2.586653	-0.541231
20	1	0	-4.880744	0.803865	-0.231771
21	7	0	2.877760	-2.314515	-0.401462
22	1	0	3.192453	-2.977567	-1.098319
23	1	0	3.554314	-1.561211	-0.356059

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357807	0.000000			
3	N	2.204343	1.390799	0.000000		
4	C	2.214560	2.226313	1.346252	0.000000	
5	N	1.386406	2.211556	2.170312	1.333877	0.000000
6	C	2.565716	3.650376	3.594079	2.481498	1.478445
7	C	3.522448	4.481112	4.295271	3.172103	2.500459
8	H	1.076372	2.213708	3.264052	3.231988	2.160365

9	H	2.212138	1.074701	2.170735	3.246775	3.268324
10	H	3.305987	4.238137	3.942439	2.705471	2.087346
11	H	2.665358	3.954351	4.237361	3.322761	2.084220
12	H	3.399662	4.352790	4.398450	3.525364	2.755609
13	H	3.869786	4.548932	4.046994	2.886564	2.706141
14	Br	5.334548	5.386803	4.202752	3.246404	4.109051
15	H	3.291868	3.306816	2.199430	1.117042	2.179930
16	C	3.599194	2.541197	1.423422	2.423218	3.529286
17	C	4.340226	3.053809	2.433540	3.650147	4.599657
18	H	4.255847	3.412462	2.085571	2.547094	3.841124
19	H	5.400615	4.129981	3.398818	4.501741	5.563208
20	H	4.196984	2.842217	2.744913	4.078868	4.773590
21	N	4.769298	5.842491	5.677475	4.477653	3.755919
22	H	5.303333	6.401029	6.347139	5.233073	4.452808
23	H	5.443765	6.407617	6.038794	4.761488	4.278345

		6	7	8	9	10
6	C	0.000000				
7	C	1.537691	0.000000			
8	H	2.864399	3.804979	0.000000		
9	H	4.676882	5.479122	2.754628	0.000000	
10	H	1.090260	2.162183	3.699336	5.286417	0.000000
11	H	1.090278	2.184961	2.539811	4.873961	1.770558
12	H	2.165190	1.096235	3.532739	5.238624	3.064138
13	H	2.147595	1.095586	4.398824	5.560777	2.486250
14	Br	4.182547	3.934391	6.235120	6.323700	3.860339
15	H	2.820800	3.217045	4.263440	4.285282	2.738346
16	C	4.875607	5.435768	4.634498	2.879098	5.083993
17	C	6.024201	6.628416	5.266801	2.904336	6.290407
18	H	4.994573	5.401819	5.327896	3.905492	5.049598
19	H	6.945134	7.475233	6.342607	3.956311	7.139777
20	H	6.248185	6.945578	4.976665	2.327361	6.620275
21	N	2.431206	1.460711	4.872194	6.842414	2.659756
22	H	3.213101	2.066668	5.280930	7.343230	3.611181
23	H	3.010571	2.057025	5.680391	7.444134	2.929552

		11	12	13	14	15
11	H	0.000000				
12	H	2.515407	0.000000			
13	H	3.066719	1.776546	0.000000		
14	Br	5.267700	4.651429	2.944312	0.000000	
15	H	3.834646	3.788100	2.615103	2.156351	0.000000
16	C	5.608142	5.568460	4.971228	4.332996	2.779882
17	C	6.647661	6.647509	6.220108	5.596431	4.102961
18	H	5.869766	5.672413	4.753857	3.526362	2.433612
19	H	7.631820	7.528624	6.960169	5.950934	4.762795

20	H	6.716331	6.853529	6.689038	6.448771	4.750336
21	N	2.709211	2.117307	2.124369	4.670341	4.377247
22	H	3.314992	2.248918	2.741103	5.429740	5.195112
23	H	3.483035	2.870354	2.245018	4.257800	4.419593

		16	17	18	19	20
16	C	0.000000				
17	C	1.326434	0.000000			
18	H	1.084077	2.128447	0.000000		
19	H	2.079596	1.081182	2.454633	0.000000	
20	H	2.126644	1.082866	3.105036	1.847589	0.000000
21	N	6.810096	8.032969	6.699912	8.864514	8.363460
22	H	7.492496	8.673765	7.421915	9.516122	8.956932
23	H	7.038685	8.316774	6.773372	9.067974	8.761234

		21	22	23
21	N	0.000000		
22	H	1.012066	0.000000	
23	H	1.013535	1.639498	0.000000

Stoichiometry C7H12BrN3
Framework group C1[X(C7H12BrN3)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.567273	2.300622	-0.099335
2	6	0	-2.593200	1.438293	0.118615
3	7	0	-2.073007	0.156388	-0.024355
4	6	0	-0.763337	0.249180	-0.321927
5	7	0	-0.439953	1.542172	-0.375061
6	6	0	0.933295	2.037029	-0.609805
7	6	0	1.847309	1.795585	0.602951
8	1	0	-1.544057	3.376677	-0.087451
9	1	0	-3.623745	1.626287	0.358653
10	1	0	1.332164	1.511243	-1.477629
11	1	0	0.862931	3.098462	-0.848796
12	1	0	1.446574	2.327900	1.473459
13	1	0	1.843325	0.722568	0.824142
14	35	0	1.492096	-2.069104	-0.043140
15	1	0	-0.044481	-0.601307	-0.409678
16	6	0	-2.727886	-1.099333	0.118576

17	6	0	-4.033072	-1.248502	0.302052
18	1	0	-2.029783	-1.926884	0.063487
19	1	0	-4.438967	-2.244783	0.409893
20	1	0	-4.730147	-0.421252	0.350454
21	7	0	3.187620	2.271321	0.269903
22	1	0	3.591157	2.825550	1.014394
23	1	0	3.814017	1.497782	0.078809

Rotational constants (GHZ): 0.7100243 0.5235547 0.3095386

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 365 symmetry adapted cartesian basis functions of A symmetry.

There are 352 symmetry adapted basis functions of A symmetry.

352 basis functions, 562 primitive gaussians, 365 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 833.8270860035 Hartrees.

NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 352 RedAO= T EigKep= 4.76D-06 NBF= 352

NBsUse= 352 1.00D-06 EigRej= -1.00D+00 NBFU= 352

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999964 0.004217 0.001027 -0.007341 Ang= 0.98 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3012.46610569 A.U. after 13 cycles

NFock= 13 Conv=0.34D-08 -V/T= 2.0017

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000069217	-0.000114650	0.000065877
2	6	0.000018870	0.000005847	0.000209944
3	7	0.000111415	0.000139575	-0.000509319
4	6	0.000178530	-0.000274889	0.000853297
5	7	-0.000096625	0.000397723	-0.000192559
6	6	-0.000663744	-0.000160099	0.000326705
7	6	-0.000662220	0.001843434	-0.000450665
8	1	0.000012355	-0.000019134	-0.000050533
9	1	0.000028292	-0.000007040	-0.000032406
10	1	-0.000065266	-0.000222448	0.000079299
11	1	0.000359786	0.000053647	-0.000114802
12	1	0.000969931	0.000132453	0.001060985
13	1	-0.001254582	-0.000081702	-0.000940813
14	35	0.000096582	-0.000216046	-0.000003587
15	1	-0.000294033	0.000371083	-0.000111863
16	6	0.000124297	0.000037551	0.000112271
17	6	-0.000020064	0.000005449	0.000012877
18	1	-0.000001138	-0.000113074	-0.000172966
19	1	-0.000000742	-0.000007300	0.000000643
20	1	-0.000016653	0.000012046	-0.000022134
21	7	0.001276524	-0.002462306	-0.000855225
22	1	0.000230490	0.000828291	0.000382788
23	1	-0.000262787	-0.000148411	0.000352187

Cartesian Forces: Max 0.002462306 RMS 0.000547225

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.001739067 RMS 0.000330972

Search for a local minimum.

Step number 11 out of a maximum of 121

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 8 9 10 11

DE= 1.45D-04 DEPred=-1.86D-04 R=-7.79D-01

Trust test=-7.79D-01 RLast= 1.34D+00 DXMaxT set to 1.50D+00

ITU= -1 1 1 1 1 1 1 0 1 0 0

Eigenvalues ---	0.00069	0.00241	0.00381	0.00886	0.01379
Eigenvalues ---	0.01452	0.01876	0.02002	0.02238	0.02328
Eigenvalues ---	0.02387	0.02574	0.03062	0.03062	0.03435
Eigenvalues ---	0.03667	0.03871	0.04549	0.04767	0.05326
Eigenvalues ---	0.05800	0.09257	0.09633	0.12414	0.12909
Eigenvalues ---	0.14793	0.15926	0.15992	0.16000	0.16001
Eigenvalues ---	0.16009	0.16030	0.17442	0.20694	0.21994
Eigenvalues ---	0.22037	0.22799	0.23599	0.24024	0.25036
Eigenvalues ---	0.28151	0.31514	0.34076	0.34648	0.34704
Eigenvalues ---	0.34822	0.34986	0.35685	0.35690	0.35858
Eigenvalues ---	0.36437	0.36658	0.37214	0.42052	0.42246
Eigenvalues ---	0.43382	0.47157	0.47715	0.48343	0.50462
Eigenvalues ---	0.54332	0.60343	0.60453		

En-DIIS/RFO-DIIS IScMMF= 0 using points: 11 10 9 8 7

RFO step: Lambda=-4.41956571D-05.

DidBck=T Rises=F RFO-DIIS coefs: 0.48461 0.75193 -0.61074 -0.40782 0.78202

Iteration 1 RMS(Cart)= 0.03633702 RMS(Int)= 0.00171932

Iteration 2 RMS(Cart)= 0.00168299 RMS(Int)= 0.00016393

Iteration 3 RMS(Cart)= 0.00000263 RMS(Int)= 0.00016391

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00016391

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56588	0.00009	0.00027	-0.00023	0.00007	2.56596
R2	2.61993	0.00002	0.00027	-0.00004	0.00023	2.62016
R3	2.03405	0.00001	-0.00005	0.00005	0.00000	2.03405
R4	2.62823	0.00014	0.00014	-0.00017	-0.00002	2.62821
R5	2.03089	-0.00002	0.00002	-0.00001	0.00002	2.03091
R6	2.54405	-0.00017	-0.00046	-0.00017	-0.00065	2.54340
R7	2.68988	-0.00008	0.00064	0.00011	0.00075	2.69062
R8	2.52066	-0.00029	0.00048	-0.00019	0.00027	2.52093
R9	2.11090	-0.00001	0.00245	-0.00205	0.00040	2.11130
R10	2.79386	-0.00001	-0.00109	0.00026	-0.00083	2.79303
R11	2.90581	0.00054	-0.00152	0.00075	-0.00077	2.90504
R12	2.06029	-0.00010	0.00011	0.00026	0.00037	2.06066
R13	2.06033	-0.00012	-0.00014	-0.00017	-0.00031	2.06002
R14	2.07158	-0.00125	-0.00178	0.00040	-0.00137	2.07021
R15	2.07036	0.00019	0.00177	-0.00072	0.00105	2.07141
R16	2.76034	0.00174	0.00046	0.00210	0.00256	2.76290
R17	4.07491	-0.00006	0.00673	-0.01026	-0.00353	4.07138
R18	2.50660	0.00004	-0.00006	-0.00002	-0.00008	2.50652

R19	2.04861	-0.00007	0.00038	-0.00002	0.00036	2.04897
R20	2.04314	-0.00001	0.00004	-0.00001	0.00003	2.04317
R21	2.04632	0.00000	0.00007	-0.00002	0.00005	2.04637
R22	1.91253	-0.00074	-0.00050	0.00120	0.00071	1.91324
R23	1.91530	-0.00027	0.00052	0.00086	0.00138	1.91668
A1	1.87430	-0.00019	-0.00039	0.00009	-0.00030	1.87400
A2	2.27763	0.00010	0.00004	0.00004	0.00008	2.27770
A3	2.13124	0.00009	0.00033	-0.00010	0.00024	2.13147
A4	1.86112	0.00004	0.00038	-0.00025	0.00013	1.86125
A5	2.27745	-0.00002	0.00007	-0.00007	0.00000	2.27744
A6	2.14462	-0.00001	-0.00044	0.00031	-0.00013	2.14449
A7	1.89975	-0.00008	-0.00018	0.00035	0.00014	1.89989
A8	2.25327	0.00019	0.00093	-0.00014	0.00081	2.25407
A9	2.13007	-0.00010	-0.00073	-0.00022	-0.00094	2.12914
A10	1.88753	0.00009	0.00023	-0.00028	0.00001	1.88754
A11	2.20301	0.00010	-0.00338	-0.00126	-0.00449	2.19852
A12	2.18816	-0.00022	0.00208	0.00178	0.00403	2.19219
A13	1.90206	0.00014	-0.00002	0.00009	0.00004	1.90210
A14	2.21897	0.00052	0.00231	-0.00157	0.00081	2.21978
A15	2.16032	-0.00067	-0.00237	0.00164	-0.00069	2.15963
A16	1.95447	-0.00052	-0.00192	0.00235	0.00042	1.95490
A17	1.88051	-0.00005	0.00204	-0.00214	-0.00010	1.88040
A18	1.87624	0.00060	0.00192	-0.00106	0.00086	1.87710
A19	1.91197	0.00025	-0.00094	0.00223	0.00127	1.91324
A20	1.94347	-0.00012	-0.00025	-0.00116	-0.00142	1.94205
A21	1.89508	-0.00014	-0.00068	-0.00038	-0.00106	1.89402
A22	1.91002	0.00016	-0.00147	0.00002	-0.00101	1.90901
A23	1.88688	-0.00028	0.00250	0.00094	0.00385	1.89073
A24	1.89067	0.00011	-0.00342	0.00095	-0.00195	1.88873
A25	1.89013	-0.00022	0.00285	-0.00193	0.00053	1.89066
A26	1.93728	-0.00068	-0.01327	0.00120	-0.01198	1.92530
A27	1.94803	0.00090	0.01172	-0.00116	0.01072	1.95874
A28	2.87049	-0.00046	0.00934	-0.00073	0.00861	2.87910
A29	2.17220	0.00008	-0.00092	-0.00002	-0.00095	2.17125
A30	1.95202	-0.00009	-0.00064	-0.00003	-0.00068	1.95135
A31	2.15895	0.00001	0.00157	0.00006	0.00163	2.16058
A32	2.07925	-0.00002	-0.00001	-0.00002	-0.00003	2.07922
A33	2.15759	0.00003	-0.00011	0.00003	-0.00007	2.15751
A34	2.04635	-0.00002	0.00012	-0.00001	0.00010	2.04645
A35	1.95680	0.00048	-0.00780	-0.00065	-0.00798	1.94883
A36	1.94068	-0.00014	-0.00830	0.00156	-0.00626	1.93442
A37	1.88622	-0.00017	-0.00481	-0.00313	-0.00705	1.87917
D1	0.00297	0.00006	0.00081	-0.00262	-0.00183	0.00114
D2	-3.14006	-0.00011	0.00105	-0.00375	-0.00268	3.14044

D3	3.13786	0.00017	-0.00144	0.00192	0.00040	3.13827
D4	-0.00516	0.00000	-0.00120	0.00079	-0.00045	-0.00561
D5	-0.00473	0.00009	0.00159	0.00260	0.00419	-0.00054
D6	-3.08287	0.00019	0.00216	-0.00035	0.00161	-3.08126
D7	-3.14031	-0.00001	0.00362	-0.00147	0.00219	-3.13813
D8	0.06474	0.00009	0.00419	-0.00443	-0.00040	0.06434
D9	-0.00024	-0.00019	-0.00291	0.00178	-0.00111	-0.00135
D10	3.12648	-0.00016	-0.00163	0.00118	-0.00044	3.12604
D11	-3.14053	-0.00004	-0.00313	0.00279	-0.00034	-3.14087
D12	-0.01381	-0.00001	-0.00185	0.00219	0.00033	-0.01348
D13	-0.00271	0.00025	0.00392	-0.00017	0.00373	0.00103
D14	3.04135	-0.00003	-0.00330	0.00264	-0.00074	3.04061
D15	-3.13068	0.00022	0.00271	0.00038	0.00310	-3.12758
D16	-0.08662	-0.00006	-0.00451	0.00319	-0.00137	-0.08799
D17	0.11734	0.00002	0.01346	-0.00160	0.01188	0.12922
D18	-3.02035	0.00010	0.01306	-0.00140	0.01167	-3.00868
D19	-3.04086	0.00005	0.01491	-0.00226	0.01264	-3.02822
D20	0.10463	0.00013	0.01451	-0.00206	0.01243	0.11706
D21	0.00458	-0.00021	-0.00341	-0.00149	-0.00489	-0.00031
D22	3.08532	-0.00025	-0.00337	0.00121	-0.00235	3.08297
D23	-3.04052	0.00004	0.00421	-0.00406	0.00017	-3.04036
D24	0.04021	0.00000	0.00426	-0.00137	0.00270	0.04292
D25	-1.75410	0.00004	0.10416	-0.01272	0.09149	-1.66262
D26	1.27376	-0.00026	0.09555	-0.00959	0.08592	1.35968
D27	1.82567	-0.00001	0.01236	0.00145	0.01381	1.83948
D28	-2.35382	-0.00006	0.01135	0.00423	0.01558	-2.33824
D29	-0.31437	0.00006	0.01261	0.00213	0.01474	-0.29964
D30	-1.24372	0.00007	0.01267	-0.00184	0.01084	-1.23288
D31	0.85997	0.00002	0.01166	0.00094	0.01261	0.87259
D32	2.89942	0.00014	0.01293	-0.00115	0.01177	2.91119
D33	-1.05979	-0.00044	-0.04198	0.00238	-0.03963	-1.09942
D34	0.99539	-0.00077	-0.03805	0.00063	-0.03736	0.95803
D35	3.10905	0.00021	-0.02362	0.00033	-0.02331	3.08574
D36	3.13809	-0.00020	-0.04268	0.00209	-0.04062	3.09747
D37	-1.08992	-0.00053	-0.03875	0.00034	-0.03835	-1.12827
D38	1.02374	0.00045	-0.02432	0.00004	-0.02430	0.99944
D39	1.04156	-0.00011	-0.04103	0.00184	-0.03923	1.00233
D40	3.09674	-0.00044	-0.03709	0.00008	-0.03696	3.05978
D41	-1.07278	0.00054	-0.02266	-0.00022	-0.02291	-1.09569
D42	2.34175	0.00012	0.10604	0.02129	0.12753	2.46928
D43	-1.82762	0.00014	0.09108	0.01792	0.10874	-1.71888
D44	0.24434	0.00026	0.11666	0.01993	0.13713	0.38147
D45	2.35815	0.00027	0.10171	0.01656	0.11834	2.47649
D46	-1.86602	0.00039	0.11518	0.02236	0.13749	-1.72853

D47	0.24779	0.00040	0.10023	0.01899	0.11870	0.36649
D48	-3.13125	0.00005	0.00012	0.00059	0.00071	-3.13054
D49	0.01155	0.00003	0.00111	-0.00023	0.00087	0.01242
D50	0.00599	-0.00005	0.00057	0.00037	0.00094	0.00693
D51	-3.13439	-0.00006	0.00155	-0.00045	0.00110	-3.13329

Item	Value	Threshold	Converged?
Maximum Force	0.001739	0.000450	NO
RMS Force	0.000331	0.000300	NO
Maximum Displacement	0.190352	0.001800	NO
RMS Displacement	0.036334	0.001200	NO

Predicted change in Energy=-2.186222D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.836987	-2.026807	0.329439
2	6	0	-2.828491	-1.133385	0.079517
3	7	0	-2.228164	0.119358	0.012173
4	6	0	-0.905610	-0.020390	0.219047
5	7	0	-0.649922	-1.315227	0.413041
6	6	0	0.709297	-1.864285	0.601623
7	6	0	1.533264	-1.820702	-0.695456
8	1	0	-1.874245	-3.094929	0.457123
9	1	0	-3.884394	-1.282145	-0.054415
10	1	0	1.204230	-1.269517	1.369989
11	1	0	0.603385	-2.885244	0.968746
12	1	0	1.056572	-2.455481	-1.450413
13	1	0	1.538539	-0.789113	-1.066028
14	35	0	1.395206	2.139940	-0.541596
15	1	0	-0.139532	0.788720	0.137068
16	6	0	-2.821624	1.387923	-0.244347
17	6	0	-4.127958	1.600111	-0.332573
18	1	0	-2.075029	2.165101	-0.363600
19	1	0	-4.486079	2.598750	-0.541035
20	1	0	-4.871466	0.823108	-0.205614
21	7	0	2.879154	-2.308625	-0.398562
22	1	0	3.245360	-2.876836	-1.152262
23	1	0	3.520021	-1.535409	-0.256583

Distance matrix (angstroms):

	1	2	3	4	5

1	C	0.000000				
2	C	1.357845	0.000000			
3	N	2.204473	1.390788	0.000000		
4	C	2.214804	2.226139	1.345910	0.000000	
5	N	1.386528	2.211440	2.170156	1.334021	0.000000
6	C	2.565942	3.650034	3.593183	2.480773	1.478007
7	C	3.528666	4.483067	4.291027	3.166314	2.500114
8	H	1.076371	2.213781	3.264181	3.232294	2.160613
9	H	2.212180	1.074709	2.170655	3.246531	3.268244
10	H	3.302308	4.236353	3.943852	2.708581	2.087036
11	H	2.664779	3.954429	4.237963	3.323628	2.084356
12	H	3.424079	4.379765	4.422493	3.544986	2.772140
13	H	3.856603	4.527885	4.021926	2.866394	2.693288
14	Br	5.344862	5.379596	4.185477	3.246438	4.126991
15	H	3.293259	3.305798	2.196822	1.117254	2.182487
16	C	3.599878	2.542032	1.423817	2.422641	3.529230
17	C	4.340661	3.054575	2.433247	3.648812	4.599115
18	H	4.255474	3.412341	2.085599	2.546250	3.840154
19	H	5.401036	4.130558	3.398765	4.500819	5.562874
20	H	4.197185	2.843046	2.744038	4.076744	4.772488
21	N	4.780313	5.846961	5.669964	4.465635	3.754985
22	H	5.361739	6.438056	6.347642	5.222100	4.479065
23	H	5.411325	6.370101	5.987664	4.701885	4.229102

		6	7	8	9	10
6	C	0.000000				
7	C	1.537282	0.000000			
8	H	2.865319	3.816178	0.000000		
9	H	4.676673	5.481970	2.754733	0.000000	
10	H	1.090456	2.162899	3.693571	5.284240	0.000000
11	H	1.090117	2.183459	2.538578	4.874110	1.769910
12	H	2.163554	1.095509	3.554895	5.266752	3.063165
13	H	2.150510	1.096141	4.391340	5.538469	2.505340
14	Br	4.220336	3.966033	6.252248	6.310482	3.913442
15	H	2.823961	3.209428	4.265489	4.283590	2.749933
16	C	4.874415	5.428059	4.635251	2.880073	5.086804
17	C	6.022772	6.624430	5.267469	2.905872	6.290127
18	H	4.992001	5.386700	5.327459	3.905497	5.055242
19	H	6.943793	7.469129	6.343183	3.957293	7.141086
20	H	6.246489	6.946240	4.977305	2.330078	6.616320
21	N	2.430244	1.462065	4.893391	6.849648	2.648186
22	H	3.245457	2.062854	5.371037	7.387943	3.620972
23	H	2.957169	2.054558	5.660352	7.411504	2.842415

		11	12	13	14	15
11	H	0.000000				

12	H	2.498480	0.000000			
13	H	3.067341	1.776746	0.000000		
14	Br	5.306655	4.696650	2.979081	0.000000	
15	H	3.839482	3.804682	2.598638	2.154484	0.000000
16	C	5.609121	5.591669	4.942233	4.293663	2.774552
17	C	6.648115	6.676582	6.193184	5.553417	4.097128
18	H	5.869841	5.686640	4.720027	3.474888	2.427188
19	H	7.632579	7.556004	6.931756	5.899154	4.756942
20	H	6.716025	6.887693	6.665413	6.412340	4.744451
21	N	2.716826	2.109445	2.133465	4.691726	4.358085
22	H	3.388035	2.248828	2.698011	5.381824	5.153268
23	H	3.439513	2.887966	2.266811	4.254911	4.353030

		16	17	18	19	20
16	C	0.000000				
17	C	1.326391	0.000000			
18	H	1.084266	2.129482	0.000000		
19	H	2.079551	1.081197	2.456155	0.000000	
20	H	2.126586	1.082893	3.105796	1.847683	0.000000
21	N	6.796110	8.023850	6.675281	8.851512	8.361644
22	H	7.471331	8.664915	7.372222	9.493724	8.970429
23	H	6.983015	8.266126	6.708936	9.014978	8.716781

		21	22	23
21	N	0.000000		
22	H	1.012441	0.000000	
23	H	1.014264	1.636187	0.000000

Stoichiometry C7H12BrN3
Framework group C1[X(C7H12BrN3)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.558895	2.318035	-0.093850
2	6	0	-2.582327	1.452409	0.122997
3	7	0	-2.058724	0.172166	-0.022291
4	6	0	-0.750052	0.268811	-0.321477
5	7	0	-0.429110	1.562782	-0.368875
6	6	0	0.943256	2.060186	-0.600615
7	6	0	1.861043	1.801461	0.605190
8	1	0	-1.538570	3.394123	-0.079843

9	1	0	-3.613168	1.637064	0.364391
10	1	0	1.338580	1.547813	-1.478276
11	1	0	0.873712	3.125028	-0.823391
12	1	0	1.485351	2.354265	1.473178
13	1	0	1.830053	0.730904	0.838585
14	35	0	1.462149	-2.090850	-0.043046
15	1	0	-0.032436	-0.582969	-0.409530
16	6	0	-2.709236	-1.086450	0.119041
17	6	0	-4.015544	-1.239861	0.290320
18	1	0	-2.006099	-1.910563	0.073572
19	1	0	-4.418618	-2.237241	0.398732
20	1	0	-4.716220	-0.415059	0.327889
21	7	0	3.207887	2.253458	0.259724
22	1	0	3.666576	2.696454	1.046105
23	1	0	3.785796	1.473537	-0.034343

Rotational constants (GHZ): 0.7021927 0.5285011 0.3096310

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 365 symmetry adapted cartesian basis functions of A symmetry.

There are 352 symmetry adapted basis functions of A symmetry.

352 basis functions, 562 primitive gaussians, 365 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 833.6362801912 Hartrees.

NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 352 RedAO= T EigKep= 4.87D-06 NBF= 352

NBsUse= 352 1.00D-06 EigRej= -1.00D+00 NBFU= 352

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999993 -0.000785 -0.000397 0.003598 Ang= -0.42 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0

NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3012.46636416 A.U. after 11 cycles

NFock= 11 Conv=0.81D-08 -V/T= 2.0017

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000003048	-0.000139841	-0.000220634
2	6	0.000002833	0.000036484	0.000272563
3	7	-0.000003099	0.000189540	-0.000238109
4	6	0.000320678	-0.000349945	0.000193739
5	7	-0.000095996	0.000458661	0.000180586
6	6	-0.000405753	-0.000170711	0.000317321
7	6	-0.000453076	0.001406782	-0.000437962
8	1	0.000032340	-0.000026256	-0.000098514
9	1	0.000026376	-0.000011979	-0.000017066
10	1	-0.000134291	-0.000133158	0.000094316
11	1	0.000400987	0.000050497	-0.000039414
12	1	0.000722385	0.000122940	0.000917546
13	1	-0.000962683	-0.000077443	-0.000814305
14	35	0.000084054	-0.000316051	0.000007434
15	1	-0.000287739	0.000357178	-0.000007607
16	6	0.000130746	-0.000036312	0.000159025
17	6	-0.000016086	0.000024188	-0.000021092
18	1	-0.000025986	-0.000083525	-0.000147964
19	1	-0.000000883	-0.000010621	-0.000000511
20	1	-0.000019935	0.000010841	-0.000018972
21	7	0.000763843	-0.001886340	-0.000822523
22	1	0.000143541	0.000690235	0.000354916
23	1	-0.000219209	-0.000105163	0.000387227

Cartesian Forces: Max 0.001886340 RMS 0.000428381

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.001053365 RMS 0.000281435
Search for a local minimum.
Step number 12 out of a maximum of 121
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 9 11 12
DE= -2.58D-04 DEPred=-2.19D-04 R= 1.18D+00
TightC=F SS= 1.41D+00 RLast= 3.50D-01 DXNew= 2.5227D+00 1.0506D+00
Trust test= 1.18D+00 RLast= 3.50D-01 DXMaxT set to 1.50D+00
ITU= 1 -1 1 1 1 1 1 1 0 1 0 0
Eigenvalues --- 0.00019 0.00218 0.00405 0.00889 0.01383
Eigenvalues --- 0.01505 0.01877 0.02077 0.02247 0.02329
Eigenvalues --- 0.02393 0.02746 0.03062 0.03063 0.03426
Eigenvalues --- 0.03761 0.04067 0.04509 0.04734 0.05332
Eigenvalues --- 0.05769 0.09277 0.09712 0.12377 0.13292
Eigenvalues --- 0.15039 0.15920 0.15995 0.16000 0.16000
Eigenvalues --- 0.16010 0.16063 0.17541 0.20851 0.21989
Eigenvalues --- 0.22060 0.22831 0.23657 0.24137 0.25036
Eigenvalues --- 0.28222 0.31587 0.34069 0.34585 0.34735
Eigenvalues --- 0.34811 0.35019 0.35688 0.35689 0.35858
Eigenvalues --- 0.36437 0.36658 0.38396 0.41786 0.42199
Eigenvalues --- 0.43333 0.47240 0.47694 0.48325 0.50536
Eigenvalues --- 0.54342 0.60352 0.60987
En-DIIS/RFO-DIIS IScMMF= 0 using points: 12 11 10 9 8
RFO step: Lambda=-5.31957548D-05.
DidBck=T Rises=F En-DIIS coefs: 0.53546 0.00000 0.46454 0.00000 0.00000
Iteration 1 RMS(Cart)= 0.08814372 RMS(Int)= 0.09086035
Iteration 2 RMS(Cart)= 0.04635872 RMS(Int)= 0.04277503
Iteration 3 RMS(Cart)= 0.04061861 RMS(Int)= 0.00369013
Iteration 4 RMS(Cart)= 0.00355964 RMS(Int)= 0.00030776
Iteration 5 RMS(Cart)= 0.00001831 RMS(Int)= 0.00030714
Iteration 6 RMS(Cart)= 0.00000001 RMS(Int)= 0.00030714

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56596	0.00012	0.00080	-0.00018	0.00065	2.56661
R2	2.62016	-0.00002	-0.00014	0.00090	0.00075	2.62091
R3	2.03405	0.00001	0.00010	-0.00013	-0.00003	2.03402
R4	2.62821	0.00015	0.00104	-0.00092	0.00015	2.62835
R5	2.03091	-0.00002	0.00000	0.00008	0.00008	2.03099
R6	2.54340	-0.00010	-0.00174	-0.00076	-0.00251	2.54089
R7	2.69062	-0.00010	0.00067	0.00237	0.00304	2.69366

R8	2.52093	-0.00042	0.00002	0.00058	0.00057	2.52150
R9	2.11130	-0.00011	0.00314	-0.00031	0.00282	2.11412
R10	2.79303	-0.00010	-0.00168	-0.00248	-0.00416	2.78887
R11	2.90504	0.00034	0.00177	-0.00626	-0.00448	2.90056
R12	2.06066	-0.00007	0.00041	0.00142	0.00183	2.06250
R13	2.06002	-0.00010	-0.00065	-0.00085	-0.00150	2.05853
R14	2.07021	-0.00102	-0.00254	-0.00269	-0.00523	2.06498
R15	2.07141	0.00020	0.00144	0.00332	0.00476	2.07617
R16	2.76290	0.00105	0.00004	0.00635	0.00639	2.76929
R17	4.07138	-0.00014	-0.02508	0.00527	-0.01982	4.05157
R18	2.50652	0.00004	-0.00003	-0.00028	-0.00032	2.50620
R19	2.04897	-0.00006	0.00061	0.00089	0.00149	2.05046
R20	2.04317	-0.00001	0.00002	0.00010	0.00013	2.04329
R21	2.04637	0.00000	0.00013	0.00009	0.00022	2.04659
R22	1.91324	-0.00060	-0.00073	0.00361	0.00288	1.91611
R23	1.91668	-0.00017	0.00034	0.00580	0.00614	1.92282
A1	1.87400	-0.00019	-0.00145	-0.00003	-0.00150	1.87250
A2	2.27770	0.00011	-0.00030	0.00084	0.00055	2.27826
A3	2.13147	0.00008	0.00173	-0.00078	0.00096	2.13243
A4	1.86125	0.00003	0.00069	0.00008	0.00078	1.86203
A5	2.27744	-0.00003	-0.00032	0.00014	-0.00018	2.27726
A6	2.14449	-0.00001	-0.00038	-0.00022	-0.00060	2.14388
A7	1.89989	-0.00013	-0.00053	0.00054	-0.00001	1.89988
A8	2.25407	0.00018	0.00173	0.00179	0.00353	2.25760
A9	2.12914	-0.00005	-0.00124	-0.00235	-0.00358	2.12556
A10	1.88754	0.00012	0.00041	0.00005	0.00048	1.88802
A11	2.19852	0.00032	0.00339	-0.01766	-0.01414	2.18439
A12	2.19219	-0.00045	-0.00568	0.01900	0.01345	2.20564
A13	1.90210	0.00018	0.00085	-0.00063	0.00025	1.90235
A14	2.21978	0.00059	0.00900	-0.00277	0.00640	2.22618
A15	2.15963	-0.00078	-0.01117	0.00443	-0.00662	2.15301
A16	1.95490	-0.00071	-0.00444	0.00352	-0.00092	1.95397
A17	1.88040	-0.00005	-0.00302	0.00199	-0.00106	1.87935
A18	1.87710	0.00066	0.00786	-0.00251	0.00534	1.88244
A19	1.91324	0.00034	0.00435	0.00409	0.00845	1.92169
A20	1.94205	-0.00007	-0.00300	-0.00379	-0.00680	1.93525
A21	1.89402	-0.00017	-0.00167	-0.00344	-0.00511	1.88891
A22	1.90901	0.00015	-0.00527	0.00185	-0.00428	1.90473
A23	1.89073	-0.00015	0.00674	0.01008	0.01667	1.90740
A24	1.88873	-0.00011	0.00039	-0.01176	-0.01183	1.87690
A25	1.89066	-0.00019	-0.00371	0.00913	0.00578	1.89643
A26	1.92530	-0.00046	-0.01415	-0.03697	-0.05133	1.87397
A27	1.95874	0.00076	0.01550	0.02809	0.04375	2.00249
A28	2.87910	-0.00054	0.02690	0.01261	0.03951	2.91861

A29	2.17125	0.00010	-0.00113	-0.00266	-0.00378	2.16747
A30	1.95135	-0.00007	-0.00109	-0.00169	-0.00278	1.94857
A31	2.16058	-0.00003	0.00221	0.00434	0.00656	2.16713
A32	2.07922	-0.00002	-0.00021	0.00011	-0.00010	2.07912
A33	2.15751	0.00004	0.00011	-0.00043	-0.00032	2.15719
A34	2.04645	-0.00002	0.00010	0.00033	0.00042	2.04688
A35	1.94883	0.00035	-0.00578	-0.03121	-0.03795	1.91088
A36	1.93442	-0.00011	-0.00339	-0.02545	-0.02981	1.90461
A37	1.87917	-0.00010	-0.00651	-0.02283	-0.03141	1.84776
D1	0.00114	0.00014	0.00421	-0.00771	-0.00355	-0.00241
D2	3.14044	-0.00003	0.00234	-0.00722	-0.00486	3.13558
D3	3.13827	0.00016	0.00147	-0.00217	-0.00080	3.13747
D4	-0.00561	-0.00001	-0.00039	-0.00169	-0.00211	-0.00772
D5	-0.00054	-0.00008	-0.00368	0.00460	0.00095	0.00041
D6	-3.08126	0.00008	0.01518	-0.01430	0.00065	-3.08061
D7	-3.13813	-0.00010	-0.00121	-0.00037	-0.00152	-3.13965
D8	0.06434	0.00007	0.01765	-0.01927	-0.00182	0.06252
D9	-0.00135	-0.00016	-0.00334	0.00823	0.00495	0.00360
D10	3.12604	-0.00016	-0.00661	0.00725	0.00069	3.12673
D11	-3.14087	0.00000	-0.00165	0.00779	0.00614	-3.13474
D12	-0.01348	0.00000	-0.00492	0.00681	0.00188	-0.01161
D13	0.00103	0.00011	0.00107	-0.00544	-0.00440	-0.00337
D14	3.04061	-0.00005	-0.01594	0.01030	-0.00558	3.03503
D15	-3.12758	0.00011	0.00402	-0.00458	-0.00059	-3.12817
D16	-0.08799	-0.00005	-0.01299	0.01116	-0.00177	-0.08977
D17	0.12922	0.00001	0.02259	0.03044	0.05304	0.18226
D18	-3.00868	0.00009	0.02367	0.03033	0.05400	-2.95468
D19	-3.02822	0.00000	0.01896	0.02938	0.04833	-2.97989
D20	0.11706	0.00009	0.02004	0.02926	0.04929	0.16636
D21	-0.00031	-0.00002	0.00159	0.00056	0.00216	0.00185
D22	3.08297	-0.00012	-0.01511	0.01837	0.00298	3.08595
D23	-3.04036	0.00008	0.01763	-0.01241	0.00540	-3.03496
D24	0.04292	-0.00002	0.00093	0.00540	0.00622	0.04914
D25	-1.66262	-0.00007	0.22746	0.13567	0.36318	-1.29943
D26	1.35968	-0.00021	0.20820	0.15247	0.36063	1.72031
D27	1.83948	-0.00007	0.01304	0.02774	0.04078	1.88026
D28	-2.33824	-0.00011	0.01376	0.03627	0.04999	-2.28825
D29	-0.29964	0.00000	0.01429	0.03197	0.04623	-0.25340
D30	-1.23288	0.00007	0.03364	0.00645	0.04013	-1.19275
D31	0.87259	0.00004	0.03436	0.01499	0.04935	0.92193
D32	2.91119	0.00015	0.03489	0.01068	0.04559	2.95678
D33	-1.09942	-0.00041	-0.02892	-0.12727	-0.15617	-1.25559
D34	0.95803	-0.00063	-0.03251	-0.10951	-0.14199	0.81603
D35	3.08574	0.00013	-0.00915	-0.07654	-0.08571	3.00003

D36	3.09747	-0.00013	-0.02517	-0.13474	-0.15990	2.93756
D37	-1.12827	-0.00035	-0.02876	-0.11697	-0.14573	-1.27400
D38	0.99944	0.00041	-0.00540	-0.08401	-0.08945	0.90999
D39	1.00233	-0.00009	-0.02401	-0.13071	-0.15471	0.84763
D40	3.05978	-0.00032	-0.02761	-0.11294	-0.14053	2.91925
D41	-1.09569	0.00044	-0.00424	-0.07998	-0.08425	-1.17994
D42	2.46928	0.00013	0.13253	0.45259	0.58483	3.05411
D43	-1.71888	0.00016	0.11839	0.38551	0.50477	-1.21411
D44	0.38147	0.00029	0.14670	0.47932	0.62494	1.00642
D45	2.47649	0.00032	0.13257	0.41224	0.54488	3.02138
D46	-1.72853	0.00033	0.15115	0.47450	0.62528	-1.10325
D47	0.36649	0.00037	0.13702	0.40742	0.54522	0.91171
D48	-3.13054	0.00005	0.00173	0.00315	0.00488	-3.12566
D49	0.01242	0.00003	0.00270	0.00258	0.00527	0.01770
D50	0.00693	-0.00005	0.00052	0.00326	0.00378	0.01071
D51	-3.13329	-0.00006	0.00148	0.00269	0.00417	-3.12912

Item	Value	Threshold	Converged?
Maximum Force	0.001053	0.000450	NO
RMS Force	0.000281	0.000300	YES
Maximum Displacement	1.006241	0.001800	NO
RMS Displacement	0.155931	0.001200	NO

Predicted change in Energy=-8.354484D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.864840	-2.043701	0.356097
2	6	0	-2.836912	-1.129417	0.103419
3	7	0	-2.205783	0.105419	-0.003166
4	6	0	-0.884266	-0.065030	0.176938
5	7	0	-0.658063	-1.361403	0.397541
6	6	0	0.692051	-1.931561	0.571066
7	6	0	1.506632	-1.883705	-0.728980
8	1	0	-1.927600	-3.107238	0.509373
9	1	0	-3.898560	-1.252947	-0.009457
10	1	0	1.196222	-1.358236	1.351015
11	1	0	0.579159	-2.956953	0.921003
12	1	0	1.107083	-2.621226	-1.429341
13	1	0	1.413941	-0.885621	-1.178749
14	35	0	1.294424	2.191897	-0.651504
15	1	0	-0.109070	0.731930	0.052359

16	6	0	-2.767105	1.386680	-0.277257
17	6	0	-4.068230	1.643197	-0.288952
18	1	0	-1.998518	2.125337	-0.479760
19	1	0	-4.405284	2.643775	-0.522127
20	1	0	-4.827315	0.901118	-0.074431
21	7	0	2.878314	-2.285576	-0.405688
22	1	0	3.423462	-2.344357	-1.258613
23	1	0	3.315781	-1.557466	0.154501

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.358191	0.000000			
3	N	2.205454	1.390865	0.000000		
4	C	2.215573	2.225119	1.344581	0.000000	
5	N	1.386924	2.210816	2.169693	1.334322	0.000000
6	C	2.568362	3.649070	3.588381	2.474683	1.475805
7	C	3.545393	4.486448	4.273810	3.137620	2.495547
8	H	1.076357	2.214367	3.265157	3.233278	2.161520
9	H	2.212450	1.074754	2.170413	3.245282	3.267756
10	H	3.290870	4.227887	3.943315	2.716481	2.085065
11	H	2.669510	3.959530	4.241240	3.325428	2.085789
12	H	3.514776	4.486640	4.521466	3.616593	2.835559
13	H	3.800961	4.446700	3.932754	2.791597	2.646555
14	Br	5.379266	5.354342	4.126159	3.244492	4.187916
15	H	3.298350	3.302779	2.189019	1.118747	2.191480
16	C	3.603155	2.545689	1.425425	2.420503	3.529216
17	C	4.343297	3.059001	2.432107	3.643174	4.596535
18	H	4.254103	3.411221	2.085705	2.543721	3.837164
19	H	5.403477	4.133773	3.398584	4.497097	5.561376
20	H	4.199234	2.848931	2.740555	4.067464	4.767014
21	N	4.810024	5.853179	5.632666	4.407640	3.742357
22	H	5.537492	6.521004	6.266255	5.080616	4.513080
23	H	5.207293	6.167777	5.768685	4.457384	3.986094

		6	7	8	9	10
6	C	0.000000				
7	C	1.534911	0.000000			
8	H	2.872037	3.850259	0.000000		
9	H	4.676669	5.489232	2.755406	0.000000	
10	H	1.091426	2.167683	3.677721	5.274350	0.000000
11	H	1.089325	2.175893	2.544772	4.880508	1.766798
12	H	2.156273	1.092740	3.633747	5.380029	3.055072
13	H	2.162629	1.098661	4.353301	5.452048	2.582725
14	Br	4.342861	4.081859	6.309509	6.264684	4.077152

15	H	2.829318	3.172149	4.272601	4.278293	2.785514
16	C	4.867868	5.400397	4.638841	2.884361	5.088594
17	C	6.014882	6.611486	5.271267	2.914542	6.277942
18	H	4.980143	5.331098	5.325716	3.904375	5.068864
19	H	6.936253	7.449269	6.346421	3.962833	7.134538
20	H	6.237319	6.950004	4.981575	2.346658	6.589354
21	N	2.420561	1.465446	4.960773	6.866538	2.602959
22	H	3.313416	2.041311	5.686970	7.507567	3.569760
23	H	2.682803	2.039606	5.479121	7.222626	2.442103

		11	12	13	14	15
11	H	0.000000				
12	H	2.432187	0.000000			
13	H	3.065328	1.780248	0.000000		
14	Br	5.430934	4.879168	3.124642	0.000000	
15	H	3.851761	3.862398	2.540011	2.143997	0.000000
16	C	5.612527	5.692094	4.843261	4.157458	2.757262
17	C	6.650083	6.802180	6.102529	5.402831	4.076991
18	H	5.868239	5.751201	4.604273	3.298090	2.407228
19	H	7.635146	7.676553	6.837482	5.719056	4.737366
20	H	6.716068	7.032764	6.585228	6.282899	4.722980
21	N	2.738059	2.073110	2.168384	4.755723	4.270786
22	H	3.635390	2.339106	2.484444	5.047671	4.864254
23	H	3.167837	2.918645	2.417836	4.335119	4.120846

		16	17	18	19	20
16	C	0.000000				
17	C	1.326222	0.000000			
18	H	1.085056	2.133676	0.000000		
19	H	2.079395	1.081265	2.462335	0.000000	
20	H	2.126353	1.083010	3.108873	1.848079	0.000000
21	N	6.735927	7.981439	6.576103	8.795616	8.345146
22	H	7.294299	8.542030	7.069840	9.311989	8.944871
23	H	6.771699	8.060057	6.496699	8.816071	8.509234

		21	22	23
21	N	0.000000		
22	H	1.013964	0.000000	
23	H	1.017513	1.621013	0.000000

Stoichiometry C7H12BrN3
Framework group C1[X(C7H12BrN3)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.522246	2.380704	-0.074823
2	6	0	-2.539724	1.505941	0.135446
3	7	0	-2.005806	0.229893	-0.009942
4	6	0	-0.696452	0.336757	-0.296418
5	7	0	-0.384727	1.633373	-0.341481
6	6	0	0.986652	2.131042	-0.564294
7	6	0	1.908744	1.823720	0.623666
8	1	0	-1.510466	3.456882	-0.059179
9	1	0	-3.572943	1.681705	0.373480
10	1	0	1.369061	1.655100	-1.468979
11	1	0	0.927732	3.204051	-0.742648
12	1	0	1.636544	2.466890	1.464094
13	1	0	1.774920	0.775787	0.925297
14	35	0	1.354160	-2.164825	-0.043805
15	1	0	0.018279	-0.520503	-0.372973
16	6	0	-2.644034	-1.037585	0.124228
17	6	0	-3.955502	-1.204060	0.230075
18	1	0	-1.923993	-1.849248	0.133741
19	1	0	-4.351647	-2.203750	0.343312
20	1	0	-4.666916	-0.387773	0.208288
21	7	0	3.274066	2.177759	0.226067
22	1	0	3.897125	2.064247	1.017923
23	1	0	3.597358	1.519186	-0.478984

Rotational constants (GHZ): 0.6778707 0.5467830 0.3103244
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 365 symmetry adapted cartesian basis functions of A symmetry.
There are 352 symmetry adapted basis functions of A symmetry.
352 basis functions, 562 primitive gaussians, 365 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 833.6684737515 Hartrees.
NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 352 RedAO= T EigKep= 5.13D-06 NBF= 352
NBsUse= 352 1.00D-06 EigRej= -1.00D+00 NBFU= 352
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"
B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999907 -0.002745 -0.001292 0.013310 Ang= -1.56 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3012.46578895 A.U. after 13 cycles
NFock= 13 Conv=0.24D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000008082	-0.000137610	-0.000187796
2	6	-0.000090019	0.000103114	0.000913984
3	7	0.000076667	-0.000072417	-0.000522495
4	6	0.000427788	0.000011614	-0.000188702
5	7	0.000068455	0.000224293	-0.000181251
6	6	-0.000240365	-0.000581569	-0.001064630
7	6	0.000358665	-0.002728821	0.000856116
8	1	0.000049527	-0.000057302	-0.000207489
9	1	0.000006064	-0.000029484	0.000011761
10	1	-0.000426778	0.000583610	-0.000121849
11	1	-0.000096902	-0.000121914	0.000558889
12	1	-0.002170425	0.000647158	-0.001443854
13	1	0.001422355	0.000103331	0.001195689
14	35	-0.000091736	-0.000506634	-0.000038593
15	1	-0.000250618	0.000494151	0.000693214
16	6	0.000076860	-0.000400923	-0.000231072
17	6	0.000018831	0.000040511	-0.000155712
18	1	-0.000113838	0.000136747	0.000158196

19	1	0.000009228	-0.000000337	0.000090540
20	1	-0.000023019	-0.000012605	-0.000011965
21	7	-0.000928569	0.003725332	0.000992636
22	1	0.000852605	-0.001508043	-0.000390982
23	1	0.001073306	0.000087798	-0.000724632

Cartesian Forces: Max 0.003725332 RMS 0.000806396

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.001643424 RMS 0.000477095

Search for a local minimum.

Step number 13 out of a maximum of 121

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 12 13

DE= 5.75D-04 DEPred=-8.35D-04 R=-6.89D-01

Trust test=-6.89D-01 RLast= 1.56D+00 DXMaxT set to 7.50D-01

ITU= -1 1 -1 1 1 1 1 1 1 0 1 0 0

Eigenvalues ---	0.00138	0.00260	0.00405	0.00889	0.01385
Eigenvalues ---	0.01504	0.01876	0.02077	0.02247	0.02334
Eigenvalues ---	0.02394	0.02752	0.03062	0.03064	0.03464
Eigenvalues ---	0.04024	0.04167	0.04675	0.04793	0.05322
Eigenvalues ---	0.05800	0.09264	0.09657	0.12606	0.13291
Eigenvalues ---	0.14904	0.15921	0.15996	0.16000	0.16001
Eigenvalues ---	0.16010	0.16063	0.17552	0.20923	0.21985
Eigenvalues ---	0.22066	0.22831	0.23660	0.24134	0.25036
Eigenvalues ---	0.28194	0.31583	0.34080	0.34648	0.34735
Eigenvalues ---	0.34823	0.35015	0.35688	0.35690	0.35859
Eigenvalues ---	0.36437	0.36658	0.38387	0.41687	0.42198
Eigenvalues ---	0.43324	0.47236	0.47705	0.48340	0.50520
Eigenvalues ---	0.54341	0.60352	0.60967		

En-DIIS/RFO-DIIS IScMMF= 0 using points: 13 12 11 10 9

RFO step: Lambda=-1.57302787D-04.

EnCoef did 100 forward-backward iterations

DidBck=T Rises=T En-DIIS coefs: 0.45920 0.00426 0.37236 0.00000 0.16418

Iteration 1 RMS(Cart)= 0.08172979 RMS(Int)= 0.07053908

Iteration 2 RMS(Cart)= 0.04743991 RMS(Int)= 0.02050231

Iteration 3 RMS(Cart)= 0.01948196 RMS(Int)= 0.00090894

Iteration 4 RMS(Cart)= 0.00088686 RMS(Int)= 0.00002543

Iteration 5 RMS(Cart)= 0.00000127 RMS(Int)= 0.00002540

Iteration 6 RMS(Cart)= 0.00000000 RMS(Int)= 0.00002540

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56661	-0.00017	-0.00022	-0.00032	-0.00053	2.56608
R2	2.62091	-0.00002	-0.00066	0.00004	-0.00062	2.62028
R3	2.03402	0.00002	0.00005	-0.00001	0.00004	2.03406
R4	2.62835	0.00003	0.00018	-0.00011	0.00008	2.62843
R5	2.03099	0.00000	-0.00007	-0.00003	-0.00009	2.03090
R6	2.54089	0.00013	0.00134	0.00084	0.00218	2.54307
R7	2.69366	-0.00016	-0.00207	-0.00080	-0.00287	2.69079
R8	2.52150	-0.00023	-0.00052	-0.00018	-0.00070	2.52080
R9	2.11412	-0.00032	-0.00141	-0.00036	-0.00177	2.11235
R10	2.78887	-0.00024	0.00255	0.00087	0.00342	2.79229
R11	2.90056	-0.00008	0.00358	0.00139	0.00497	2.90553
R12	2.06250	0.00002	-0.00115	-0.00052	-0.00167	2.06083
R13	2.05853	0.00031	0.00086	0.00034	0.00120	2.05973
R14	2.06498	0.00128	0.00289	0.00062	0.00352	2.06849
R15	2.07617	-0.00052	-0.00298	-0.00125	-0.00422	2.07195
R16	2.76929	0.00027	-0.00444	0.00035	-0.00408	2.76521
R17	4.05157	-0.00039	0.00440	0.01109	0.01549	4.06706
R18	2.50620	0.00000	0.00024	0.00008	0.00032	2.50651
R19	2.05046	-0.00001	-0.00095	-0.00048	-0.00143	2.04903
R20	2.04329	-0.00002	-0.00009	-0.00003	-0.00012	2.04317
R21	2.04659	0.00002	-0.00012	-0.00006	-0.00018	2.04641
R22	1.91611	0.00087	-0.00219	-0.00092	-0.00310	1.91301
R23	1.92282	0.00012	-0.00414	-0.00147	-0.00561	1.91721
A1	1.87250	-0.00005	0.00065	0.00034	0.00098	1.87348
A2	2.27826	0.00005	-0.00040	0.00011	-0.00028	2.27798
A3	2.13243	0.00000	-0.00026	-0.00045	-0.00070	2.13173
A4	1.86203	-0.00002	-0.00032	-0.00029	-0.00061	1.86142
A5	2.27726	-0.00002	-0.00002	0.00007	0.00005	2.27731
A6	2.14388	0.00004	0.00034	0.00021	0.00055	2.14444
A7	1.89988	0.00005	-0.00026	0.00033	0.00006	1.89993
A8	2.25760	-0.00024	-0.00203	-0.00100	-0.00303	2.25457
A9	2.12556	0.00019	0.00230	0.00073	0.00303	2.12858
A10	1.88802	-0.00018	-0.00013	-0.00051	-0.00065	1.88737
A11	2.18439	0.00047	0.01166	0.00144	0.01312	2.19751
A12	2.20564	-0.00030	-0.01159	-0.00112	-0.01269	2.19295
A13	1.90235	0.00020	0.00005	0.00015	0.00022	1.90257
A14	2.22618	-0.00045	-0.00189	-0.00280	-0.00464	2.22153
A15	2.15301	0.00025	0.00133	0.00286	0.00424	2.15725
A16	1.95397	0.00025	-0.00105	0.00081	-0.00023	1.95374
A17	1.87935	-0.00028	-0.00069	0.00062	-0.00006	1.87928

A18	1.88244	-0.00036	-0.00079	-0.00221	-0.00301	1.87944
A19	1.92169	0.00008	-0.00395	-0.00235	-0.00629	1.91540
A20	1.93525	0.00024	0.00364	0.00214	0.00578	1.94103
A21	1.88891	0.00004	0.00291	0.00097	0.00387	1.89278
A22	1.90473	-0.00124	0.00091	0.00108	0.00202	1.90675
A23	1.90740	0.00026	-0.00996	-0.00370	-0.01361	1.89379
A24	1.87690	0.00113	0.00812	0.00404	0.01220	1.88909
A25	1.89643	0.00007	-0.00547	-0.00128	-0.00676	1.88967
A26	1.87397	0.00140	0.03318	0.00942	0.04258	1.91655
A27	2.00249	-0.00164	-0.02628	-0.00898	-0.03524	1.96725
A28	2.91861	-0.00067	-0.02081	-0.01373	-0.03453	2.88408
A29	2.16747	0.00000	0.00255	0.00097	0.00353	2.17100
A30	1.94857	0.00016	0.00168	0.00068	0.00237	1.95094
A31	2.16713	-0.00016	-0.00424	-0.00166	-0.00590	2.16124
A32	2.07912	-0.00001	0.00001	0.00003	0.00005	2.07916
A33	2.15719	0.00002	0.00029	0.00010	0.00039	2.15758
A34	2.04688	-0.00001	-0.00030	-0.00013	-0.00044	2.04644
A35	1.91088	0.00136	0.02610	0.00939	0.03558	1.94645
A36	1.90461	0.00125	0.02083	0.00557	0.02648	1.93110
A37	1.84776	-0.00073	0.02042	0.00659	0.02718	1.87494
D1	-0.00241	0.00024	0.00375	0.00102	0.00476	0.00235
D2	3.13558	-0.00001	0.00396	-0.00150	0.00246	3.13804
D3	3.13747	0.00021	0.00147	0.00284	0.00430	-3.14142
D4	-0.00772	-0.00003	0.00169	0.00032	0.00200	-0.00572
D5	0.00041	-0.00009	-0.00356	0.00334	-0.00022	0.00019
D6	-3.08061	-0.00013	0.00374	-0.00072	0.00299	-3.07762
D7	-3.13965	-0.00007	-0.00152	0.00171	0.00019	-3.13945
D8	0.06252	-0.00011	0.00578	-0.00236	0.00340	0.06592
D9	0.00360	-0.00031	-0.00269	-0.00500	-0.00768	-0.00409
D10	3.12673	-0.00018	-0.00218	-0.00183	-0.00402	3.12271
D11	-3.13474	-0.00009	-0.00288	-0.00272	-0.00560	-3.14034
D12	-0.01161	0.00004	-0.00237	0.00045	-0.00193	-0.01354
D13	-0.00337	0.00026	0.00049	0.00713	0.00762	0.00424
D14	3.03503	0.00019	-0.00077	0.00519	0.00442	3.03945
D15	-3.12817	0.00015	0.00008	0.00427	0.00434	-3.12383
D16	-0.08977	0.00008	-0.00118	0.00232	0.00114	-0.08862
D17	0.18226	-0.00016	-0.03199	-0.01332	-0.04531	0.13696
D18	-2.95468	-0.00024	-0.03155	-0.01300	-0.04455	-2.99923
D19	-2.97989	-0.00002	-0.03146	-0.00980	-0.04126	-3.02114
D20	0.16636	-0.00011	-0.03102	-0.00948	-0.04050	0.12586
D21	0.00185	-0.00010	0.00188	-0.00649	-0.00461	-0.00276
D22	3.08595	-0.00010	-0.00514	-0.00286	-0.00803	3.07791
D23	-3.03496	-0.00009	0.00133	-0.00471	-0.00336	-3.03831
D24	0.04914	-0.00008	-0.00569	-0.00108	-0.00678	0.04236

D25	-1.29943	-0.00010	-0.21762	-0.13018	-0.34780	-1.64723
D26	1.72031	-0.00016	-0.21805	-0.13240	-0.35045	1.36986
D27	1.88026	-0.00005	-0.02832	-0.01298	-0.04131	1.83895
D28	-2.28825	0.00002	-0.03429	-0.01499	-0.04929	-2.33753
D29	-0.25340	-0.00027	-0.03166	-0.01468	-0.04635	-0.29975
D30	-1.19275	-0.00009	-0.02002	-0.01746	-0.03748	-1.23023
D31	0.92193	-0.00002	-0.02599	-0.01947	-0.04546	0.87647
D32	2.95678	-0.00030	-0.02336	-0.01916	-0.04252	2.91426
D33	-1.25559	0.00096	0.10387	0.02778	0.13166	-1.12393
D34	0.81603	0.00047	0.09209	0.02469	0.11679	0.93282
D35	3.00003	-0.00066	0.05898	0.01390	0.07288	3.07290
D36	2.93756	0.00109	0.10804	0.02805	0.13610	3.07366
D37	-1.27400	0.00060	0.09626	0.02496	0.12123	-1.15278
D38	0.90999	-0.00053	0.06315	0.01417	0.07731	0.98731
D39	0.84763	0.00083	0.10467	0.02700	0.13168	0.97931
D40	2.91925	0.00034	0.09289	0.02391	0.11680	3.03606
D41	-1.17994	-0.00078	0.05978	0.01312	0.07289	-1.10705
D42	3.05411	-0.00104	-0.37720	-0.11930	-0.49645	2.55766
D43	-1.21411	-0.00047	-0.32237	-0.10313	-0.42554	-1.63965
D44	1.00642	-0.00091	-0.40148	-0.12752	-0.52893	0.47749
D45	3.02138	-0.00034	-0.34665	-0.11135	-0.45802	2.56336
D46	-1.10325	-0.00095	-0.40066	-0.12697	-0.52762	-1.63087
D47	0.91171	-0.00038	-0.34583	-0.11080	-0.45671	0.45501
D48	-3.12566	-0.00013	-0.00244	-0.00125	-0.00369	-3.12935
D49	0.01770	-0.00006	-0.00273	-0.00109	-0.00382	0.01388
D50	0.01071	-0.00003	-0.00291	-0.00160	-0.00451	0.00620
D51	-3.12912	0.00003	-0.00321	-0.00144	-0.00464	-3.13376

Item	Value	Threshold	Converged?
Maximum Force	0.001643	0.000450	NO
RMS Force	0.000477	0.000300	NO
Maximum Displacement	0.865790	0.001800	NO
RMS Displacement	0.134473	0.001200	NO

Predicted change in Energy=-1.246750D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.842172	-2.029501	0.336228
2	6	0	-2.830432	-1.132718	0.085140
3	7	0	-2.225175	0.117492	0.012641
4	6	0	-0.903478	-0.026360	0.221014

5	7	0	-0.652529	-1.321768	0.416897
6	6	0	0.706076	-1.872786	0.601070
7	6	0	1.524717	-1.829713	-0.699703
8	1	0	-1.882970	-3.097411	0.464659
9	1	0	-3.886745	-1.278000	-0.049342
10	1	0	1.202978	-1.278857	1.368939
11	1	0	0.602301	-2.893825	0.968114
12	1	0	1.056494	-2.483231	-1.442556
13	1	0	1.509940	-0.803845	-1.086394
14	35	0	1.396815	2.131886	-0.543764
15	1	0	-0.134556	0.780357	0.134623
16	6	0	-2.812854	1.387485	-0.250520
17	6	0	-4.118488	1.606161	-0.333043
18	1	0	-2.062126	2.158791	-0.381672
19	1	0	-4.472243	2.604891	-0.548423
20	1	0	-4.865598	0.834579	-0.194522
21	7	0	2.877623	-2.303129	-0.405218
22	1	0	3.275568	-2.802513	-1.190744
23	1	0	3.492378	-1.523068	-0.198139

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357911	0.000000			
3	N	2.204764	1.390906	0.000000		
4	C	2.215174	2.226127	1.345733	0.000000	
5	N	1.386594	2.211122	2.169818	1.333951	0.000000
6	C	2.566762	3.649763	3.591613	2.478788	1.477615
7	C	3.528315	4.479855	4.284942	3.161634	2.499040
8	H	1.076378	2.213987	3.264511	3.232665	2.160827
9	H	2.212171	1.074704	2.170727	3.246471	3.267942
10	H	3.301953	4.235314	3.942280	2.706221	2.085937
11	H	2.668667	3.957877	4.239762	3.323836	2.085618
12	H	3.431065	4.389297	4.432912	3.556004	2.779806
13	H	3.842231	4.507713	4.000978	2.852785	2.684101
14	Br	5.346266	5.377990	4.181648	3.245652	4.129214
15	H	3.294222	3.306063	2.196578	1.117809	2.183324
16	C	3.600318	2.542519	1.423903	2.422193	3.528810
17	C	4.341380	3.055393	2.433160	3.648068	4.598701
18	H	4.255062	3.412073	2.085418	2.545699	3.839136
19	H	5.401618	4.131183	3.398714	4.500178	5.562437
20	H	4.198305	2.844358	2.743896	4.075817	4.772171
21	N	4.785507	5.847410	5.663265	4.457866	3.755119
22	H	5.396336	6.457501	6.342928	5.211958	4.495226

23	H	5.385113	6.341178	5.951998	4.662550	4.195122
		6	7	8	9	10
6	C	0.000000				
7	C	1.537543	0.000000			
8	H	2.867311	3.817738	0.000000		
9	H	4.676623	5.478255	2.754917	0.000000	
10	H	1.090543	2.164771	3.694311	5.283635	0.000000
11	H	1.089960	2.182842	2.543911	4.878282	1.769066
12	H	2.161445	1.094600	3.557406	5.275342	3.062103
13	H	2.153222	1.096427	4.379275	5.515841	2.519627
14	Br	4.221985	3.966729	6.254555	6.307755	3.915249
15	H	2.821950	3.203397	4.266493	4.283643	2.748253
16	C	4.872108	5.419100	4.635780	2.880716	5.085168
17	C	6.020968	6.617056	5.268535	2.907331	6.287930
18	H	4.988219	5.373523	5.326916	3.905280	5.054005
19	H	6.941607	7.460035	6.344046	3.958375	7.139181
20	H	6.245506	6.941886	4.979070	2.332857	6.613519
21	N	2.431754	1.463284	4.904163	6.850855	2.645978
22	H	3.267611	2.062266	5.425665	7.411185	3.628930
23	H	2.919678	2.053603	5.640232	7.384690	2.785089
		11	12	13	14	15
11	H	0.000000				
12	H	2.487210	0.000000			
13	H	3.068034	1.775613	0.000000		
14	Br	5.307994	4.714122	2.987601	0.000000	
15	H	3.838917	3.815377	2.589391	2.152194	0.000000
16	C	5.610523	5.601361	4.918044	4.285025	2.773124
17	C	6.650469	6.688392	6.168863	5.544309	4.095409
18	H	5.869414	5.692067	4.693985	3.462841	2.425317
19	H	7.634577	7.566729	6.906186	5.888090	4.755103
20	H	6.719423	6.901929	6.642843	6.404904	4.742788
21	N	2.722509	2.103573	2.140657	4.677750	4.344254
22	H	3.437348	2.256023	2.668895	5.319453	5.120791
23	H	3.404654	2.898968	2.288305	4.227236	4.309426
		16	17	18	19	20
16	C	0.000000				
17	C	1.326390	0.000000			
18	H	1.084300	2.129881	0.000000		
19	H	2.079518	1.081200	2.456721	0.000000	
20	H	2.126641	1.082913	3.106127	1.847696	0.000000
21	N	6.784253	8.014570	6.656606	8.839101	8.357457
22	H	7.450435	8.651250	7.332128	9.470014	8.972150
23	H	6.944783	8.230161	6.666504	8.977635	8.684140
		21	22	23		

21 N 0.000000

22 H 1.012322 0.000000

23 H 1.014544 1.633784 0.000000

Stoichiometry C7H12BrN3

Framework group C1[X(C7H12BrN3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.570829	2.314836	-0.096565
2	6	0	-2.588869	1.442851	0.120597
3	7	0	-2.056868	0.165615	-0.021743
4	6	0	-0.749427	0.270069	-0.322886
5	7	0	-0.436461	1.565917	-0.370378
6	6	0	0.934351	2.068272	-0.598105
7	6	0	1.848887	1.810550	0.610713
8	1	0	-1.556664	3.391019	-0.081719
9	1	0	-3.620502	1.621242	0.363290
10	1	0	1.332143	1.558587	-1.476324
11	1	0	0.864187	3.133179	-0.819608
12	1	0	1.481281	2.381135	1.469461
13	1	0	1.802344	0.744138	0.861218
14	35	0	1.468609	-2.083086	-0.044974
15	1	0	-0.026531	-0.578244	-0.408218
16	6	0	-2.698041	-1.097319	0.124520
17	6	0	-4.003969	-1.259764	0.290276
18	1	0	-1.987566	-1.915677	0.089556
19	1	0	-4.399667	-2.259473	0.404282
20	1	0	-4.711409	-0.440326	0.317685
21	7	0	3.200615	2.251166	0.264465
22	1	0	3.688873	2.620332	1.070763
23	1	0	3.748588	1.476242	-0.094030

Rotational constants (GHZ): 0.7033873 0.5291748 0.3101740

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 365 symmetry adapted cartesian basis functions of A symmetry.

There are 352 symmetry adapted basis functions of A symmetry.

352 basis functions, 562 primitive gaussians, 365 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 833.9714255529 Hartrees.
NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 352 RedAO= T EigKep= 4.90D-06 NBF= 352
NBsUse= 352 1.00D-06 EigRej= -1.00D+00 NBFU= 352
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999883 0.002401 0.001252 -0.015066 Ang= 1.75 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3012.46654145 A.U. after 13 cycles
NFock= 13 Conv=0.29D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000052422	-0.000034149	-0.000265362
2	6	0.000032488	0.000029799	0.000043062
3	7	-0.000125844	0.000171999	0.000101932
4	6	0.000326581	-0.000259241	-0.000317907
5	7	0.000107586	0.000377611	0.000283466
6	6	0.000143480	-0.000163628	0.000171292
7	6	0.000008898	0.000684373	-0.000379259

8	1	0.000029074	-0.000010823	-0.000038585
9	1	0.000009032	-0.000003475	0.000006077
10	1	-0.000065485	-0.000020933	0.000035466
11	1	0.000253554	0.000005417	-0.000025452
12	1	0.000415198	-0.000161504	0.000515217
13	1	-0.000533426	0.000057635	-0.000437488
14	35	0.000110264	-0.000274216	0.000000077
15	1	-0.000380977	0.000236213	0.000123498
16	6	0.000058411	-0.000103904	0.000097655
17	6	-0.000006634	0.000050676	-0.000013342
18	1	-0.000051211	-0.000025539	-0.000052155
19	1	-0.000004648	-0.000008399	-0.000005068
20	1	0.000000533	0.000004276	-0.000003616
21	7	-0.000179620	-0.001143357	-0.000137271
22	1	-0.000055243	0.000443820	-0.000051245
23	1	-0.000144430	0.000147347	0.000349008

Cartesian Forces: Max 0.001143357 RMS 0.000252831

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000574193 RMS 0.000180033
Search for a local minimum.
Step number 14 out of a maximum of 121
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 9 11 12 13 14
DE= -7.53D-04 DEPred=-1.25D-03 R= 6.04D-01
TightC=F SS= 1.41D+00 RLast= 1.34D+00 DXNew= 1.2613D+00 4.0107D+00
Trust test= 6.04D-01 RLast= 1.34D+00 DXMaxT set to 1.26D+00
ITU= 1 -1 1 -1 1 1 1 1 1 1 0 1 0 0

Eigenvalues ---	0.00113	0.00246	0.00402	0.00840	0.01379
Eigenvalues ---	0.01484	0.01877	0.02100	0.02261	0.02327
Eigenvalues ---	0.02394	0.02810	0.03062	0.03063	0.03488
Eigenvalues ---	0.03818	0.04048	0.04585	0.04695	0.05350
Eigenvalues ---	0.05710	0.09251	0.09693	0.12641	0.12999
Eigenvalues ---	0.14847	0.15926	0.15994	0.16000	0.16001
Eigenvalues ---	0.16006	0.16123	0.17922	0.20896	0.21903
Eigenvalues ---	0.22108	0.22904	0.23562	0.24255	0.25043
Eigenvalues ---	0.28476	0.31285	0.34071	0.34627	0.34794
Eigenvalues ---	0.34822	0.35068	0.35683	0.35690	0.35858

Eigenvalues --- 0.36437 0.36658 0.39051 0.41891 0.42225
Eigenvalues --- 0.43330 0.47137 0.47694 0.48383 0.50489
Eigenvalues --- 0.54352 0.60332 0.60540
En-DIIS/RFO-DIIS IScMMF= 0 using points: 14 13 12 11 10
RFO step: Lambda=-1.50451589D-05.
DidBck=F Rises=F RFO-DIIS coefs: 1.80490 0.21513 -2.25436 1.33981 -0.10548
Iteration 1 RMS(Cart)= 0.02162598 RMS(Int)= 0.00094964
Iteration 2 RMS(Cart)= 0.00102901 RMS(Int)= 0.00009421
Iteration 3 RMS(Cart)= 0.00000885 RMS(Int)= 0.00009409
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00009409

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56608	0.00009	-0.00004	-0.00005	-0.00009	2.56599
R2	2.62028	-0.00006	-0.00001	-0.00008	-0.00009	2.62019
R3	2.03406	0.00000	-0.00002	0.00000	-0.00002	2.03404
R4	2.62843	0.00004	0.00000	-0.00002	-0.00003	2.62840
R5	2.03090	-0.00001	-0.00001	0.00001	0.00000	2.03089
R6	2.54307	0.00003	0.00045	0.00029	0.00074	2.54381
R7	2.69079	-0.00007	-0.00037	-0.00030	-0.00067	2.69012
R8	2.52080	-0.00026	-0.00035	-0.00013	-0.00048	2.52033
R9	2.11235	-0.00022	0.00020	-0.00057	-0.00037	2.11198
R10	2.79229	-0.00008	0.00000	0.00007	0.00007	2.79236
R11	2.90553	-0.00015	0.00006	-0.00059	-0.00053	2.90501
R12	2.06083	-0.00002	-0.00006	-0.00009	-0.00015	2.06068
R13	2.05973	-0.00004	0.00000	0.00011	0.00011	2.05983
R14	2.06849	-0.00043	-0.00009	0.00004	-0.00005	2.06845
R15	2.07195	0.00021	-0.00027	0.00005	-0.00023	2.07172
R16	2.76521	-0.00014	-0.00021	-0.00043	-0.00064	2.76457
R17	4.06706	-0.00009	0.00268	-0.00030	0.00238	4.06944
R18	2.50651	0.00002	0.00005	0.00001	0.00006	2.50657
R19	2.04903	-0.00005	-0.00024	-0.00024	-0.00048	2.04855
R20	2.04317	0.00000	-0.00001	0.00000	-0.00002	2.04316
R21	2.04641	-0.00001	-0.00002	-0.00004	-0.00006	2.04635
R22	1.91301	-0.00020	-0.00034	0.00001	-0.00033	1.91268
R23	1.91721	0.00010	-0.00018	0.00010	-0.00008	1.91713
A1	1.87348	-0.00006	-0.00001	0.00019	0.00019	1.87367
A2	2.27798	0.00005	0.00031	0.00000	0.00030	2.27828
A3	2.13173	0.00001	-0.00030	-0.00019	-0.00049	2.13124
A4	1.86142	0.00003	-0.00003	-0.00002	-0.00004	1.86138
A5	2.27731	-0.00002	-0.00007	0.00002	-0.00005	2.27726
A6	2.14444	-0.00001	0.00009	-0.00001	0.00008	2.14452
A7	1.89993	-0.00014	-0.00003	-0.00018	-0.00020	1.89973
A8	2.25457	0.00007	-0.00031	-0.00042	-0.00073	2.25384

A9	2.12858	0.00006	0.00032	0.00061	0.00093	2.12952
A10	1.88737	0.00012	-0.00014	0.00015	0.00002	1.88739
A11	2.19751	0.00033	0.00138	0.00217	0.00353	2.20104
A12	2.19295	-0.00044	-0.00061	-0.00278	-0.00340	2.18954
A13	1.90257	0.00005	0.00019	-0.00017	0.00002	1.90259
A14	2.22153	0.00030	-0.00034	-0.00022	-0.00060	2.22093
A15	2.15725	-0.00036	0.00013	0.00037	0.00046	2.15771
A16	1.95374	-0.00055	-0.00069	-0.00071	-0.00140	1.95235
A17	1.87928	-0.00002	-0.00031	-0.00051	-0.00081	1.87847
A18	1.87944	0.00048	0.00009	0.00085	0.00093	1.88037
A19	1.91540	0.00026	0.00086	-0.00058	0.00028	1.91569
A20	1.94103	-0.00006	0.00030	0.00015	0.00046	1.94148
A21	1.89278	-0.00010	-0.00030	0.00085	0.00056	1.89334
A22	1.90675	0.00026	-0.00020	-0.00009	-0.00002	1.90673
A23	1.89379	-0.00003	-0.00064	-0.00133	-0.00188	1.89191
A24	1.88909	-0.00052	0.00027	-0.00034	0.00011	1.88921
A25	1.88967	-0.00009	0.00059	0.00018	0.00063	1.89031
A26	1.91655	-0.00019	0.00117	-0.00018	0.00106	1.91762
A27	1.96725	0.00057	-0.00162	0.00170	0.00004	1.96729
A28	2.88408	-0.00048	-0.00514	-0.00489	-0.01002	2.87405
A29	2.17100	0.00008	0.00051	0.00035	0.00086	2.17186
A30	1.95094	-0.00001	0.00022	0.00035	0.00058	1.95152
A31	2.16124	-0.00007	-0.00074	-0.00070	-0.00144	2.15980
A32	2.07916	0.00000	0.00002	0.00011	0.00013	2.07930
A33	2.15758	0.00000	0.00006	-0.00012	-0.00006	2.15752
A34	2.04644	-0.00001	-0.00008	0.00001	-0.00007	2.04637
A35	1.94645	-0.00019	0.00193	-0.00071	0.00154	1.94799
A36	1.93110	-0.00022	0.00008	-0.00020	0.00021	1.93130
A37	1.87494	0.00015	0.00076	0.00073	0.00210	1.87705
D1	0.00235	0.00007	0.00171	-0.00185	-0.00013	0.00222
D2	3.13804	0.00002	0.00008	-0.00164	-0.00156	3.13648
D3	-3.14142	0.00004	0.00177	0.00068	0.00247	-3.13894
D4	-0.00572	0.00000	0.00015	0.00089	0.00104	-0.00468
D5	0.00019	-0.00010	-0.00398	0.00453	0.00054	0.00074
D6	-3.07762	0.00001	-0.00253	0.00489	0.00240	-3.07522
D7	-3.13945	-0.00008	-0.00405	0.00227	-0.00179	-3.14124
D8	0.06592	0.00004	-0.00260	0.00262	0.00007	0.06599
D9	-0.00409	-0.00002	0.00111	-0.00142	-0.00033	-0.00441
D10	3.12271	-0.00004	-0.00044	-0.00018	-0.00063	3.12208
D11	-3.14034	0.00003	0.00258	-0.00161	0.00097	-3.13937
D12	-0.01354	0.00000	0.00103	-0.00037	0.00067	-0.01288
D13	0.00424	-0.00005	-0.00360	0.00426	0.00067	0.00491
D14	3.03945	-0.00005	0.00248	-0.00049	0.00196	3.04141
D15	-3.12383	-0.00002	-0.00218	0.00313	0.00096	-3.12286

D16	-0.08862	-0.00002	0.00390	-0.00161	0.00225	-0.08637
D17	0.13696	0.00001	-0.00341	-0.00117	-0.00458	0.13237
D18	-2.99923	0.00005	-0.00179	-0.00223	-0.00402	-3.00325
D19	-3.02114	-0.00002	-0.00514	0.00021	-0.00493	-3.02608
D20	0.12586	0.00001	-0.00352	-0.00085	-0.00438	0.12148
D21	-0.00276	0.00009	0.00468	-0.00543	-0.00075	-0.00351
D22	3.07791	0.00001	0.00315	-0.00579	-0.00257	3.07534
D23	-3.03831	0.00003	-0.00142	-0.00108	-0.00256	-3.04087
D24	0.04236	-0.00005	-0.00295	-0.00144	-0.00438	0.03798
D25	-1.64723	-0.00015	-0.08371	-0.06432	-0.14804	-1.79527
D26	1.36986	-0.00011	-0.07662	-0.06962	-0.14623	1.22363
D27	1.83895	-0.00012	-0.01312	-0.01291	-0.02602	1.81293
D28	-2.33753	-0.00015	-0.01268	-0.01439	-0.02706	-2.36459
D29	-0.29975	-0.00003	-0.01313	-0.01322	-0.02634	-0.32609
D30	-1.23023	-0.00001	-0.01140	-0.01249	-0.02389	-1.25412
D31	0.87647	-0.00004	-0.01095	-0.01397	-0.02492	0.85155
D32	2.91426	0.00008	-0.01141	-0.01280	-0.02421	2.89004
D33	-1.12393	-0.00035	0.00634	-0.00801	-0.00168	-1.12560
D34	0.93282	-0.00032	0.00660	-0.00860	-0.00200	0.93082
D35	3.07290	0.00004	0.00454	-0.00755	-0.00301	3.06989
D36	3.07366	-0.00014	0.00658	-0.00653	0.00005	3.07371
D37	-1.15278	-0.00012	0.00684	-0.00712	-0.00028	-1.15305
D38	0.98731	0.00024	0.00477	-0.00607	-0.00129	0.98602
D39	0.97931	-0.00015	0.00619	-0.00731	-0.00112	0.97818
D40	3.03606	-0.00013	0.00645	-0.00790	-0.00145	3.03461
D41	-1.10705	0.00023	0.00439	-0.00685	-0.00246	-1.10951
D42	2.55766	0.00024	-0.00401	-0.00388	-0.00780	2.54985
D43	-1.63965	0.00015	-0.00021	-0.00356	-0.00400	-1.64366
D44	0.47749	0.00034	-0.00532	-0.00347	-0.00847	0.46902
D45	2.56336	0.00026	-0.00152	-0.00315	-0.00466	2.55869
D46	-1.63087	0.00021	-0.00540	-0.00472	-0.01005	-1.64092
D47	0.45501	0.00012	-0.00160	-0.00439	-0.00625	0.44876
D48	-3.12935	0.00002	0.00066	-0.00115	-0.00049	-3.12984
D49	0.01388	0.00001	0.00052	-0.00069	-0.00017	0.01371
D50	0.00620	-0.00001	-0.00115	0.00005	-0.00110	0.00510
D51	-3.13376	-0.00002	-0.00129	0.00051	-0.00078	-3.13454

Item	Value	Threshold	Converged?
Maximum Force	0.000574	0.000450	NO
RMS Force	0.000180	0.000300	YES
Maximum Displacement	0.106271	0.001800	NO
RMS Displacement	0.022116	0.001200	NO

Predicted change in Energy=-1.359103D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.835900	-2.024965	0.331366
2	6	0	-2.827558	-1.132083	0.080044
3	7	0	-2.228156	0.121333	0.014917
4	6	0	-0.906296	-0.017173	0.228348
5	7	0	-0.649966	-1.311993	0.419367
6	6	0	0.710530	-1.858348	0.603779
7	6	0	1.518135	-1.836889	-0.704081
8	1	0	-1.871321	-3.093805	0.453415
9	1	0	-3.882435	-1.282200	-0.060265
10	1	0	1.211779	-1.249205	1.356645
11	1	0	0.611457	-2.872789	0.990080
12	1	0	1.045652	-2.505136	-1.430922
13	1	0	1.495823	-0.817890	-1.107856
14	35	0	1.453051	2.088718	-0.497833
15	1	0	-0.138371	0.791144	0.151040
16	6	0	-2.821694	1.388634	-0.246142
17	6	0	-4.127817	1.600443	-0.338696
18	1	0	-2.075527	2.165621	-0.367313
19	1	0	-4.485508	2.598394	-0.551124
20	1	0	-4.871635	0.823870	-0.211032
21	7	0	2.875013	-2.299324	-0.412114
22	1	0	3.266926	-2.818360	-1.187645
23	1	0	3.489342	-1.513083	-0.228694

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357861	0.000000			
3	N	2.204677	1.390890	0.000000		
4	C	2.214951	2.226268	1.346124	0.000000	
5	N	1.386547	2.211203	2.169951	1.333700	0.000000
6	C	2.566375	3.649634	3.591903	2.478911	1.477654
7	C	3.515263	4.471762	4.287923	3.171538	2.497661
8	H	1.076368	2.214080	3.264463	3.232274	2.160490
9	H	2.212098	1.074703	2.170759	3.246690	3.267995
10	H	3.307772	4.237886	3.938498	2.697629	2.085312
11	H	2.672502	3.960436	4.240178	3.322402	2.086380
12	H	3.411680	4.378361	4.439212	3.571167	2.778899
13	H	3.824758	4.494603	4.001347	2.863000	2.679732

14	Br	5.331713	5.388053	4.205330	3.244786	4.102289
15	H	3.293113	3.306897	2.198722	1.117614	2.181035
16	C	3.599717	2.541741	1.423549	2.422846	3.528837
17	C	4.341134	3.054949	2.433418	3.649167	4.599173
18	H	4.255184	3.411822	2.085308	2.546862	3.839908
19	H	5.401357	4.130814	3.398805	4.501058	5.562766
20	H	4.198302	2.844068	2.744557	4.077293	4.773029
21	N	4.777106	5.841575	5.664298	4.462814	3.753886
22	H	5.382909	6.449287	6.346958	5.221826	4.493737
23	H	5.379023	6.335906	5.951507	4.665647	4.194554

		6	7	8	9	10
6	C	0.000000				
7	C	1.537265	0.000000			
8	H	2.866168	3.795793	0.000000		
9	H	4.676348	5.467023	2.755061	0.000000	
10	H	1.090465	2.164675	3.704575	5.287697	0.000000
11	H	1.090016	2.182964	2.549714	4.881420	1.769402
12	H	2.161168	1.094574	3.522213	5.259307	3.061942
13	H	2.151495	1.096308	4.353736	5.498972	2.518031
14	Br	4.164638	3.931560	6.230157	6.326292	3.826099
15	H	2.818760	3.222080	4.264665	4.285023	2.727529
16	C	4.872562	5.426585	4.635175	2.879770	5.078979
17	C	6.021719	6.620085	5.268318	2.906435	6.285377
18	H	4.989736	5.389611	5.326993	3.904698	5.043755
19	H	6.942273	7.465846	6.343832	3.957732	7.134612
20	H	6.246501	6.939157	4.979111	2.331689	6.615375
21	N	2.431354	1.462945	4.889583	6.842620	2.645299
22	H	3.265882	2.062860	5.400975	7.398928	3.627574
23	H	2.921303	2.053411	5.630333	7.377314	2.787512

		11	12	13	14	15
11	H	0.000000				
12	H	2.486954	0.000000			
13	H	3.066928	1.775901	0.000000		
14	Br	5.247734	4.705329	2.970240	0.000000	
15	H	3.832836	3.843172	2.616180	2.153453	0.000000
16	C	5.610214	5.614402	4.924658	4.338999	2.777583
17	C	6.651027	6.694289	6.169706	5.604448	4.100060
18	H	5.869240	5.717429	4.712143	3.531829	2.431143
19	H	7.634671	7.577188	6.910663	5.960629	4.759915
20	H	6.721031	6.898166	6.636580	6.456296	4.747205
21	N	2.723728	2.104018	2.140296	4.613484	4.353001
22	H	3.434671	2.256403	2.673023	5.276874	5.139712
23	H	3.408288	2.898472	2.286993	4.146310	4.314389

		16	17	18	19	20

16	C	0.000000				
17	C	1.326419	0.000000			
18	H	1.084046	2.128882	0.000000		
19	H	2.079618	1.081191	2.455420	0.000000	
20	H	2.126606	1.082880	3.105308	1.847618	0.000000
21	N	6.788302	8.015810	6.666753	8.842185	8.354958
22	H	7.460330	8.656140	7.352199	9.478745	8.969715
23	H	6.946181	8.229657	6.672320	8.978108	8.681451

		21	22	23
21	N	0.000000		
22	H	1.012148	0.000000	
23	H	1.014503	1.634871	0.000000

Stoichiometry C7H12BrN3
Framework group C1[X(C7H12BrN3)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.601736	2.280835	-0.111181
2	6	0	-2.615796	1.405511	0.110802
3	7	0	-2.077597	0.129943	-0.022772
4	6	0	-0.770143	0.238979	-0.323979
5	7	0	-0.463464	1.535773	-0.379012
6	6	0	0.905346	2.044043	-0.605901
7	6	0	1.806622	1.828511	0.620651
8	1	0	-1.591907	3.357115	-0.101438
9	1	0	-3.648197	1.580634	0.352603
10	1	0	1.317157	1.511997	-1.464070
11	1	0	0.829205	3.101525	-0.859020
12	1	0	1.424507	2.421176	1.457806
13	1	0	1.762956	0.769370	0.900301
14	35	0	1.527070	-2.035833	-0.047076
15	1	0	-0.040607	-0.603709	-0.405920
16	6	0	-2.713449	-1.134264	0.132035
17	6	0	-4.018017	-1.301760	0.303602
18	1	0	-2.000702	-1.950387	0.098994
19	1	0	-4.408965	-2.302645	0.423448
20	1	0	-4.728932	-0.485346	0.329978
21	7	0	3.159504	2.266955	0.277597

```
      22                1                0            3.634311       2.670003       1.075439
      23                1                0            3.717643       1.484576      -0.047335
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.7183347           0.5217128           0.3106827
 Standard basis: 6-311++G(d,p) (5D, 7F)
 There are     365 symmetry adapted cartesian basis functions of A      symmetry.
 There are     352 symmetry adapted basis functions of A      symmetry.
    352 basis functions,      562 primitive gaussians,      365 cartesian basis functions
     55 alpha electrons              55 beta electrons
          nuclear repulsion energy             834.6554530488 Hartrees.
 NAtoms=       23 NActive=       23 NUniq=       23 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      352 RedAO= T EigKep=    4.86D-06    NBF=      352
 NBsUse=      352 1.00D-06 EigRej= -1.00D+00 NBFU=      352
 Initial guess from the checkpoint file:    "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"
 B after Tr=          0.000000        0.000000        0.000000
             Rot=        0.999966        0.000900        0.000542      -0.008205 Ang=      0.95 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn=                5 AccDes=
0.00D+00
 Harris functional with IExCor=    402 and IRadAn=             5 diagonalized for initial guess.
 HarFok:    IExCor=    402 AccDes= 0.00D+00 IRadAn=                5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=    3500011 ScaDFX=    1.000000    1.000000    1.000000    1.000000
 FoFCou: FMM=F IPFlag=                  0 FMFlag=           100000 FMFlg1=                  0
             NFxFlg=                    0 DoJE=T BraDBF=F KetDBF=T FulRan=T
             wScrn=      0.000000  ICntrl=             500  IOpCl=      0  I1Cent=        200000004  NGrid=
0
             NMat0=         1 NMatS0=            1 NMatT0=         0 NMatD0=         1 NMtDS0=         0
NMtDT0=         0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                       energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3012.46658827          A.U. after      11 cycles
                  NFock= 11    Conv=0.58D-08         -V/T= 2.0017
 Calling FoFJK, ICntrl=             2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 ---------------------------------------------------------------------
 Center          Atomic                                Forces (Hartrees/Bohr)
```

Number	Number	X	Y	Z
1	6	0.000119574	-0.000026272	-0.000413183
2	6	-0.000016639	-0.000049986	-0.000047838
3	7	-0.000036454	0.000078474	0.000137653
4	6	-0.000023705	0.000061903	-0.000382288
5	7	-0.000046601	0.000313255	0.000527431
6	6	0.000192894	-0.000108115	0.000261372
7	6	0.000021922	0.000657118	-0.000431830
8	1	-0.000014238	-0.000009843	0.000028337
9	1	-0.000000762	-0.000000455	0.000051053
10	1	-0.000016979	0.000038406	-0.000086424
11	1	0.000153272	0.000018219	-0.000024483
12	1	0.000452267	-0.000263082	0.000450662
13	1	-0.000384530	0.000054241	-0.000382737
14	35	0.000169028	-0.000208802	0.000021188
15	1	-0.000119315	0.000023451	0.000061861
16	6	0.000048245	-0.000137092	0.000110935
17	6	-0.000017626	0.000070007	0.000017468
18	1	-0.000062292	-0.000005883	-0.000013139
19	1	-0.000003297	-0.000012973	-0.000026666
20	1	0.000011024	0.000001359	0.000004014
21	7	-0.000256142	-0.001192604	-0.000050088
22	1	-0.000010599	0.000492836	-0.000156784
23	1	-0.000159046	0.000205836	0.000343486

Cartesian Forces: Max 0.001192604 RMS 0.000251738

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000746046 RMS 0.000186026
Search for a local minimum.
Step number 15 out of a maximum of 121
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 9 11 12 14 15
DE= -4.68D-05 DEPred=-1.36D-06 R= 3.44D+01
TightC=F SS= 1.41D+00 RLast= 2.19D-01 DXNew= 2.1213D+00 6.5603D-01
Trust test= 3.44D+01 RLast= 2.19D-01 DXMaxT set to 1.26D+00
ITU= 1 1 -1 1 -1 1 1 1 1 1 0 1 0 0
Eigenvalues --- -0.02097 0.00001 0.00292 0.00461 0.01146

Eigenvalues --- 0.01396 0.01448 0.01953 0.02088 0.02320
Eigenvalues --- 0.02391 0.02650 0.03011 0.03062 0.03212
Eigenvalues --- 0.03720 0.03980 0.04248 0.04655 0.05294
Eigenvalues --- 0.05562 0.08304 0.09582 0.09687 0.12253
Eigenvalues --- 0.12676 0.15677 0.15920 0.15993 0.16000
Eigenvalues --- 0.16001 0.16041 0.16138 0.20146 0.21516
Eigenvalues --- 0.22043 0.22523 0.23251 0.23636 0.24925
Eigenvalues --- 0.27468 0.30523 0.34044 0.34470 0.34682
Eigenvalues --- 0.34796 0.35041 0.35660 0.35689 0.35858
Eigenvalues --- 0.36436 0.36657 0.37701 0.41677 0.42148
Eigenvalues --- 0.43047 0.46965 0.47669 0.48224 0.50146
Eigenvalues --- 0.54303 0.59704 0.60361
Eigenvalue 2 is 1.02D-05 Eigenvector:

	D25	D26	D46	D44	D42
1	0.65583	0.64819	0.13006	0.12328	0.11617
	D28	D29	D27	D31	D47
1	0.11410	0.11067	0.10951	0.10391	0.10199

Use linear search instead of GDIIS.
RFO step: Lambda=-2.09998255D-02 EMin=-2.09716951D-02
I= 1 Eig= -2.10D-02 Dot1= 4.61D-04
I= 1 Stepn= 6.00D-01 RXN= 6.00D-01 EDone=F
Mixed 1 eigenvectors in step. Raw Step.Grad= 4.61D-04.
RFO eigenvector is Hessian eigenvector with negative curvature.
Taking step of 6.00D-01 in eigenvector direction(s). Step.Grad= 3.15D-06.
Skip linear search -- no minimum in search direction.
Iteration 1 RMS(Cart)= 0.14618413 RMS(Int)= 0.00732718
Iteration 2 RMS(Cart)= 0.01304415 RMS(Int)= 0.00142140
Iteration 3 RMS(Cart)= 0.00010707 RMS(Int)= 0.00142034
Iteration 4 RMS(Cart)= 0.00000025 RMS(Int)= 0.00142034

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56599	0.00006	0.00000	-0.00424	-0.00404	2.56194
R2	2.62019	-0.00007	0.00000	-0.00296	-0.00287	2.61733
R3	2.03404	0.00001	0.00000	0.00191	0.00191	2.03595
R4	2.62840	0.00012	0.00000	0.01224	0.01234	2.64074
R5	2.03089	-0.00001	0.00000	0.00056	0.00056	2.03145
R6	2.54381	0.00001	0.00000	-0.00342	-0.00353	2.54027
R7	2.69012	-0.00008	0.00000	-0.00235	-0.00235	2.68776
R8	2.52033	-0.00023	0.00000	0.00660	0.00630	2.52663
R9	2.11198	-0.00011	0.00000	0.02910	0.02910	2.14108
R10	2.79236	0.00002	0.00000	0.02804	0.02804	2.82040
R11	2.90501	0.00001	0.00000	0.04450	0.04450	2.94951
R12	2.06068	-0.00005	0.00000	-0.00712	-0.00712	2.05356
R13	2.05983	-0.00004	0.00000	-0.00055	-0.00055	2.05928

R14	2.06845	-0.00034	0.00000	0.01023	0.01023	2.07867
R15	2.07172	0.00020	0.00000	-0.00018	-0.00018	2.07155
R16	2.76457	-0.00021	0.00000	0.02132	0.02132	2.78588
R17	4.06944	-0.00001	0.00000	0.15550	0.15550	4.22493
R18	2.50657	0.00002	0.00000	0.00047	0.00047	2.50704
R19	2.04855	-0.00004	0.00000	-0.00085	-0.00085	2.04770
R20	2.04316	0.00000	0.00000	-0.00039	-0.00039	2.04277
R21	2.04635	-0.00001	0.00000	-0.00063	-0.00063	2.04572
R22	1.91268	-0.00014	0.00000	0.00789	0.00789	1.92057
R23	1.91713	0.00013	0.00000	0.00484	0.00484	1.92197
A1	1.87367	-0.00007	0.00000	-0.00530	-0.00622	1.86745
A2	2.27828	0.00003	0.00000	-0.01195	-0.01379	2.26448
A3	2.13124	0.00005	0.00000	0.01729	0.01504	2.14627
A4	1.86138	0.00001	0.00000	-0.00281	-0.00285	1.85853
A5	2.27726	-0.00001	0.00000	0.00078	-0.00045	2.27681
A6	2.14452	0.00000	0.00000	0.00250	0.00137	2.14589
A7	1.89973	-0.00011	0.00000	0.00940	0.00935	1.90908
A8	2.25384	0.00001	0.00000	-0.02059	-0.02149	2.23235
A9	2.12952	0.00010	0.00000	0.01199	0.01127	2.14079
A10	1.88739	0.00007	0.00000	-0.01640	-0.01723	1.87016
A11	2.20104	0.00069	0.00000	0.15708	0.15670	2.35774
A12	2.18954	-0.00075	0.00000	-0.13381	-0.13488	2.05466
A13	1.90259	0.00010	0.00000	0.01529	0.01541	1.91800
A14	2.22093	0.00035	0.00000	0.01414	0.01375	2.23468
A15	2.15771	-0.00046	0.00000	-0.03030	-0.03017	2.12754
A16	1.95235	-0.00028	0.00000	0.09461	0.09502	2.04737
A17	1.87847	-0.00006	0.00000	-0.01247	-0.01038	1.86809
A18	1.88037	0.00032	0.00000	-0.04992	-0.05133	1.82904
A19	1.91569	0.00010	0.00000	-0.08274	-0.08189	1.83380
A20	1.94148	-0.00006	0.00000	0.01305	0.01314	1.95462
A21	1.89334	-0.00002	0.00000	0.03662	0.03624	1.92957
A22	1.90673	0.00032	0.00000	0.05406	0.05403	1.96076
A23	1.89191	-0.00003	0.00000	-0.01428	-0.01485	1.87706
A24	1.88921	-0.00047	0.00000	0.01444	0.01421	1.90342
A25	1.89031	-0.00004	0.00000	0.04097	0.03972	1.93003
A26	1.91762	-0.00024	0.00000	-0.02996	-0.03076	1.88686
A27	1.96729	0.00046	0.00000	-0.06171	-0.06217	1.90512
A28	2.87405	-0.00043	0.00000	0.00139	0.00139	2.87544
A29	2.17186	0.00006	0.00000	-0.00668	-0.00679	2.16506
A30	1.95152	0.00002	0.00000	0.01002	0.00992	1.96143
A31	2.15980	-0.00007	0.00000	-0.00320	-0.00330	2.15650
A32	2.07930	0.00001	0.00000	0.00487	0.00477	2.08406
A33	2.15752	-0.00001	0.00000	-0.00789	-0.00799	2.14953
A34	2.04637	0.00000	0.00000	0.00306	0.00296	2.04932

A35	1.94799	-0.00022	0.00000	-0.00109	-0.00173	1.94626
A36	1.93130	-0.00030	0.00000	-0.05181	-0.05251	1.87879
A37	1.87705	0.00016	0.00000	-0.03220	-0.03363	1.84342
D1	0.00222	0.00007	0.00000	0.02548	0.02414	0.02636
D2	3.13648	0.00008	0.00000	0.09937	0.09860	-3.04810
D3	-3.13894	-0.00001	0.00000	-0.08389	-0.08284	3.06140
D4	-0.00468	-0.00001	0.00000	-0.01001	-0.00838	-0.01306
D5	0.00074	-0.00013	0.00000	-0.05185	-0.05086	-0.05012
D6	-3.07522	0.00000	0.00000	-0.03605	-0.03410	-3.10932
D7	-3.14124	-0.00005	0.00000	0.04627	0.04715	-3.09409
D8	0.06599	0.00007	0.00000	0.06208	0.06391	0.12990
D9	-0.00441	0.00001	0.00000	0.00900	0.00987	0.00545
D10	3.12208	0.00000	0.00000	0.07037	0.07172	-3.08939
D11	-3.13937	0.00000	0.00000	-0.05791	-0.05764	3.08618
D12	-0.01288	-0.00001	0.00000	0.00346	0.00421	-0.00867
D13	0.00491	-0.00009	0.00000	-0.04143	-0.04106	-0.03615
D14	3.04141	-0.00007	0.00000	0.01695	0.02348	3.06489
D15	-3.12286	-0.00008	0.00000	-0.09723	-0.09868	3.06164
D16	-0.08637	-0.00006	0.00000	-0.03885	-0.03415	-0.12052
D17	0.13237	0.00001	0.00000	-0.03431	-0.03467	0.09770
D18	-3.00325	0.00002	0.00000	-0.06057	-0.06102	-3.06427
D19	-3.02608	-0.00001	0.00000	0.03412	0.03457	-2.99151
D20	0.12148	0.00001	0.00000	0.00786	0.00822	0.12970
D21	-0.00351	0.00013	0.00000	0.05753	0.05671	0.05320
D22	3.07534	0.00005	0.00000	0.04436	0.04303	3.11837
D23	-3.04087	0.00001	0.00000	-0.02231	-0.01517	-3.05604
D24	0.03798	-0.00007	0.00000	-0.03548	-0.02885	0.00912
D25	-1.79527	-0.00018	0.00000	-0.04848	-0.04827	-1.84355
D26	1.22363	-0.00009	0.00000	0.03084	0.03063	1.25426
D27	1.81293	-0.00010	0.00000	-0.08385	-0.08498	1.72795
D28	-2.36459	-0.00019	0.00000	-0.13690	-0.13715	-2.50174
D29	-0.32609	-0.00008	0.00000	-0.12635	-0.12600	-0.45209
D30	-1.25412	0.00001	0.00000	-0.06778	-0.06823	-1.32236
D31	0.85155	-0.00008	0.00000	-0.12084	-0.12040	0.73114
D32	2.89004	0.00004	0.00000	-0.11029	-0.10925	2.78079
D33	-1.12560	-0.00037	0.00000	-0.04972	-0.05087	-1.17647
D34	0.93082	-0.00025	0.00000	0.02152	0.02047	0.95129
D35	3.06989	0.00001	0.00000	-0.05331	-0.05472	3.01517
D36	3.07371	-0.00018	0.00000	-0.03965	-0.03890	3.03480
D37	-1.15305	-0.00006	0.00000	0.03159	0.03243	-1.12062
D38	0.98602	0.00020	0.00000	-0.04324	-0.04276	0.94326
D39	0.97818	-0.00019	0.00000	-0.03939	-0.03881	0.93937
D40	3.03461	-0.00007	0.00000	0.03186	0.03252	3.06713
D41	-1.10951	0.00019	0.00000	-0.04297	-0.04267	-1.15218

D42	2.54985	0.00033	0.00000	0.19057	0.18980	2.73965
D43	-1.64366	0.00019	0.00000	0.11441	0.11442	-1.52923
D44	0.46902	0.00036	0.00000	0.13383	0.13398	0.60300
D45	2.55869	0.00022	0.00000	0.05766	0.05861	2.61730
D46	-1.64092	0.00027	0.00000	0.14413	0.14356	-1.49735
D47	0.44876	0.00012	0.00000	0.06796	0.06819	0.51694
D48	-3.12984	0.00004	0.00000	0.01834	0.01838	-3.11146
D49	0.01371	0.00001	0.00000	-0.00938	-0.00934	0.00437
D50	0.00510	0.00002	0.00000	0.04770	0.04766	0.05275
D51	-3.13454	-0.00001	0.00000	0.01998	0.01994	-3.11460

Item	Value	Threshold	Converged?
Maximum Force	0.000746	0.000450	NO
RMS Force	0.000186	0.000300	YES
Maximum Displacement	0.632719	0.001800	NO
RMS Displacement	0.150223	0.001200	NO

Predicted change in Energy=-4.200008D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.886418	-1.998769	0.234614
2	6	0	-2.881027	-1.104032	0.015113
3	7	0	-2.275453	0.153580	-0.051832
4	6	0	-0.948509	0.019272	0.116102
5	7	0	-0.707679	-1.278065	0.331910
6	6	0	0.675837	-1.800623	0.532779
7	6	0	1.581267	-1.934404	-0.731511
8	1	0	-1.941397	-3.059800	0.413316
9	1	0	-3.945305	-1.244298	-0.041996
10	1	0	1.192554	-1.094173	1.176859
11	1	0	0.541745	-2.754939	1.041501
12	1	0	1.221138	-2.709822	-1.423613
13	1	0	1.604284	-0.956586	-1.226515
14	35	0	1.787872	1.833710	-0.508510
15	1	0	-0.060037	0.721446	0.080244
16	6	0	-2.904948	1.419242	-0.209253
17	6	0	-4.219260	1.599848	-0.212786
18	1	0	-2.189079	2.226882	-0.306380
19	1	0	-4.618196	2.592720	-0.366365
20	1	0	-4.928408	0.791030	-0.091006
21	7	0	2.946945	-2.295260	-0.309555

22	1	0	3.460588	-2.750448	-1.059147
23	1	0	3.449010	-1.431595	-0.118683

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.355722	0.000000			
3	N	2.205903	1.397422	0.000000		
4	C	2.228499	2.237551	1.344255	0.000000	
5	N	1.385030	2.203200	2.157495	1.337033	0.000000
6	C	2.587145	3.661215	3.587589	2.474699	1.492491
7	C	3.600331	4.599895	4.438010	3.306821	2.607857
8	H	1.077378	2.206014	3.264011	3.248823	2.168702
9	H	2.210147	1.075000	2.177743	3.256131	3.259320
10	H	3.344576	4.236013	3.885054	2.636118	2.087735
11	H	2.668115	3.936284	4.194218	3.282296	2.060518
12	H	3.593358	4.634247	4.723029	3.811305	2.975252
13	H	3.925054	4.656328	4.202941	3.044943	2.806637
14	Br	5.361020	5.541039	4.420634	3.342171	4.076423
15	H	3.280102	3.360743	2.290848	1.133013	2.116795
16	C	3.594054	2.533342	1.422303	2.427638	3.520840
17	C	4.311886	3.025520	2.428164	3.647492	4.572776
18	H	4.270878	3.417182	2.090654	2.567303	3.858318
19	H	5.376389	4.102348	3.396584	4.507994	5.546415
20	H	4.140376	2.791826	2.728745	4.059323	4.719595
21	N	4.872928	5.957322	5.773793	4.551132	3.847394
22	H	5.552415	6.639337	6.507705	5.337855	4.634371
23	H	5.377109	6.339918	5.940264	4.636628	4.183858

		6	7	8	9	10
6	C	0.000000				
7	C	1.560811	0.000000			
8	H	2.906839	3.871216	0.000000		
9	H	4.689863	5.612012	2.742079	0.000000	
10	H	1.086695	2.121076	3.777346	5.282588	0.000000
11	H	1.089724	2.213020	2.579448	4.856914	1.788859
12	H	2.225189	1.099986	3.674020	5.545156	3.061632
13	H	2.160909	1.096215	4.436712	5.681884	2.442265
14	Br	3.940721	3.780357	6.221226	6.523886	3.430360
15	H	2.665920	3.225890	4.236541	4.355961	2.463336
16	C	4.872388	5.625462	4.623618	2.864397	5.002808
17	C	6.006750	6.812205	5.224269	2.862410	6.202951
18	H	5.013255	5.631390	5.341190	3.899143	4.966371
19	H	6.938063	7.685150	6.302709	3.909055	7.052627
20	H	6.205912	7.086192	4.899538	2.260854	6.528986

21	N	2.472271	1.474225	5.000296	6.977049	2.594210
22	H	3.345330	2.074878	5.607610	7.625636	3.589839
23	H	2.872469	2.028999	5.656021	7.397084	2.623714

		11	12	13	14	15
11	H	0.000000				
12	H	2.557420	0.000000			
13	H	3.083336	1.805404	0.000000		
14	Br	5.001106	4.669291	2.887038	0.000000	
15	H	3.656694	3.959368	2.700625	2.235739	0.000000
16	C	5.555885	5.962250	5.197361	4.720582	2.943509
17	C	6.573019	7.045374	6.440239	6.018952	4.261055
18	H	5.838897	6.103182	5.036936	4.001447	2.636026
19	H	7.563368	7.958175	7.215033	6.452442	4.947519
20	H	6.616574	7.200606	6.857085	6.809546	4.871879
21	N	2.796721	2.095566	2.106087	4.293184	4.277196
22	H	3.596163	2.269277	2.586854	4.910772	5.074156
23	H	3.398450	2.880993	2.203619	3.684231	4.121719

		16	17	18	19	20
16	C	0.000000				
17	C	1.326668	0.000000			
18	H	1.083597	2.126868	0.000000		
19	H	2.082536	1.080987	2.457244	0.000000	
20	H	2.122033	1.082547	3.100319	1.848822	0.000000
21	N	6.931972	8.156944	6.843137	9.007050	8.461332
22	H	7.656937	8.866875	7.566981	9.710620	9.157217
23	H	6.964787	8.246264	6.723669	9.018663	8.667293

		21	22	23
21	N	0.000000		
22	H	1.016323	0.000000	
23	H	1.017064	1.619871	0.000000

Stoichiometry C7H12BrN3
Framework group C1[X(C7H12BrN3)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.788333	2.139003	-0.058550
2	6	0	-2.787633	1.245228	0.142816
3	7	0	-2.214190	-0.023751	0.026010

4	6	0	-0.901007	0.102173	-0.232285
5	7	0	-0.641348	1.410359	-0.326526
6	6	0	0.736547	1.924632	-0.580418
7	6	0	1.740621	1.902195	0.614347
8	1	0	-1.827226	3.214057	-0.117634
9	1	0	-3.839933	1.399150	0.299648
10	1	0	1.181789	1.282631	-1.335732
11	1	0	0.590243	2.931126	-0.971651
12	1	0	1.457089	2.604457	1.412099
13	1	0	1.774505	0.876003	0.998363
14	35	0	1.823600	-1.822494	-0.026669
15	1	0	-0.032464	-0.616907	-0.343075
16	6	0	-2.864828	-1.286521	0.096900
17	6	0	-4.179460	-1.440791	0.186302
18	1	0	-2.166510	-2.113730	0.049356
19	1	0	-4.592973	-2.436522	0.264133
20	1	0	-4.872957	-0.609855	0.209003
21	7	0	3.079072	2.280196	0.125467
22	1	0	3.661817	2.640905	0.875940
23	1	0	3.540425	1.432851	-0.196370

Rotational constants (GHZ): 0.8049924 0.4648118 0.3012423

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 365 symmetry adapted cartesian basis functions of A symmetry.

There are 352 symmetry adapted basis functions of A symmetry.

352 basis functions, 562 primitive gaussians, 365 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 830.1083271095 Hartrees.

NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 352 RedAO= T EigKep= 5.04D-06 NBF= 352

NBsUse= 352 1.00D-06 EigRej= -1.00D+00 NBFU= 352

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999450 0.003742 -0.000921 -0.032946 Ang= 3.80 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3012.46036542 A.U. after 12 cycles
NFock= 12 Conv=0.92D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000692414	0.000716240	0.006440409
2	6	0.002948254	0.004061177	0.001590956
3	7	-0.003326688	0.006297818	-0.001788397
4	6	0.012228996	-0.011639280	0.007926880
5	7	0.014651983	-0.001429580	-0.012669820
6	6	0.003094846	-0.007281953	-0.003251976
7	6	-0.001985859	-0.000171628	-0.005233798
8	1	0.001670809	0.000207912	-0.002026722
9	1	0.000616705	0.000424112	-0.001963622
10	1	-0.002371239	0.000072223	0.005659370
11	1	0.005372135	-0.000413844	0.001083992
12	1	-0.002778834	0.004252714	0.003810929
13	1	-0.006803704	-0.001532108	-0.002750082
14	35	-0.002738234	-0.003415069	0.002028980
15	1	-0.013802975	0.007351350	-0.004396669
16	6	-0.000545514	0.000659257	0.000010676
17	6	0.000397984	0.000165726	-0.001948051
18	1	-0.000102022	-0.000654057	-0.001116796
19	1	-0.000004464	0.000219665	0.001277373
20	1	-0.000549190	0.000505318	-0.000270706
21	7	-0.003368424	0.002689888	0.004262807
22	1	-0.004462969	-0.000397057	0.000740393
23	1	0.001165990	-0.000688824	0.002583876

Cartesian Forces: Max 0.014651983 RMS 0.004648964

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.020280318 RMS 0.004228606
Search for a local minimum.
Step number 16 out of a maximum of 121
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 9 11 12 14 16
15
ITU= 0 1 1 -1 1 -1 1 1 1 1 1 0 1 0 0
Use linear search instead of GDIIS.
Energy rises -- skip Quadratic/GDIIS search.
Quartic linear search produced a step of -0.96623.
Iteration 1 RMS(Cart)= 0.14553043 RMS(Int)= 0.00742855
Iteration 2 RMS(Cart)= 0.01199931 RMS(Int)= 0.00006018
Iteration 3 RMS(Cart)= 0.00006805 RMS(Int)= 0.00004600
Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00004600

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56194	0.00338	0.00391	0.00000	0.00390	2.56584
R2	2.61733	-0.00266	0.00277	0.00000	0.00277	2.62010
R3	2.03595	-0.00063	-0.00184	0.00000	-0.00184	2.03411
R4	2.64074	-0.00376	-0.01193	0.00000	-0.01193	2.62881
R5	2.03145	-0.00056	-0.00054	0.00000	-0.00054	2.03091
R6	2.54027	0.00007	0.00341	0.00000	0.00342	2.54369
R7	2.68776	0.00137	0.00228	0.00000	0.00228	2.69004
R8	2.52663	0.00121	-0.00609	0.00000	-0.00608	2.52055
R9	2.14108	-0.01046	-0.02812	0.00000	-0.02812	2.11297
R10	2.82040	-0.00910	-0.02709	0.00000	-0.02709	2.79331
R11	2.94951	-0.01369	-0.04299	0.00000	-0.04299	2.90651
R12	2.05356	0.00227	0.00688	0.00000	0.00688	2.06044
R13	2.05928	0.00021	0.00053	0.00000	0.00053	2.05981
R14	2.07867	-0.00449	-0.00988	0.00000	-0.00988	2.06879
R15	2.07155	-0.00027	0.00017	0.00000	0.00017	2.07172
R16	2.78588	-0.00439	-0.02060	0.00000	-0.02060	2.76529
R17	4.22493	-0.00450	-0.15025	0.00000	-0.15025	4.07469
R18	2.50704	0.00028	-0.00045	0.00000	-0.00045	2.50659
R19	2.04770	-0.00046	0.00082	0.00000	0.00082	2.04852
R20	2.04277	0.00002	0.00037	0.00000	0.00037	2.04314
R21	2.04572	-0.00004	0.00061	0.00000	0.00061	2.04632

R22	1.92057	-0.00262	-0.00762	0.00000	-0.00762	1.91295
R23	1.92197	0.00048	-0.00468	0.00000	-0.00468	1.91730
A1	1.86745	0.00105	0.00601	0.00000	0.00604	1.87350
A2	2.26448	0.00105	0.01333	0.00000	0.01339	2.27788
A3	2.14627	-0.00184	-0.01453	0.00000	-0.01446	2.13181
A4	1.85853	0.00195	0.00276	0.00000	0.00276	1.86128
A5	2.27681	-0.00031	0.00043	0.00000	0.00047	2.27729
A6	2.14589	-0.00156	-0.00132	0.00000	-0.00128	2.14460
A7	1.90908	-0.00396	-0.00903	0.00000	-0.00903	1.90005
A8	2.23235	0.00365	0.02076	0.00000	0.02079	2.25314
A9	2.14079	0.00032	-0.01089	0.00000	-0.01086	2.12992
A10	1.87016	0.00534	0.01665	0.00000	0.01667	1.88683
A11	2.35774	-0.01388	-0.15140	0.00000	-0.15141	2.20632
A12	2.05466	0.00849	0.13033	0.00000	0.13038	2.18504
A13	1.91800	-0.00425	-0.01489	0.00000	-0.01489	1.90311
A14	2.23468	-0.00114	-0.01328	0.00000	-0.01327	2.22141
A15	2.12754	0.00542	0.02916	0.00000	0.02915	2.15669
A16	2.04737	-0.02028	-0.09181	0.00000	-0.09183	1.95554
A17	1.86809	0.00167	0.01003	0.00000	0.00996	1.87805
A18	1.82904	0.01146	0.04960	0.00000	0.04965	1.87869
A19	1.83380	0.01022	0.07912	0.00000	0.07910	1.91290
A20	1.95462	0.00125	-0.01269	0.00000	-0.01270	1.94192
A21	1.92957	-0.00462	-0.03501	0.00000	-0.03500	1.89457
A22	1.96076	-0.00044	-0.05221	0.00000	-0.05221	1.90855
A23	1.87706	0.00186	0.01435	0.00000	0.01437	1.89143
A24	1.90342	-0.01237	-0.01373	0.00000	-0.01373	1.88969
A25	1.93003	-0.00292	-0.03838	0.00000	-0.03834	1.89169
A26	1.88686	0.00625	0.02972	0.00000	0.02975	1.91660
A27	1.90512	0.00766	0.06007	0.00000	0.06008	1.96521
A28	2.87544	0.00018	-0.00134	0.00000	-0.00134	2.87410
A29	2.16506	0.00282	0.00656	0.00000	0.00656	2.17163
A30	1.96143	-0.00169	-0.00958	0.00000	-0.00958	1.95185
A31	2.15650	-0.00112	0.00319	0.00000	0.00319	2.15969
A32	2.08406	-0.00048	-0.00461	0.00000	-0.00460	2.07946
A33	2.14953	0.00103	0.00772	0.00000	0.00773	2.15725
A34	2.04932	-0.00053	-0.00286	0.00000	-0.00285	2.04647
A35	1.94626	-0.00522	0.00167	0.00000	0.00169	1.94796
A36	1.87879	0.00447	0.05074	0.00000	0.05076	1.92955
A37	1.84342	0.00155	0.03249	0.00000	0.03254	1.87596
D1	0.02636	-0.00091	-0.02333	0.00000	-0.02328	0.00308
D2	-3.04810	-0.00229	-0.09527	0.00000	-0.09526	3.13983
D3	3.06140	0.00176	0.08005	0.00000	0.08002	3.14142
D4	-0.01306	0.00037	0.00810	0.00000	0.00805	-0.00502
D5	-0.05012	0.00220	0.04915	0.00000	0.04912	-0.00100

D6	-3.10932	0.00166	0.03295	0.00000	0.03289	-3.07643
D7	-3.09409	-0.00044	-0.04556	0.00000	-0.04559	-3.13968
D8	0.12990	-0.00098	-0.06176	0.00000	-0.06182	0.06808
D9	0.00545	-0.00047	-0.00953	0.00000	-0.00957	-0.00412
D10	-3.08939	-0.00090	-0.06929	0.00000	-0.06934	3.12445
D11	3.08618	0.00083	0.05569	0.00000	0.05568	-3.14132
D12	-0.00867	0.00040	-0.00407	0.00000	-0.00409	-0.01276
D13	-0.03615	0.00168	0.03967	0.00000	0.03967	0.00353
D14	3.06489	0.00030	-0.02269	0.00000	-0.02291	3.04197
D15	3.06164	0.00220	0.09535	0.00000	0.09541	-3.12614
D16	-0.12052	0.00082	0.03299	0.00000	0.03282	-0.08769
D17	0.09770	0.00000	0.03350	0.00000	0.03351	0.13121
D18	-3.06427	0.00037	0.05896	0.00000	0.05897	-3.00530
D19	-2.99151	-0.00040	-0.03340	0.00000	-0.03341	-3.02492
D20	0.12970	-0.00003	-0.00794	0.00000	-0.00795	0.12175
D21	0.05320	-0.00232	-0.05480	0.00000	-0.05478	-0.00158
D22	3.11837	-0.00214	-0.04157	0.00000	-0.04154	3.07683
D23	-3.05604	-0.00063	0.01466	0.00000	0.01444	-3.04160
D24	0.00912	-0.00045	0.02788	0.00000	0.02768	0.03681
D25	-1.84355	-0.00017	0.04664	0.00000	0.04666	-1.79689
D26	1.25426	-0.00178	-0.02959	0.00000	-0.02960	1.22465
D27	1.72795	-0.00189	0.08211	0.00000	0.08214	1.81009
D28	-2.50174	-0.00004	0.13252	0.00000	0.13253	-2.36921
D29	-0.45209	0.00098	0.12174	0.00000	0.12173	-0.33035
D30	-1.32236	-0.00204	0.06593	0.00000	0.06594	-1.25642
D31	0.73114	-0.00019	0.11634	0.00000	0.11632	0.84747
D32	2.78079	0.00083	0.10557	0.00000	0.10553	2.88632
D33	-1.17647	-0.00082	0.04915	0.00000	0.04919	-1.12728
D34	0.95129	-0.00348	-0.01978	0.00000	-0.01974	0.93155
D35	3.01517	-0.00007	0.05287	0.00000	0.05292	3.06809
D36	3.03480	0.00149	0.03759	0.00000	0.03757	3.07237
D37	-1.12062	-0.00117	-0.03133	0.00000	-0.03136	-1.15198
D38	0.94326	0.00225	0.04132	0.00000	0.04130	0.98456
D39	0.93937	0.00004	0.03750	0.00000	0.03748	0.97685
D40	3.06713	-0.00263	-0.03142	0.00000	-0.03144	3.03568
D41	-1.15218	0.00079	0.04123	0.00000	0.04122	-1.11096
D42	2.73965	-0.00204	-0.18339	0.00000	-0.18337	2.55629
D43	-1.52923	-0.00037	-0.11056	0.00000	-0.11056	-1.63979
D44	0.60300	0.00214	-0.12946	0.00000	-0.12946	0.47354
D45	2.61730	0.00382	-0.05663	0.00000	-0.05666	2.56064
D46	-1.49735	-0.00250	-0.13871	0.00000	-0.13870	-1.63605
D47	0.51694	-0.00083	-0.06588	0.00000	-0.06589	0.45105
D48	-3.11146	-0.00095	-0.01776	0.00000	-0.01776	-3.12922
D49	0.00437	0.00003	0.00902	0.00000	0.00902	0.01339

D50	0.05275	-0.00136	-0.04605	0.00000	-0.04605	0.00671
D51	-3.11460	-0.00038	-0.01927	0.00000	-0.01927	-3.13387

Item	Value	Threshold	Converged?
Maximum Force	0.020280	0.000450	NO
RMS Force	0.004229	0.000300	NO
Maximum Displacement	0.610442	0.001800	NO
RMS Displacement	0.145175	0.001200	NO

Predicted change in Energy=-5.776290D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.837595	-2.024111	0.328146
2	6	0	-2.829388	-1.131186	0.077928
3	7	0	-2.229811	0.122384	0.012753
4	6	0	-0.907750	-0.015947	0.224668
5	7	0	-0.651912	-1.310865	0.416506
6	6	0	0.709376	-1.856399	0.601520
7	6	0	1.520293	-1.840223	-0.705300
8	1	0	-1.873684	-3.092746	0.452080
9	1	0	-3.884687	-1.280990	-0.059591
10	1	0	1.211136	-1.243689	1.350959
11	1	0	0.609145	-2.869098	0.992042
12	1	0	1.051492	-2.512067	-1.431484
13	1	0	1.499554	-0.822449	-1.112229
14	35	0	1.464840	2.081303	-0.498063
15	1	0	-0.135566	0.789158	0.148772
16	6	0	-2.824709	1.389695	-0.244912
17	6	0	-4.131216	1.600482	-0.334457
18	1	0	-2.079619	2.167802	-0.365384
19	1	0	-4.490380	2.598297	-0.544998
20	1	0	-4.873846	0.822776	-0.206871
21	7	0	2.877593	-2.299674	-0.408708
22	1	0	3.273809	-2.816741	-1.183552
23	1	0	3.488449	-1.510796	-0.224539

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357784	0.000000			
3	N	2.204711	1.391108	0.000000		

4	C	2.215410	2.226653	1.346064	0.000000	
5	N	1.386496	2.210955	2.169559	1.333817	0.000000
6	C	2.567084	3.650060	3.591803	2.478785	1.478155
7	C	3.518130	4.476149	4.293100	3.176195	2.501428
8	H	1.076402	2.213838	3.264490	3.232868	2.160808
9	H	2.212048	1.074713	2.171015	3.247043	3.267782
10	H	3.309073	4.237818	3.936632	2.695470	2.085345
11	H	2.672320	3.959729	4.238826	3.321190	2.085568
12	H	3.417780	4.387071	4.448944	3.579397	2.785595
13	H	3.828215	4.500170	4.008298	2.869294	2.684099
14	Br	5.333209	5.393723	4.212925	3.248073	4.101692
15	H	3.292956	3.308991	2.202033	1.118134	2.179081
16	C	3.599565	2.541474	1.423507	2.423029	3.528675
17	C	4.340210	3.053986	2.433243	3.649137	4.598418
18	H	4.255784	3.412038	2.085492	2.547587	3.840680
19	H	5.400584	4.129888	3.398735	4.501322	5.562363
20	H	4.196407	2.842338	2.744031	4.076714	4.771347
21	N	4.780364	5.845666	5.668295	4.466027	3.757143
22	H	5.388872	6.456117	6.352908	5.226181	4.498792
23	H	5.379191	6.336455	5.951645	4.665075	4.194461

		6	7	8	9	10
6	C	0.000000				
7	C	1.538060	0.000000			
8	H	2.867592	3.798345	0.000000		
9	H	4.676920	5.472065	2.754706	0.000000	
10	H	1.090337	2.163245	3.707170	5.287576	0.000000
11	H	1.090006	2.183975	2.550689	4.880834	1.770077
12	H	2.163342	1.094757	3.527274	5.269109	3.062067
13	H	2.151829	1.096305	4.356609	5.505302	2.515536
14	Br	4.157560	3.927389	6.230513	6.333617	3.812980
15	H	2.813873	3.222569	4.264063	4.287754	2.718700
16	C	4.872713	5.433541	4.634925	2.879315	5.076373
17	C	6.021413	6.626880	5.267019	2.905032	6.282569
18	H	4.990750	5.398071	5.327666	3.904605	5.041148
19	H	6.942354	7.473577	6.342652	3.956179	7.131816
20	H	6.245305	6.944423	4.976595	2.329368	6.612421
21	N	2.432739	1.463326	4.893317	6.847483	2.643598
22	H	3.268800	2.063281	5.408156	7.407151	3.626687
23	H	2.919771	2.052630	5.631416	7.378561	2.782030

		11	12	13	14	15
11	H	0.000000				
12	H	2.489301	0.000000			
13	H	3.067500	1.776933	0.000000		
14	Br	5.240143	4.705441	2.968195	0.000000	

15	H	3.827341	3.847649	2.619355	2.156231	0.000000
16	C	5.608808	5.626423	4.934072	4.352314	2.783365
17	C	6.648893	6.706489	6.179086	5.619057	4.105725
18	H	5.868766	5.730759	4.723331	3.547996	2.438105
19	H	7.632828	7.590391	6.921168	5.977803	4.766414
20	H	6.717925	6.908725	6.644295	6.468973	4.751727
21	N	2.726207	2.103764	2.139188	4.604000	4.350954
22	H	3.440405	2.256765	2.670256	5.266223	5.138233
23	H	3.408144	2.897933	2.284189	4.131947	4.308438

		16	17	18	19	20
16	C	0.000000				
17	C	1.326428	0.000000			
18	H	1.084031	2.128816	0.000000		
19	H	2.079719	1.081185	2.455475	0.000000	
20	H	2.126454	1.082868	3.105145	1.847661	0.000000
21	N	6.793712	8.021230	6.673393	8.848487	8.359141
22	H	7.467736	8.664134	7.360317	9.487519	8.976874
23	H	6.947606	8.231126	6.674976	8.980482	8.681811

		21	22	23
21	N	0.000000		
22	H	1.012289	0.000000	
23	H	1.014590	1.634402	0.000000

Stoichiometry C7H12BrN3
Framework group C1[X(C7H12BrN3)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.611499	2.274189	-0.109540
2	6	0	-2.623847	1.396827	0.111745
3	7	0	-2.082655	0.122223	-0.021201
4	6	0	-0.775132	0.233642	-0.320965
5	7	0	-0.471867	1.531300	-0.377361
6	6	0	0.896525	2.041718	-0.605217
7	6	0	1.801723	1.833994	0.620791
8	1	0	-1.604869	3.350545	-0.102141
9	1	0	-3.657284	1.569828	0.350675
10	1	0	1.310125	1.506202	-1.460198
11	1	0	0.816496	3.097745	-0.863126

12	1	0	1.422072	2.429711	1.457140
13	1	0	1.762255	0.775659	0.904080
14	35	0	1.540448	-2.027481	-0.046390
15	1	0	-0.039441	-0.604279	-0.403852
16	6	0	-2.717324	-1.142855	0.130938
17	6	0	-4.022082	-1.311758	0.299728
18	1	0	-2.003953	-1.958397	0.097560
19	1	0	-4.412421	-2.313024	0.418303
20	1	0	-4.733557	-0.495837	0.325820
21	7	0	3.153567	2.272858	0.272596
22	1	0	3.631601	2.675294	1.068998
23	1	0	3.709800	1.489174	-0.052730

Rotational constants (GHZ): 0.7207643 0.5195626 0.3103134

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 365 symmetry adapted cartesian basis functions of A symmetry.

There are 352 symmetry adapted basis functions of A symmetry.

352 basis functions, 562 primitive gaussians, 365 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 834.4203257673 Hartrees.

NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 352 RedAO= T EigKep= 4.86D-06 NBF= 352

NBsUse= 352 1.00D-06 EigRej= -1.00D+00 NBFU= 352

Lowest energy guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999998 0.000128 -0.000024 -0.001823 Ang= 0.21 deg.

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999509 -0.003616 0.000893 0.031124 Ang= -3.59 deg.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3012.46659570 A.U. after 9 cycles

NFock= 9 Conv=0.34D-08 -V/T= 2.0017

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000143457	-0.000002760	-0.000180072
2	6	0.000085562	0.000089357	0.000012078
3	7	-0.000112364	0.000304188	0.000063990
4	6	0.000395664	-0.000272306	-0.000120847
5	7	0.000489868	0.000295983	0.000079085
6	6	0.000292147	-0.000318415	0.000071176
7	6	-0.000100991	0.000649392	-0.000557565
8	1	0.000046362	0.000004519	-0.000038871
9	1	0.000025692	0.000015534	-0.000016428
10	1	-0.000097796	0.000003430	0.000099774
11	1	0.000329570	0.000008491	0.000010054
12	1	0.000362898	-0.000117196	0.000596276
13	1	-0.000610353	0.000011061	-0.000444804
14	35	0.000052438	-0.000369621	0.000109767
15	1	-0.000620413	0.000201072	-0.000097625
16	6	0.000040337	-0.000111861	0.000106888
17	6	0.000001924	0.000072302	-0.000048505
18	1	-0.000069639	-0.000035872	-0.000046757
19	1	-0.000005848	-0.000003920	0.000017448
20	1	-0.000004060	0.000016775	-0.000006728
21	7	-0.000364588	-0.001083948	0.000090212
22	1	-0.000157204	0.000482415	-0.000107067
23	1	-0.000122665	0.000161378	0.000408520

Cartesian Forces: Max 0.001083948 RMS 0.000277605

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.001013106 RMS 0.000243616
Search for a local minimum.
Step number 17 out of a maximum of 121
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Update second derivatives using D2CorX and points 9 11 12 14 16
15 17
ITU= 0 0 1 1 -1 1 -1 1 1 1 1 1 1 0 1 0 0
Use linear search instead of GDIIS.
Eigenvalues --- -0.00105 0.00000 0.00391 0.00697 0.01236
Eigenvalues --- 0.01406 0.01817 0.02055 0.02163 0.02315

Eigenvalues --- 0.02391 0.02927 0.03062 0.03083 0.03300
Eigenvalues --- 0.03790 0.03901 0.04348 0.04548 0.05233
Eigenvalues --- 0.05494 0.08977 0.09145 0.10076 0.12277
Eigenvalues --- 0.12776 0.15233 0.15920 0.15990 0.16000
Eigenvalues --- 0.16002 0.16047 0.16087 0.20576 0.21647
Eigenvalues --- 0.22026 0.22939 0.23440 0.24685 0.24920
Eigenvalues --- 0.28514 0.30580 0.34029 0.34385 0.34610
Eigenvalues --- 0.34788 0.35003 0.35674 0.35689 0.35858
Eigenvalues --- 0.36437 0.36658 0.37876 0.40276 0.42166
Eigenvalues --- 0.42901 0.46795 0.47679 0.48191 0.50068
Eigenvalues --- 0.54251 0.59429 0.60360

RFO step: Lambda=-1.49760559D-03 EMin=-1.04831770D-03

Quartic linear search produced a step of -0.01374.

Iteration 1 RMS(Cart)= 0.09722948 RMS(Int)= 0.03539721
Iteration 2 RMS(Cart)= 0.03303819 RMS(Int)= 0.00205455
Iteration 3 RMS(Cart)= 0.00210309 RMS(Int)= 0.00014070
Iteration 4 RMS(Cart)= 0.00000620 RMS(Int)= 0.00014062
Iteration 5 RMS(Cart)= 0.00000000 RMS(Int)= 0.00014062

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56584	0.00017	0.00000	0.00075	0.00076	2.56660
R2	2.62010	-0.00017	0.00000	-0.00223	-0.00223	2.61787
R3	2.03411	-0.00001	0.00000	-0.00013	-0.00013	2.03397
R4	2.62881	-0.00001	-0.00001	0.00151	0.00151	2.63032
R5	2.03091	-0.00002	0.00000	-0.00022	-0.00022	2.03069
R6	2.54369	-0.00003	0.00000	-0.00086	-0.00086	2.54283
R7	2.69004	-0.00004	0.00000	-0.00130	-0.00130	2.68873
R8	2.52055	-0.00023	0.00000	-0.00034	-0.00035	2.52020
R9	2.11297	-0.00051	-0.00001	0.00012	0.00011	2.11308
R10	2.79331	-0.00033	-0.00001	-0.00321	-0.00322	2.79009
R11	2.90651	-0.00052	-0.00002	-0.00539	-0.00541	2.90110
R12	2.06044	0.00002	0.00000	0.00001	0.00002	2.06045
R13	2.05981	-0.00003	0.00000	-0.00115	-0.00115	2.05867
R14	2.06879	-0.00048	0.00000	-0.00598	-0.00599	2.06280
R15	2.07172	0.00019	0.00000	0.00130	0.00130	2.07301
R16	2.76529	-0.00038	-0.00001	0.00292	0.00291	2.76819
R17	4.07469	-0.00022	-0.00007	-0.00280	-0.00287	4.07182
R18	2.50659	0.00002	0.00000	0.00025	0.00025	2.50683
R19	2.04852	-0.00007	0.00000	-0.00210	-0.00210	2.04642
R20	2.04314	0.00000	0.00000	-0.00008	-0.00008	2.04307
R21	2.04632	-0.00001	0.00000	-0.00034	-0.00034	2.04598
R22	1.91295	-0.00023	0.00000	-0.00066	-0.00066	1.91229
R23	1.91730	0.00013	0.00000	0.00361	0.00361	1.92091
A1	1.87350	-0.00005	0.00000	-0.00100	-0.00101	1.87248

A2	2.27788	0.00006	0.00001	0.00010	0.00011	2.27798
A3	2.13181	-0.00001	-0.00001	0.00091	0.00091	2.13272
A4	1.86128	0.00007	0.00000	0.00144	0.00143	1.86271
A5	2.27729	-0.00002	0.00000	-0.00006	-0.00006	2.27723
A6	2.14460	-0.00005	0.00000	-0.00136	-0.00136	2.14324
A7	1.90005	-0.00025	0.00000	-0.00266	-0.00270	1.89735
A8	2.25314	0.00014	0.00001	-0.00196	-0.00197	2.25117
A9	2.12992	0.00011	-0.00001	0.00477	0.00474	2.13467
A10	1.88683	0.00026	0.00001	0.00175	0.00174	1.88857
A11	2.20632	0.00021	-0.00007	0.02982	0.02973	2.23605
A12	2.18504	-0.00047	0.00006	-0.03222	-0.03213	2.15291
A13	1.90311	-0.00004	-0.00001	0.00045	0.00039	1.90350
A14	2.22141	0.00032	-0.00001	0.00781	0.00779	2.22920
A15	2.15669	-0.00029	0.00001	-0.00913	-0.00914	2.14756
A16	1.95554	-0.00101	-0.00004	-0.00929	-0.00936	1.94618
A17	1.87805	0.00005	0.00001	-0.00702	-0.00705	1.87100
A18	1.87869	0.00071	0.00002	0.01096	0.01100	1.88968
A19	1.91290	0.00045	0.00004	-0.00027	-0.00030	1.91260
A20	1.94192	0.00001	-0.00001	0.00143	0.00144	1.94336
A21	1.89457	-0.00019	-0.00002	0.00443	0.00443	1.89900
A22	1.90855	0.00030	-0.00003	0.00419	0.00368	1.91223
A23	1.89143	0.00004	0.00001	0.00103	0.00104	1.89247
A24	1.88969	-0.00087	-0.00001	-0.01350	-0.01371	1.87599
A25	1.89169	-0.00014	-0.00002	0.01071	0.01088	1.90257
A26	1.91660	-0.00004	0.00001	-0.03326	-0.03332	1.88328
A27	1.96521	0.00071	0.00003	0.03086	0.03102	1.99623
A28	2.87410	-0.00044	0.00000	-0.01312	-0.01312	2.86098
A29	2.17163	0.00015	0.00000	0.00278	0.00278	2.17441
A30	1.95185	-0.00004	0.00000	0.00108	0.00107	1.95293
A31	2.15969	-0.00011	0.00000	-0.00385	-0.00385	2.15584
A32	2.07946	0.00000	0.00000	0.00113	0.00112	2.08058
A33	2.15725	0.00002	0.00000	-0.00113	-0.00112	2.15613
A34	2.04647	-0.00001	0.00000	0.00000	0.00000	2.04647
A35	1.94796	-0.00038	0.00000	-0.02153	-0.02195	1.92601
A36	1.92955	-0.00015	0.00002	-0.02386	-0.02426	1.90529
A37	1.87596	0.00020	0.00001	-0.01310	-0.01396	1.86199
D1	0.00308	0.00003	-0.00001	-0.00591	-0.00589	-0.00282
D2	3.13983	-0.00001	-0.00005	-0.00170	-0.00175	3.13808
D3	3.14142	0.00005	0.00004	-0.00002	0.00004	3.14145
D4	-0.00502	0.00001	0.00000	0.00419	0.00418	-0.00083
D5	-0.00100	-0.00005	0.00002	0.01360	0.01359	0.01258
D6	-3.07643	0.00006	0.00002	0.02849	0.02853	-3.04790
D7	-3.13968	-0.00007	-0.00002	0.00831	0.00826	-3.13141
D8	0.06808	0.00005	-0.00003	0.02320	0.02321	0.09129

D9	-0.00412	0.00000	0.00000	-0.00364	-0.00366	-0.00778
D10	3.12445	-0.00003	-0.00003	0.00943	0.00933	3.13378
D11	-3.14132	0.00003	0.00003	-0.00746	-0.00742	3.13444
D12	-0.01276	0.00001	0.00000	0.00561	0.00557	-0.00719
D13	0.00353	-0.00003	0.00002	0.01213	0.01216	0.01568
D14	3.04197	-0.00004	-0.00001	0.00306	0.00293	3.04491
D15	-3.12614	-0.00001	0.00004	0.00022	0.00026	-3.12588
D16	-0.08769	-0.00002	0.00002	-0.00886	-0.00896	-0.09665
D17	0.13121	0.00001	0.00002	0.00295	0.00297	0.13418
D18	-3.00530	0.00003	0.00003	0.00154	0.00157	-3.00374
D19	-3.02492	-0.00002	-0.00002	0.01749	0.01747	-3.00745
D20	0.12175	0.00000	0.00000	0.01607	0.01607	0.13781
D21	-0.00158	0.00005	-0.00003	-0.01588	-0.01592	-0.01750
D22	3.07683	-0.00003	-0.00002	-0.02934	-0.02926	3.04757
D23	-3.04160	0.00001	0.00001	-0.01150	-0.01167	-3.05328
D24	0.03681	-0.00007	0.00002	-0.02496	-0.02502	0.01179
D25	-1.79689	-0.00018	0.00002	-0.28802	-0.28798	-2.08488
D26	1.22465	-0.00015	-0.00001	-0.29579	-0.29581	0.92885
D27	1.81009	-0.00017	0.00004	-0.10707	-0.10705	1.70304
D28	-2.36921	-0.00019	0.00006	-0.11765	-0.11755	-2.48676
D29	-0.33035	-0.00002	0.00006	-0.11044	-0.11037	-0.44072
D30	-1.25642	-0.00006	0.00003	-0.09063	-0.09065	-1.34706
D31	0.84747	-0.00008	0.00006	-0.10122	-0.10114	0.74632
D32	2.88632	0.00009	0.00005	-0.09401	-0.09396	2.79236
D33	-1.12728	-0.00039	0.00002	-0.12744	-0.12742	-1.25470
D34	0.93155	-0.00037	-0.00001	-0.11163	-0.11163	0.81992
D35	3.06809	-0.00001	0.00002	-0.08170	-0.08167	2.98642
D36	3.07237	-0.00011	0.00002	-0.11256	-0.11256	2.95981
D37	-1.15198	-0.00008	-0.00001	-0.09675	-0.09676	-1.24875
D38	0.98456	0.00028	0.00002	-0.06682	-0.06681	0.91775
D39	0.97685	-0.00018	0.00002	-0.11882	-0.11881	0.85804
D40	3.03568	-0.00015	-0.00001	-0.10301	-0.10302	2.93267
D41	-1.11096	0.00021	0.00002	-0.07308	-0.07306	-1.18402
D42	2.55629	0.00026	-0.00009	0.34586	0.34574	2.90203
D43	-1.63979	0.00017	-0.00005	0.29928	0.29968	-1.34011
D44	0.47354	0.00043	-0.00006	0.36819	0.36760	0.84114
D45	2.56064	0.00035	-0.00003	0.32162	0.32154	2.88218
D46	-1.63605	0.00017	-0.00007	0.35722	0.35699	-1.27906
D47	0.45105	0.00008	-0.00003	0.31064	0.31093	0.76198
D48	-3.12922	0.00000	-0.00001	-0.00019	-0.00020	-3.12942
D49	0.01339	0.00001	0.00000	0.00069	0.00069	0.01408
D50	0.00671	-0.00003	-0.00002	0.00140	0.00138	0.00809
D51	-3.13387	-0.00002	-0.00001	0.00228	0.00227	-3.13160

Item	Value	Threshold	Converged?

Maximum Force	0.001013	0.000450	NO
RMS Force	0.000244	0.000300	YES
Maximum Displacement	0.524633	0.001800	NO
RMS Displacement	0.115863	0.001200	NO

Predicted change in Energy=-1.362295D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.830351	-2.018470	0.329059
2	6	0	-2.819526	-1.126763	0.062490
3	7	0	-2.222232	0.129228	0.006566
4	6	0	-0.905022	-0.008219	0.244740
5	7	0	-0.647798	-1.303813	0.428717
6	6	0	0.718343	-1.837090	0.599550
7	6	0	1.460948	-1.922576	-0.741367
8	1	0	-1.866769	-3.087080	0.452488
9	1	0	-3.872631	-1.277782	-0.088891
10	1	0	1.248246	-1.158093	1.268145
11	1	0	0.646490	-2.814113	1.076049
12	1	0	1.042436	-2.733865	-1.339884
13	1	0	1.321149	-0.975087	-1.276261
14	35	0	1.644981	1.914582	-0.324240
15	1	0	-0.109004	0.775456	0.194139
16	6	0	-2.820468	1.394175	-0.251176
17	6	0	-4.126839	1.603725	-0.347283
18	1	0	-2.079473	2.175637	-0.365026
19	1	0	-4.487131	2.601203	-0.557285
20	1	0	-4.868281	0.824343	-0.224656
21	7	0	2.858297	-2.252120	-0.450429
22	1	0	3.335487	-2.539118	-1.295381
23	1	0	3.334668	-1.419242	-0.114781

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.358185	0.000000			
3	N	2.206848	1.391905	0.000000		
4	C	2.214600	2.224788	1.345608	0.000000	
5	N	1.385315	2.209496	2.170406	1.333633	0.000000
6	C	2.569417	3.648220	3.586783	2.471026	1.476451

7	C	3.462319	4.427409	4.281952	3.199215	2.489733
8	H	1.076331	2.214202	3.266472	3.232260	2.160208
9	H	2.212285	1.074595	2.170854	3.244966	3.266213
10	H	3.331650	4.242800	3.910626	2.646910	2.078667
11	H	2.706619	3.985940	4.246954	3.312296	2.091704
12	H	3.398538	4.411822	4.546238	3.705775	2.833705
13	H	3.687500	4.354360	3.926921	2.864283	2.625217
14	Br	5.289010	5.415825	4.272266	3.243982	4.022667
15	H	3.284397	3.314015	2.217775	1.118191	2.160715
16	C	3.600438	2.540377	1.422817	2.425196	3.530141
17	C	4.341842	3.054922	2.434518	3.650885	4.599966
18	H	4.258445	3.411201	2.084767	2.553503	3.845296
19	H	5.402357	4.130709	3.399758	4.503758	5.564336
20	H	4.197285	2.843706	2.745583	4.076875	4.771627
21	N	4.758741	5.810954	5.629515	4.436319	3.736962
22	H	5.440198	6.459314	6.301061	5.172942	4.512765
23	H	5.218572	6.163690	5.769889	4.482769	4.021038

		6	7	8	9	10
6	C	0.000000				
7	C	1.535196	0.000000			
8	H	2.875223	3.722238	0.000000		
9	H	4.675876	5.411889	2.755020	0.000000	
10	H	1.090345	2.160512	3.753612	5.298986	0.000000
11	H	1.089399	2.182013	2.603807	4.913233	1.772403
12	H	2.161167	1.091588	3.435233	5.276650	3.054051
13	H	2.150602	1.096991	4.196655	5.336368	2.552021
14	Br	3.973296	3.864148	6.160545	6.378920	3.483449
15	H	2.770245	3.258726	4.251549	4.296601	2.595039
16	C	4.867031	5.437981	4.635336	2.876237	5.037543
17	C	6.017598	6.619174	5.267941	2.904216	6.255301
18	H	4.985996	5.428772	5.330082	3.900997	4.985451
19	H	6.937843	7.475166	6.343698	3.955190	7.096411
20	H	6.242828	6.918937	4.976628	2.329953	6.600788
21	N	2.419527	1.464865	4.882486	6.810686	2.596663
22	H	3.306516	2.049622	5.515321	7.416437	3.582662
23	H	2.744089	2.038819	5.491669	7.208734	2.516713

		11	12	13	14	15
11	H	0.000000				
12	H	2.449478	0.000000			
13	H	3.061135	1.781861	0.000000		
14	Br	5.031735	4.796108	3.059640	0.000000	
15	H	3.772737	3.999297	2.696631	2.154713	0.000000
16	C	5.611686	5.757432	4.880287	4.496265	2.816586
17	C	6.657916	6.820656	6.098676	5.780232	4.137894

18	H	5.865593	5.899142	4.724579	3.733815	2.481113
19	H	7.638553	7.723440	6.858783	6.174833	4.802706
20	H	6.733713	6.988644	6.530916	6.604629	4.777918
21	N	2.745553	2.078596	2.162322	4.341597	4.287956
22	H	3.595832	2.301736	2.550316	4.861724	5.006954
23	H	3.254235	2.912634	2.366552	3.743434	4.095243

		16	17	18	19	20
16	C	0.000000				
17	C	1.326557	0.000000			
18	H	1.082921	2.125819	0.000000		
19	H	2.080477	1.081145	2.452527	0.000000	
20	H	2.125783	1.082686	3.102120	1.847471	0.000000
21	N	6.751559	7.979368	6.632790	8.804628	8.319592
22	H	7.379494	8.587685	7.239908	9.389410	8.930908
23	H	6.769019	8.053973	6.503746	8.805699	8.504947

		21	22	23
21	N	0.000000		
22	H	1.011940	0.000000	
23	H	1.016501	1.627249	0.000000

Stoichiometry C7H12BrN3
Framework group C1[X(C7H12BrN3)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.696187	2.178825	-0.181782
2	6	0	-2.692809	1.291261	0.070492
3	7	0	-2.128684	0.021460	-0.011778
4	6	0	-0.824183	0.147609	-0.316777
5	7	0	-0.541887	1.447679	-0.410071
6	6	0	0.826436	1.961491	-0.618871
7	6	0	1.647703	1.918550	0.677471
8	1	0	-1.709765	3.254539	-0.215613
9	1	0	-3.730712	1.453578	0.296685
10	1	0	1.297426	1.328043	-1.371046
11	1	0	0.754443	2.975983	-1.009273
12	1	0	1.287511	2.687020	1.363971
13	1	0	1.512700	0.933553	1.141094
14	35	0	1.699692	-1.874181	-0.060182

15	1	0	-0.048829	-0.655782	-0.377938
16	6	0	-2.746144	-1.246284	0.177896
17	6	0	-4.050093	-1.432768	0.335048
18	1	0	-2.021967	-2.051429	0.183149
19	1	0	-4.425384	-2.435590	0.484639
20	1	0	-4.775284	-0.628959	0.320921
21	7	0	3.034495	2.238596	0.330760
22	1	0	3.567761	2.443592	1.166000
23	1	0	3.467075	1.425533	-0.099448

Rotational constants (GHZ): 0.7751261 0.5003997 0.3138248

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 365 symmetry adapted cartesian basis functions of A symmetry.

There are 352 symmetry adapted basis functions of A symmetry.

352 basis functions, 562 primitive gaussians, 365 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 838.2889948072 Hartrees.

NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 352 RedAO= T EigKep= 4.80D-06 NBF= 352

NBsUse= 352 1.00D-06 EigRej= -1.00D+00 NBFU= 352

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999747 0.002499 0.002051 -0.022252 Ang= 2.58 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3012.46696184 A.U. after 12 cycles
NFock= 12 Conv=0.68D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000184571	-0.000072662	-0.001335221
2	6	-0.000204136	-0.000116724	0.000354645
3	7	-0.000492889	-0.000248140	0.001314500
4	6	0.002588104	-0.001019874	-0.001721145
5	7	-0.000968887	0.000680094	0.002054221
6	6	0.000200745	0.000013030	-0.000736482
7	6	0.002223025	-0.002357661	0.001886293
8	1	0.000000734	-0.000100733	-0.000230340
9	1	-0.000076442	-0.000058053	-0.000016125
10	1	-0.000116076	0.000243384	-0.000064864
11	1	-0.000293558	-0.000126009	0.000390154
12	1	-0.002149831	-0.000581821	-0.001433630
13	1	0.001458732	0.000238206	0.000042040
14	35	0.000555455	-0.000626593	0.000244170
15	1	-0.001900910	0.001641008	-0.000464024
16	6	-0.000132595	-0.000078376	0.000208391
17	6	0.000113300	-0.000207058	-0.000027951
18	1	0.000217399	0.000295093	0.000027646
19	1	0.000055644	0.000010464	-0.000015300
20	1	-0.000082027	-0.000031027	-0.000018879
21	7	-0.002569759	0.002544189	0.001006067
22	1	0.000939436	-0.000838973	-0.001281483
23	1	0.000819108	0.000798237	-0.000182685

Cartesian Forces: Max 0.002588104 RMS 0.001013076

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.002040345 RMS 0.000539586
Search for a local minimum.
Step number 18 out of a maximum of 121
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.
Update second derivatives using D2CorX and points 17 18
DE= -3.66D-04 DEPred=-1.36D-03 R= 2.69D-01
Trust test= 2.69D-01 RLast= 1.00D+00 DXMaxT set to 1.26D+00
ITU= 0 0 0 1 1 -1 1 -1 1 1 1 1 1 1 0 1 0 0
Eigenvalues --- 0.00000 0.00179 0.00418 0.00705 0.01255
Eigenvalues --- 0.01407 0.01817 0.02071 0.02166 0.02314
Eigenvalues --- 0.02391 0.02947 0.03062 0.03086 0.03362
Eigenvalues --- 0.03880 0.04079 0.04574 0.04736 0.05264
Eigenvalues --- 0.05639 0.08953 0.09100 0.10008 0.12621
Eigenvalues --- 0.13281 0.15153 0.15924 0.15997 0.16002
Eigenvalues --- 0.16002 0.16046 0.16088 0.20844 0.21653
Eigenvalues --- 0.22030 0.22964 0.23468 0.24904 0.25171
Eigenvalues --- 0.28798 0.30586 0.34033 0.34621 0.34783
Eigenvalues --- 0.34915 0.35043 0.35689 0.35730 0.35858
Eigenvalues --- 0.36438 0.36659 0.38149 0.40522 0.42169
Eigenvalues --- 0.42930 0.46796 0.47697 0.48492 0.50111
Eigenvalues --- 0.54256 0.59447 0.60362
Eigenvalue 1 is 5.14D-07 Eigenvector:

	D25	D26	D28	D29	D27
1	0.62401	0.61770	0.17094	0.16198	0.15547
	D31	D32	D30	D44	D42
1	0.14793	0.13896	0.13245	-0.11070	-0.10874

En-DIIS/RFO-DIIS IScMMF= 0 using points: 18 17
RFO step: Lambda=-1.21635987D-04.
DidBck=T Rises=F RFO-DIIS coefs: 0.36229 0.63771
Iteration 1 RMS(Cart)= 0.23615767 RMS(Int)= 0.42498883
Iteration 2 RMS(Cart)= 0.11287350 RMS(Int)= 0.38512586
Iteration 3 RMS(Cart)= 0.12679303 RMS(Int)= 0.35062942
Iteration 4 RMS(Cart)= 0.11761668 RMS(Int)= 0.32114719
Iteration 5 RMS(Cart)= 0.03586926 RMS(Int)= 0.29415899
Iteration 6 RMS(Cart)= 0.03566508 RMS(Int)= 0.26730919
Iteration 7 RMS(Cart)= 0.03522386 RMS(Int)= 0.24046041
Iteration 8 RMS(Cart)= 0.03456662 RMS(Int)= 0.21361110
Iteration 9 RMS(Cart)= 0.03376330 RMS(Int)= 0.18676175
Iteration 10 RMS(Cart)= 0.03291470 RMS(Int)= 0.15991302
Iteration 11 RMS(Cart)= 0.03213757 RMS(Int)= 0.13306566
Iteration 12 RMS(Cart)= 0.03154709 RMS(Int)= 0.10622062
Iteration 13 RMS(Cart)= 0.03123529 RMS(Int)= 0.07937955
Iteration 14 RMS(Cart)= 0.03125156 RMS(Int)= 0.05254705
Iteration 15 RMS(Cart)= 0.03158956 RMS(Int)= 0.02574614
Iteration 16 RMS(Cart)= 0.03081714 RMS(Int)= 0.00202834
Iteration 17 RMS(Cart)= 0.00303463 RMS(Int)= 0.00139757
Iteration 18 RMS(Cart)= 0.00001300 RMS(Int)= 0.00139753

```
 Iteration 19 RMS(Cart)=    0.00000000 RMS(Int)=    0.00139753
 Iteration    1 RMS(Cart)=    0.24046655 RMS(Int)=    0.38807826
 Iteration    2 RMS(Cart)=    0.12706103 RMS(Int)=    0.34831455
 Iteration    3 RMS(Cart)=    0.12848189 RMS(Int)=    0.31500240
 Iteration    4 RMS(Cart)=    0.07349103 RMS(Int)=    0.28710671
 Iteration    5 RMS(Cart)=    0.03096970 RMS(Int)=    0.26023044
 Iteration    6 RMS(Cart)=    0.03181178 RMS(Int)=    0.23338699
 Iteration    7 RMS(Cart)=    0.03233161 RMS(Int)=    0.20654301
 Iteration    8 RMS(Cart)=    0.03292277 RMS(Int)=    0.17969984
 Iteration    9 RMS(Cart)=    0.03348275 RMS(Int)=    0.15285726
 Iteration 10 RMS(Cart)=    0.03391233 RMS(Int)=    0.12601512
 Iteration 11 RMS(Cart)=    0.03413813 RMS(Int)=    0.09917366
 Iteration 12 RMS(Cart)=    0.03411863 RMS(Int)=    0.07233430
 Iteration 13 RMS(Cart)=    0.03384582 RMS(Int)=    0.04550254
 Iteration 14 RMS(Cart)=    0.03334372 RMS(Int)=    0.01871597
 Iteration 15 RMS(Cart)=    0.02252426 RMS(Int)=    0.00137438
 Iteration 16 RMS(Cart)=    0.00150447 RMS(Int)=    0.00113106
 Iteration 17 RMS(Cart)=    0.00000332 RMS(Int)=    0.00113106
 Iteration 18 RMS(Cart)=    0.00000000 RMS(Int)=    0.00113106
 ITry= 2 IFail=0 DXMaxC= 3.67D+00 DCOld= 3.38D+00 DXMaxT= 1.26D+00 DXLimC= 3.00D+00
Rises=F
 Iteration    1 RMS(Cart)=    0.22292990 RMS(Int)=    0.33679661
 Iteration    2 RMS(Cart)=    0.12602276 RMS(Int)=    0.29872487
 Iteration    3 RMS(Cart)=    0.12766974 RMS(Int)=    0.26774244
 Iteration    4 RMS(Cart)=    0.03296474 RMS(Int)=    0.24074950
 Iteration    5 RMS(Cart)=    0.02999001 RMS(Int)=    0.21390209
 Iteration    6 RMS(Cart)=    0.03035189 RMS(Int)=    0.18705706
 Iteration    7 RMS(Cart)=    0.03084266 RMS(Int)=    0.16021302
 Iteration    8 RMS(Cart)=    0.03141342 RMS(Int)=    0.13337004
 Iteration    9 RMS(Cart)=    0.03195651 RMS(Int)=    0.10652821
 Iteration 10 RMS(Cart)=    0.03237679 RMS(Int)=    0.07968819
 Iteration 11 RMS(Cart)=    0.03260334 RMS(Int)=    0.05285283
 Iteration 12 RMS(Cart)=    0.03259590 RMS(Int)=    0.02603824
 Iteration 13 RMS(Cart)=    0.03128486 RMS(Int)=    0.00172508
 Iteration 14 RMS(Cart)=    0.00272870 RMS(Int)=    0.00089352
 Iteration 15 RMS(Cart)=    0.00001081 RMS(Int)=    0.00089348
 Iteration 16 RMS(Cart)=    0.00000000 RMS(Int)=    0.00089348
 ITry= 3 IFail=0 DXMaxC= 3.50D+00 DCOld= 3.38D+00 DXMaxT= 1.26D+00 DXLimC= 3.00D+00
Rises=F
 Iteration    1 RMS(Cart)=    0.20157063 RMS(Int)=    0.28608953
 Iteration    2 RMS(Cart)=    0.12828440 RMS(Int)=    0.24984058
 Iteration    3 RMS(Cart)=    0.08485821 RMS(Int)=    0.22108044
 Iteration    4 RMS(Cart)=    0.02798729 RMS(Int)=    0.19419015
 Iteration    5 RMS(Cart)=    0.02856625 RMS(Int)=    0.16734529
```

```
 Iteration    6 RMS(Cart)=    0.02887695 RMS(Int)=    0.14050034
 Iteration    7 RMS(Cart)=    0.02934897 RMS(Int)=    0.11365668
 Iteration    8 RMS(Cart)=    0.02989892 RMS(Int)=    0.08681482
 Iteration    9 RMS(Cart)=    0.03042347 RMS(Int)=    0.05997631
 Iteration 10 RMS(Cart)=    0.03083291 RMS(Int)=    0.03314871
 Iteration 11 RMS(Cart)=    0.03105840 RMS(Int)=    0.00647132
 Iteration 12 RMS(Cart)=    0.00767322 RMS(Int)=    0.00069383
 Iteration 13 RMS(Cart)=    0.00018849 RMS(Int)=    0.00068522
 Iteration 14 RMS(Cart)=    0.00000007 RMS(Int)=    0.00068522
 ITry= 4 IFail=0 DXMaxC= 3.19D+00 DCOld= 3.38D+00 DXMaxT= 1.26D+00 DXLimC= 3.00D+00
Rises=F
 Iteration    1 RMS(Cart)=    0.17896089 RMS(Int)=    0.23591702
 Iteration    2 RMS(Cart)=    0.12722641 RMS(Int)=    0.20193471
 Iteration    3 RMS(Cart)=    0.03938166 RMS(Int)=    0.17469501
 Iteration    4 RMS(Cart)=    0.02692419 RMS(Int)=    0.14784206
 Iteration    5 RMS(Cart)=    0.02710861 RMS(Int)=    0.12099646
 Iteration    6 RMS(Cart)=    0.02739318 RMS(Int)=    0.09415215
 Iteration    7 RMS(Cart)=    0.02784335 RMS(Int)=    0.06731027
 Iteration    8 RMS(Cart)=    0.02837055 RMS(Int)=    0.04047453
 Iteration    9 RMS(Cart)=    0.02887693 RMS(Int)=    0.01367876
 Iteration 10 RMS(Cart)=    0.01501059 RMS(Int)=    0.00062610
 Iteration 11 RMS(Cart)=    0.00072417 RMS(Int)=    0.00050678
 Iteration 12 RMS(Cart)=    0.00000077 RMS(Int)=    0.00050678
 ITry= 5 IFail=0 DXMaxC= 2.76D+00 DCOld= 3.19D+00 DXMaxT= 1.26D+00 DXLimC= 3.00D+00
Rises=F
```

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56660	-0.00027	-0.00048	0.00051	-0.00024	2.56636
R2	2.61787	0.00041	0.00142	-0.01324	-0.00648	2.61139
R3	2.03397	0.00007	0.00009	-0.00008	0.00004	2.03401
R4	2.63032	0.00008	-0.00096	0.00994	0.00492	2.63524
R5	2.03069	0.00009	0.00014	-0.00084	-0.00036	2.03033
R6	2.54283	0.00037	0.00055	0.00740	0.00499	2.54782
R7	2.68873	-0.00012	0.00083	-0.01876	-0.01042	2.67831
R8	2.52020	-0.00025	0.00022	-0.00662	-0.00364	2.51656
R9	2.11308	-0.00024	-0.00007	-0.00059	-0.00042	2.11265
R10	2.79009	0.00046	0.00205	0.00146	0.00293	2.79301
R11	2.90110	0.00032	0.00345	-0.01232	-0.00394	2.89716
R12	2.06045	0.00006	-0.00001	-0.00592	-0.00356	2.05690
R13	2.05867	0.00030	0.00073	-0.00161	-0.00024	2.05843
R14	2.06280	0.00204	0.00382	-0.01264	-0.00376	2.05904
R15	2.07301	0.00000	-0.00083	-0.00278	-0.00249	2.07052
R16	2.76819	-0.00142	-0.00185	-0.00845	-0.00692	2.76127
R17	4.07182	0.00006	0.00183	0.06113	0.03851	4.11032

R18	2.50683	-0.00011	-0.00016	0.00226	0.00120	2.50803
R19	2.04642	0.00036	0.00134	-0.01662	-0.00863	2.03779
R20	2.04307	-0.00001	0.00005	-0.00082	-0.00044	2.04263
R21	2.04598	0.00008	0.00022	-0.00267	-0.00138	2.04460
R22	1.91229	0.00175	0.00042	-0.00666	-0.00358	1.90871
R23	1.92091	0.00098	-0.00230	0.00886	0.00301	1.92392
A1	1.87248	0.00005	0.00065	-0.00119	0.00008	1.87256
A2	2.27798	-0.00006	-0.00007	-0.00103	-0.00076	2.27722
A3	2.13272	0.00001	-0.00058	0.00221	0.00068	2.13339
A4	1.86271	-0.00020	-0.00091	0.00405	0.00150	1.86422
A5	2.27723	0.00005	0.00004	-0.00063	-0.00040	2.27683
A6	2.14324	0.00015	0.00087	-0.00340	-0.00123	2.14201
A7	1.89735	0.00036	0.00172	-0.01266	-0.00588	1.89147
A8	2.25117	-0.00017	0.00125	-0.02814	-0.01579	2.23538
A9	2.13467	-0.00019	-0.00302	0.04081	0.02133	2.15600
A10	1.88857	-0.00041	-0.00111	0.00413	0.00149	1.89006
A11	2.23605	0.00021	-0.01896	0.24813	0.12997	2.36602
A12	2.15291	0.00027	0.02049	-0.24831	-0.12899	2.02392
A13	1.90350	0.00022	-0.00025	0.00531	0.00275	1.90624
A14	2.22920	-0.00011	-0.00496	0.02777	0.01075	2.23994
A15	2.14756	-0.00013	0.00583	-0.04156	-0.01961	2.12795
A16	1.94618	0.00122	0.00597	-0.03175	-0.01340	1.93278
A17	1.87100	-0.00054	0.00450	-0.04674	-0.02404	1.84695
A18	1.88968	-0.00056	-0.00701	0.04277	0.01872	1.90840
A19	1.91260	-0.00011	0.00019	-0.03047	-0.01857	1.89403
A20	1.94336	-0.00020	-0.00092	0.02212	0.01241	1.95577
A21	1.89900	0.00016	-0.00282	0.04403	0.02380	1.92280
A22	1.91223	-0.00093	-0.00235	0.03651	0.01988	1.93211
A23	1.89247	0.00076	-0.00066	-0.04520	-0.02783	1.86465
A24	1.87599	0.00052	0.00874	-0.04422	-0.01783	1.85816
A25	1.90257	-0.00007	-0.00694	0.05971	0.02890	1.93147
A26	1.88328	0.00143	0.02125	-0.05576	-0.01206	1.87122
A27	1.99623	-0.00174	-0.01978	0.04902	0.00904	2.00526
A28	2.86098	-0.00167	0.00837	-0.22019	-0.12374	2.73723
A29	2.17441	-0.00023	-0.00177	0.02558	0.01357	2.18798
A30	1.95293	0.00015	-0.00069	0.01867	0.01051	1.96344
A31	2.15584	0.00008	0.00246	-0.04422	-0.02408	2.13176
A32	2.08058	-0.00010	-0.00072	0.00785	0.00399	2.08458
A33	2.15613	0.00009	0.00072	-0.00735	-0.00369	2.15244
A34	2.04647	0.00001	0.00000	-0.00049	-0.00030	2.04617
A35	1.92601	0.00031	0.01400	-0.02803	-0.00262	1.92339
A36	1.90529	0.00035	0.01547	-0.07313	-0.02820	1.87710
A37	1.86199	-0.00030	0.00890	0.00148	0.01024	1.87223
D1	-0.00282	0.00029	0.00376	-0.01192	-0.00379	-0.00660

D2	3.13808	0.00026	0.00111	0.02184	0.01400	-3.13110
D3	3.14145	-0.00003	-0.00002	-0.00214	-0.00110	3.14035
D4	-0.00083	-0.00006	-0.00267	0.03162	0.01669	0.01585
D5	0.01258	-0.00064	-0.00866	0.02086	0.00429	0.01687
D6	-3.04790	-0.00043	-0.01819	0.14007	0.06714	-2.98075
D7	-3.13141	-0.00036	-0.00527	0.01208	0.00187	-3.12954
D8	0.09129	-0.00015	-0.01480	0.13128	0.06473	0.15602
D9	-0.00778	0.00016	0.00234	-0.00077	0.00209	-0.00569
D10	3.13378	0.00003	-0.00595	0.05879	0.02961	-3.11980
D11	3.13444	0.00019	0.00473	-0.03132	-0.01400	3.12044
D12	-0.00719	0.00006	-0.00355	0.02824	0.01352	0.00633
D13	0.01568	-0.00057	-0.00775	0.01374	0.00054	0.01622
D14	3.04491	0.00002	-0.00187	0.03261	0.02013	3.06504
D15	-3.12588	-0.00044	-0.00017	-0.04104	-0.02545	3.13186
D16	-0.09665	0.00014	0.00571	-0.02217	-0.00585	-0.10250
D17	0.13418	-0.00004	-0.00189	-0.12086	-0.07465	0.05953
D18	-3.00374	-0.00001	-0.00100	-0.12866	-0.07848	-3.08222
D19	-3.00745	-0.00019	-0.01114	-0.05411	-0.04332	-3.05077
D20	0.13781	-0.00016	-0.01025	-0.06192	-0.04715	0.09066
D21	-0.01750	0.00075	0.01015	-0.02148	-0.00302	-0.02051
D22	3.04757	0.00055	0.01866	-0.13021	-0.05946	2.98811
D23	-3.05328	0.00021	0.00744	-0.07727	-0.03663	-3.08990
D24	0.01179	0.00001	0.01595	-0.18600	-0.09307	-0.08129
D25	-2.08488	-0.00074	0.18365	-3.41463	-1.86477	2.33354
D26	0.92885	-0.00012	0.18864	-3.37194	-1.83488	-0.90604
D27	1.70304	-0.00040	0.06827	-0.86542	-0.45119	1.25185
D28	-2.48676	-0.00016	0.07496	-0.95082	-0.49541	-2.98217
D29	-0.44072	-0.00055	0.07038	-0.90179	-0.47081	-0.91154
D30	-1.34706	-0.00018	0.05781	-0.73353	-0.38238	-1.72944
D31	0.74632	0.00006	0.06450	-0.81893	-0.42660	0.31973
D32	2.79236	-0.00033	0.05992	-0.76991	-0.40200	2.39035
D33	-1.25470	0.00055	0.08126	-0.34984	-0.12853	-1.38324
D34	0.81992	0.00037	0.07119	-0.28332	-0.09890	0.72102
D35	2.98642	-0.00095	0.05208	-0.27836	-0.11461	2.87181
D36	2.95981	0.00053	0.07178	-0.25266	-0.07995	2.87987
D37	-1.24875	0.00035	0.06171	-0.18614	-0.05032	-1.29906
D38	0.91775	-0.00097	0.04260	-0.18118	-0.06603	0.85172
D39	0.85804	0.00053	0.07577	-0.30177	-0.10528	0.75276
D40	2.93267	0.00036	0.06570	-0.23525	-0.07565	2.85702
D41	-1.18402	-0.00097	0.04659	-0.23029	-0.09136	-1.27538
D42	2.90203	-0.00038	-0.22048	0.61133	0.14642	3.04845
D43	-1.34011	-0.00036	-0.19111	0.55357	0.14089	-1.19922
D44	0.84114	-0.00032	-0.23442	0.62151	0.13874	0.97988
D45	2.88218	-0.00030	-0.20505	0.56375	0.13321	3.01539

D46	-1.27906	-0.00013	-0.22766	0.55363	0.10453	-1.17453
D47	0.76198	-0.00011	-0.19828	0.49586	0.09899	0.86098
D48	-3.12942	0.00003	0.00013	-0.00622	-0.00359	-3.13301
D49	0.01408	0.00000	-0.00044	-0.00841	-0.00547	0.00862
D50	0.00809	0.00000	-0.00088	0.00261	0.00067	0.00876
D51	-3.13160	-0.00004	-0.00145	0.00043	-0.00121	-3.13281

Item	Value	Threshold	Converged?
Maximum Force	0.002040	0.000450	NO
RMS Force	0.000540	0.000300	NO
Maximum Displacement	2.759033	0.001800	NO
RMS Displacement	0.383366	0.001200	NO

Predicted change in Energy=-1.858612D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.717750	-1.944991	0.275779
2	6	0	-2.737884	-1.093864	-0.005707
3	7	0	-2.198739	0.192156	-0.017021
4	6	0	-0.882350	0.103553	0.260545
5	7	0	-0.575205	-1.181918	0.423845
6	6	0	0.823893	-1.641112	0.550917
7	6	0	1.340688	-2.184098	-0.786437
8	1	0	-1.709634	-3.016517	0.377252
9	1	0	-3.779912	-1.288436	-0.180807
10	1	0	1.403552	-0.757788	0.812613
11	1	0	0.889466	-2.382535	1.346222
12	1	0	0.979619	-3.198077	-0.955837
13	1	0	0.974043	-1.507710	-1.566545
14	35	0	1.748882	1.765659	1.135778
15	1	0	-0.026168	0.820975	0.306450
16	6	0	-2.871082	1.419902	-0.239142
17	6	0	-4.178909	1.558068	-0.417860
18	1	0	-2.198393	2.262647	-0.249952
19	1	0	-4.590686	2.542829	-0.588310
20	1	0	-4.871941	0.727340	-0.402884
21	7	0	2.795375	-2.256985	-0.669467
22	1	0	3.190075	-2.691348	-1.491498
23	1	0	3.148587	-1.302834	-0.632651

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.358059	0.000000			
3	N	2.210086	1.394509	0.000000		
4	C	2.212387	2.224344	1.348248	0.000000	
5	N	1.381888	2.206683	2.172166	1.331706	0.000000
6	C	2.574489	3.646309	3.580465	2.457526	1.478000
7	C	3.246463	4.293355	4.331989	3.357293	2.477861
8	H	1.076350	2.213718	3.269596	3.229993	2.157511
9	H	2.211797	1.074402	2.172346	3.244733	3.262989
10	H	3.382332	4.234866	3.816699	2.504403	2.060706
11	H	2.852169	4.079957	4.245524	3.240164	2.106543
12	H	3.219146	4.376104	4.740993	3.980863	2.895841
13	H	3.291067	4.047948	3.918815	3.062779	2.543219
14	Br	5.150346	5.441593	4.403245	3.232957	3.820529
15	H	3.242370	3.334285	2.284756	1.117967	2.080097
16	C	3.594138	2.528094	1.417302	2.436703	3.532715
17	C	4.337034	3.046173	2.438742	3.666490	4.604636
18	H	4.267509	3.408354	2.083552	2.579586	3.867010
19	H	5.398235	4.122844	3.401977	4.519113	5.569765
20	H	4.189375	2.833503	2.753420	4.092198	4.773959
21	N	4.621594	5.693012	5.600460	4.467966	3.702960
22	H	5.269446	6.316663	6.287129	5.240779	4.486006
23	H	4.991878	5.923450	5.586402	4.361671	3.872652

		6	7	8	9	10
6	C	0.000000				
7	C	1.533110	0.000000			
8	H	2.888020	3.369208	0.000000		
9	H	4.674914	5.233502	2.753860	0.000000	
10	H	1.088462	2.143658	3.870830	5.304411	0.000000
11	H	1.089274	2.188884	2.845375	5.033087	1.785729
12	H	2.172256	1.089597	3.007020	5.186573	3.043377
13	H	2.126966	1.095672	3.641011	4.956656	2.531255
14	Br	3.578233	4.411588	5.950286	6.452012	2.567387
15	H	2.616150	3.477522	4.191111	4.333316	2.189245
16	C	4.862802	5.570221	4.627172	2.857354	4.911316
17	C	6.016753	6.678743	5.258930	2.884090	6.167749
18	H	5.001494	5.708454	5.338711	3.887952	4.819345
19	H	6.936921	7.587114	6.335542	3.937258	6.984809
20	H	6.241941	6.871707	4.962385	2.303302	6.562382
21	N	2.399037	1.461201	4.686962	6.664179	2.526128
22	H	3.297464	2.043195	5.254056	7.229578	3.498463
23	H	2.630488	2.017120	5.249659	6.943232	2.330452

		11	12	13	14	15

11	H	0.000000				
12	H	2.443913	0.000000			
13	H	3.042480	1.797313	0.000000		
14	Br	4.241509	5.441075	4.314843	0.000000	
15	H	3.490271	4.331022	3.151397	2.175089	0.000000
16	C	5.577960	6.055352	5.011776	4.832600	2.958027
17	C	6.657985	7.037098	6.105030	6.131524	4.279391
18	H	5.801755	6.357479	5.100329	4.212864	2.665814
19	H	7.617985	8.007582	6.951980	6.615632	4.959859
20	H	6.776763	7.067914	6.365932	6.876109	4.898310
21	N	2.776915	2.065098	2.164119	4.531636	4.288049
22	H	3.666173	2.330198	2.513450	5.370711	5.090506
23	H	3.191445	2.898416	2.375452	3.808171	3.933388

		16	17	18	19	20
16	C	0.000000				
17	C	1.327193	0.000000			
18	H	1.078353	2.108808	0.000000		
19	H	2.083248	1.080911	2.432294	0.000000	
20	H	2.123650	1.081954	3.086813	1.846479	0.000000
21	N	6.768561	7.953526	6.748392	8.809013	8.231950
22	H	7.430236	8.573924	7.424224	9.420860	8.824320
23	H	6.618501	7.869123	6.438113	8.642189	8.276670

		21	22	23
21	N	0.000000		
22	H	1.010046	0.000000	
23	H	1.018096	1.633191	0.000000

Stoichiometry C7H12BrN3
Framework group C1[X(C7H12BrN3)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.586176	1.931947	-0.721417
2	6	0	-2.658695	1.181922	-0.358802
3	7	0	-2.164300	-0.053001	0.059758
4	6	0	-0.821519	-0.036032	-0.060346
5	7	0	-0.457692	1.161359	-0.515676
6	6	0	0.959583	1.575870	-0.578886
7	6	0	1.321989	2.455910	0.623037

8	1	0	-1.533083	2.938274	-1.099591
9	1	0	-3.708052	1.411902	-0.376101
10	1	0	1.540337	0.657032	-0.522228
11	1	0	1.146083	2.080223	-1.526179
12	1	0	0.973468	3.477114	0.471722
13	1	0	0.840758	2.009071	1.500105
14	35	0	1.846744	-1.860457	-0.122429
15	1	0	0.011622	-0.736635	0.194372
16	6	0	-2.895894	-1.180558	0.509346
17	6	0	-4.219372	-1.271483	0.549086
18	1	0	-2.255586	-1.987679	0.827793
19	1	0	-4.678764	-2.177433	0.918656
20	1	0	-4.879699	-0.477132	0.227215
21	7	0	2.781452	2.500829	0.678342
22	1	0	3.083662	3.139068	1.400501
23	1	0	3.107478	1.572424	0.939665

Rotational constants (GHZ): 0.7583693 0.4770702 0.3091576

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 365 symmetry adapted cartesian basis functions of A symmetry.

There are 352 symmetry adapted basis functions of A symmetry.

352 basis functions, 562 primitive gaussians, 365 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 835.2397498685 Hartrees.

NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 352 RedAO= T EigKep= 4.38D-06 NBF= 352

NBsUse= 352 1.00D-06 EigRej= -1.00D+00 NBFU= 352

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999156 0.035557 0.014121 -0.014973 Ang= 4.71 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3012.46055738 A.U. after 16 cycles

NFock= 16 Conv=0.24D-08 -V/T= 2.0016

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.001520740	-0.001873849	-0.001363633
2	6	0.000525931	-0.000324032	0.002244593
3	7	0.000515482	-0.000624894	0.003236821
4	6	0.012151418	-0.007542616	-0.008349450
5	7	-0.002276488	-0.001671177	0.001898800
6	6	-0.004934533	-0.005903747	-0.002811704
7	6	0.004240479	-0.001312055	0.009758475
8	1	-0.000479626	-0.000163953	-0.000212742
9	1	-0.000209713	0.000188253	0.000196571
10	1	0.001163229	0.002985362	0.005228388
11	1	-0.000227779	0.000325481	0.000688063
12	1	-0.004884345	-0.000685603	-0.004029152
13	1	-0.000259072	-0.001794958	-0.005399250
14	35	0.001680774	0.001086808	-0.001777128
15	1	-0.011227920	0.012283467	0.003371111
16	6	-0.001713737	0.002785077	-0.000761552
17	6	0.000285463	-0.002244159	-0.000063570
18	1	0.002906974	0.001654058	0.000620597
19	1	0.000367093	0.000140151	0.000131587
20	1	-0.000725915	-0.000156754	0.000001215
21	7	-0.003033145	0.006773260	-0.001735098
22	1	0.002917284	-0.002224720	-0.002580000
23	1	0.004738887	-0.001699402	0.001707058

Cartesian Forces: Max 0.012283467 RMS 0.003871871

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.019206743 RMS 0.003397808
Search for a local minimum.
Step number 19 out of a maximum of 121
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 19 18
DE= 6.40D-03 DEPred=-1.86D-03 R=-3.45D+00
Trust test=-3.45D+00 RLast= 2.88D+00 DXMaxT set to 6.31D-01
ITU= -1 0 0 0 1 1 -1 1 -1 1 1 1 1 1 1 0 1 0 0
Use linear search instead of GDIIS.
Energy rises -- skip Quadratic/GDIIS search.
Quartic linear search produced a step of -0.86826.
Iteration 1 RMS(Cart)= 0.15643428 RMS(Int)= 0.18965788
Iteration 2 RMS(Cart)= 0.12123480 RMS(Int)= 0.15537269
Iteration 3 RMS(Cart)= 0.02481122 RMS(Int)= 0.12834452
Iteration 4 RMS(Cart)= 0.02016211 RMS(Int)= 0.10149536
Iteration 5 RMS(Cart)= 0.01992663 RMS(Int)= 0.07464881
Iteration 6 RMS(Cart)= 0.01987293 RMS(Int)= 0.04780372
Iteration 7 RMS(Cart)= 0.02000091 RMS(Int)= 0.02096490
Iteration 8 RMS(Cart)= 0.01583932 RMS(Int)= 0.00049234
Iteration 9 RMS(Cart)= 0.00134067 RMS(Int)= 0.00005590
Iteration 10 RMS(Cart)= 0.00000249 RMS(Int)= 0.00005585
Iteration 11 RMS(Cart)= 0.00000000 RMS(Int)= 0.00005585

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56636	-0.00190	0.00021	0.00000	0.00021	2.56657
R2	2.61139	0.00280	0.00562	0.00000	0.00562	2.61701
R3	2.03401	0.00014	-0.00003	0.00000	-0.00003	2.03398
R4	2.63524	-0.00093	-0.00427	0.00000	-0.00426	2.63098
R5	2.03033	0.00014	0.00032	0.00000	0.00032	2.03064
R6	2.54782	-0.00163	-0.00433	0.00000	-0.00433	2.54349
R7	2.67831	0.00136	0.00905	0.00000	0.00905	2.68736
R8	2.51656	0.00783	0.00316	0.00000	0.00315	2.51971
R9	2.11265	0.00134	0.00037	0.00000	0.00037	2.11302
R10	2.79301	0.00091	-0.00254	0.00000	-0.00254	2.79047
R11	2.89716	0.00357	0.00342	0.00000	0.00342	2.90058
R12	2.05690	0.00430	0.00309	0.00000	0.00309	2.05999
R13	2.05843	0.00027	0.00020	0.00000	0.00020	2.05863
R14	2.05904	0.00288	0.00327	0.00000	0.00327	2.06231
R15	2.07052	0.00282	0.00217	0.00000	0.00217	2.07268
R16	2.76127	0.00425	0.00601	0.00000	0.00601	2.76728
R17	4.11032	0.00116	-0.03343	0.00000	-0.03343	4.07689

R18	2.50803	-0.00017	-0.00104	0.00000	-0.00104	2.50699
R19	2.03779	0.00310	0.00749	0.00000	0.00749	2.04529
R20	2.04263	-0.00004	0.00038	0.00000	0.00038	2.04301
R21	2.04460	0.00059	0.00120	0.00000	0.00120	2.04580
R22	1.90871	0.00420	0.00311	0.00000	0.00311	1.91182
R23	1.92392	0.00012	-0.00262	0.00000	-0.00262	1.92131
A1	1.87256	0.00058	-0.00007	0.00000	-0.00008	1.87247
A2	2.27722	-0.00080	0.00066	0.00000	0.00067	2.27789
A3	2.13339	0.00023	-0.00059	0.00000	-0.00058	2.13281
A4	1.86422	0.00030	-0.00131	0.00000	-0.00130	1.86291
A5	2.27683	0.00004	0.00035	0.00000	0.00035	2.27718
A6	2.14201	-0.00034	0.00107	0.00000	0.00108	2.14309
A7	1.89147	0.00328	0.00510	0.00000	0.00511	1.89658
A8	2.23538	0.00043	0.01371	0.00000	0.01373	2.24911
A9	2.15600	-0.00371	-0.01852	0.00000	-0.01850	2.13749
A10	1.89006	-0.00281	-0.00130	0.00000	-0.00131	1.88875
A11	2.36602	-0.01630	-0.11285	0.00000	-0.11286	2.25316
A12	2.02392	0.01921	0.11200	0.00000	0.11206	2.13598
A13	1.90624	-0.00131	-0.00239	0.00000	-0.00236	1.90389
A14	2.23994	-0.00615	-0.00933	0.00000	-0.00923	2.23071
A15	2.12795	0.00754	0.01703	0.00000	0.01709	2.14504
A16	1.93278	0.00479	0.01163	0.00000	0.01167	1.94446
A17	1.84695	-0.00130	0.02088	0.00000	0.02094	1.86789
A18	1.90840	-0.00315	-0.01625	0.00000	-0.01626	1.89214
A19	1.89403	0.00092	0.01612	0.00000	0.01618	1.91021
A20	1.95577	-0.00041	-0.01077	0.00000	-0.01078	1.94499
A21	1.92280	-0.00087	-0.02066	0.00000	-0.02069	1.90211
A22	1.93211	-0.00073	-0.01726	0.00000	-0.01726	1.91485
A23	1.86465	0.00245	0.02416	0.00000	0.02417	1.88881
A24	1.85816	0.00170	0.01548	0.00000	0.01550	1.87366
A25	1.93147	-0.00270	-0.02509	0.00000	-0.02511	1.90636
A26	1.87122	0.00120	0.01047	0.00000	0.01046	1.88168
A27	2.00526	-0.00179	-0.00785	0.00000	-0.00779	1.99748
A28	2.73723	0.00880	0.10744	0.00000	0.10744	2.84467
A29	2.18798	-0.00173	-0.01179	0.00000	-0.01178	2.17620
A30	1.96344	-0.00049	-0.00913	0.00000	-0.00913	1.95431
A31	2.13176	0.00222	0.02091	0.00000	0.02091	2.15267
A32	2.08458	-0.00084	-0.00347	0.00000	-0.00347	2.08111
A33	2.15244	0.00088	0.00321	0.00000	0.00321	2.15564
A34	2.04617	-0.00004	0.00026	0.00000	0.00026	2.04643
A35	1.92339	0.00159	0.00227	0.00000	0.00228	1.92567
A36	1.87710	0.00865	0.02448	0.00000	0.02449	1.90158
A37	1.87223	-0.00262	-0.00889	0.00000	-0.00888	1.86336
D1	-0.00660	0.00080	0.00329	0.00000	0.00333	-0.00327

D2	-3.13110	0.00105	-0.01216	0.00000	-0.01214	3.13995
D3	3.14035	-0.00083	0.00096	0.00000	0.00094	3.14129
D4	0.01585	-0.00058	-0.01449	0.00000	-0.01453	0.00132
D5	0.01687	-0.00170	-0.00372	0.00000	-0.00376	0.01311
D6	-2.98075	-0.00302	-0.05830	0.00000	-0.05844	-3.03920
D7	-3.12954	-0.00023	-0.00163	0.00000	-0.00161	-3.13115
D8	0.15602	-0.00156	-0.05620	0.00000	-0.05629	0.09973
D9	-0.00569	0.00030	-0.00182	0.00000	-0.00185	-0.00753
D10	-3.11980	0.00023	-0.02571	0.00000	-0.02574	3.13765
D11	3.12044	0.00008	0.01216	0.00000	0.01214	3.13259
D12	0.00633	0.00000	-0.01174	0.00000	-0.01175	-0.00542
D13	0.01622	-0.00138	-0.00047	0.00000	-0.00046	0.01576
D14	3.06504	0.00124	-0.01748	0.00000	-0.01777	3.04727
D15	3.13186	-0.00124	0.02210	0.00000	0.02218	-3.12914
D16	-0.10250	0.00138	0.00508	0.00000	0.00487	-0.09763
D17	0.05953	-0.00010	0.06482	0.00000	0.06485	0.12438
D18	-3.08222	-0.00024	0.06814	0.00000	0.06817	-3.01404
D19	-3.05077	-0.00030	0.03762	0.00000	0.03758	-3.01319
D20	0.09066	-0.00044	0.04094	0.00000	0.04091	0.13158
D21	-0.02051	0.00193	0.00262	0.00000	0.00264	-0.01787
D22	2.98811	0.00188	0.05163	0.00000	0.05161	3.03972
D23	-3.08990	0.00178	0.03180	0.00000	0.03157	-3.05833
D24	-0.08129	0.00172	0.08081	0.00000	0.08054	-0.00074
D25	2.33354	0.00003	1.61910	0.00000	1.61907	-2.33057
D26	-0.90604	0.00178	1.59315	0.00000	1.59317	0.68714
D27	1.25185	0.00099	0.39175	0.00000	0.39178	1.64363
D28	-2.98217	0.00381	0.43014	0.00000	0.43013	-2.55204
D29	-0.91154	0.00045	0.40879	0.00000	0.40880	-0.50273
D30	-1.72944	0.00035	0.33200	0.00000	0.33201	-1.39743
D31	0.31973	0.00317	0.37040	0.00000	0.37036	0.69009
D32	2.39035	-0.00020	0.34904	0.00000	0.34904	2.73939
D33	-1.38324	0.00297	0.11160	0.00000	0.11159	-1.27165
D34	0.72102	0.00078	0.08587	0.00000	0.08588	0.80690
D35	2.87181	0.00096	0.09951	0.00000	0.09948	2.97128
D36	2.87987	0.00135	0.06942	0.00000	0.06943	2.94930
D37	-1.29906	-0.00085	0.04369	0.00000	0.04373	-1.25534
D38	0.85172	-0.00067	0.05733	0.00000	0.05732	0.90904
D39	0.75276	0.00207	0.09141	0.00000	0.09141	0.84417
D40	2.85702	-0.00013	0.06568	0.00000	0.06570	2.92272
D41	-1.27538	0.00005	0.07932	0.00000	0.07930	-1.19608
D42	3.04845	-0.00196	-0.12713	0.00000	-0.12714	2.92131
D43	-1.19922	0.00070	-0.12233	0.00000	-0.12234	-1.32157
D44	0.97988	-0.00259	-0.12047	0.00000	-0.12046	0.85943
D45	3.01539	0.00007	-0.11566	0.00000	-0.11566	2.89974

D46	-1.17453	0.00121	-0.09076	0.00000	-0.09074	-1.26528
D47	0.86098	0.00387	-0.08595	0.00000	-0.08595	0.77503
D48	-3.13301	-0.00016	0.00312	0.00000	0.00311	-3.12989
D49	0.00862	-0.00002	0.00475	0.00000	0.00474	0.01336
D50	0.00876	-0.00001	-0.00058	0.00000	-0.00058	0.00818
D51	-3.13281	0.00014	0.00105	0.00000	0.00105	-3.13175

Item	Value	Threshold	Converged?
Maximum Force	0.019207	0.000450	NO
RMS Force	0.003398	0.000300	NO
Maximum Displacement	2.412436	0.001800	NO
RMS Displacement	0.338052	0.001200	NO

Predicted change in Energy=-4.121868D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.818655	-2.014744	0.302893
2	6	0	-2.812834	-1.125711	0.046260
3	7	0	-2.224859	0.135960	0.017296
4	6	0	-0.907897	0.003182	0.261382
5	7	0	-0.642527	-1.293507	0.422809
6	6	0	0.728636	-1.817823	0.582544
7	6	0	1.442844	-1.940248	-0.770564
8	1	0	-1.847861	-3.085678	0.406538
9	1	0	-3.864045	-1.281647	-0.112921
10	1	0	1.268155	-1.112890	1.215238
11	1	0	0.672208	-2.779374	1.091456
12	1	0	1.028217	-2.779869	-1.331022
13	1	0	1.275038	-1.013115	-1.332057
14	35	0	1.745384	1.824309	-0.140828
15	1	0	-0.104397	0.780416	0.237276
16	6	0	-2.834297	1.399281	-0.217111
17	6	0	-4.141517	1.598752	-0.323719
18	1	0	-2.102610	2.192124	-0.303420
19	1	0	-4.509560	2.597386	-0.513670
20	1	0	-4.876242	0.809302	-0.229121
21	7	0	2.850510	-2.236271	-0.496220
22	1	0	3.319706	-2.529178	-1.343319
23	1	0	3.312126	-1.385741	-0.184434

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.358172	0.000000			
3	N	2.207283	1.392253	0.000000		
4	C	2.214324	2.224739	1.345956	0.000000	
5	N	1.384861	2.209112	2.170621	1.333373	0.000000
6	C	2.570151	3.648099	3.586071	2.469301	1.476655
7	C	3.434419	4.409247	4.287588	3.219909	2.488209
8	H	1.076334	2.214145	3.266893	3.231975	2.159855
9	H	2.212228	1.074569	2.171059	3.244950	3.265781
10	H	3.342770	4.245132	3.898184	2.625007	2.076360
11	H	2.722295	3.996567	4.248057	3.305809	2.093661
12	H	3.370426	4.403045	4.571927	3.745619	2.841932
13	H	3.639678	4.315452	3.923060	2.887405	2.614427
14	Br	5.257146	5.432768	4.317216	3.243174	3.967440
15	H	3.279620	3.317445	2.227122	1.118162	2.150619
16	C	3.599653	2.538782	1.422091	2.426740	3.530505
17	C	4.341161	3.053683	2.435083	3.653010	4.600587
18	H	4.259810	3.410971	2.084613	2.556914	3.848231
19	H	5.401804	4.129631	3.400059	4.505838	5.565068
20	H	4.196083	2.842141	2.746624	4.078994	4.771915
21	N	4.742231	5.796644	5.625882	4.440127	3.732924
22	H	5.420093	6.442724	6.300511	5.182716	4.510585
23	H	5.192113	6.134816	5.745822	4.465025	4.002065

		6	7	8	9	10
6	C	0.000000				
7	C	1.534921	0.000000			
8	H	2.876938	3.677815	0.000000		
9	H	4.675882	5.387886	2.754879	0.000000	
10	H	1.090097	2.158343	3.775638	5.303957	0.000000
11	H	1.089383	2.182917	2.629389	4.926591	1.774159
12	H	2.162641	1.091326	3.374086	5.259530	3.052839
13	H	2.147512	1.096818	4.131674	5.288532	2.549257
14	Br	3.849957	3.828836	6.108927	6.411976	3.270138
15	H	2.750272	3.288116	4.244408	4.302290	2.534742
16	C	4.866591	5.454604	4.634312	2.873780	5.019238
17	C	6.017698	6.626407	5.266689	2.901400	6.243873
18	H	4.988042	5.464885	5.331429	3.899491	4.958982
19	H	6.937900	7.489140	6.342605	3.952744	7.080767
20	H	6.243016	6.912600	4.974537	2.325965	6.598077
21	N	2.416853	1.464383	4.859131	6.792898	2.587454
22	H	3.305846	2.048780	5.484108	7.394355	3.572247
23	H	2.729353	2.035986	5.464842	7.177282	2.492257

		11	12	13	14	15

11	H	0.000000				
12	H	2.448498	0.000000			
13	H	3.058837	1.783912	0.000000		
14	Br	4.885092	4.809298	3.113073	0.000000	
15	H	3.742304	4.051913	2.753615	2.157398	0.000000
16	C	5.609731	5.798716	4.893812	4.599995	2.835811
17	C	6.659028	6.849315	6.097348	5.894059	4.157250
18	H	5.861833	5.964793	4.768664	3.868951	2.505620
19	H	7.637846	7.762080	6.867826	6.313555	4.823978
20	H	6.738533	6.997068	6.509679	6.699550	4.794671
21	N	2.749667	2.076811	2.162602	4.223259	4.286011
22	H	3.605547	2.305194	2.545436	4.783025	5.017586
23	H	3.246424	2.911099	2.367618	3.572254	4.067272

		16	17	18	19	20
16	C	0.000000				
17	C	1.326641	0.000000			
18	H	1.082319	2.123592	0.000000		
19	H	2.080843	1.081114	2.449867	0.000000	
20	H	2.125502	1.082590	3.100121	1.847341	0.000000
21	N	6.753678	7.976565	6.646898	8.805405	8.309606
22	H	7.387347	8.587738	7.264544	9.395072	8.919667
23	H	6.748032	8.030155	6.491120	8.783647	8.477593

		21	22	23
21	N	0.000000		
22	H	1.011690	0.000000	
23	H	1.016711	1.628042	0.000000

Stoichiometry C7H12BrN3
Framework group C1[X(C7H12BrN3)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.706853	2.135928	-0.237207
2	6	0	-2.713653	1.264702	0.031027
3	7	0	-2.159660	-0.012038	-0.006336
4	6	0	-0.850607	0.094835	-0.300539
5	7	0	-0.556725	1.388975	-0.429838
6	6	0	0.820594	1.882733	-0.629098
7	6	0	1.592438	1.940226	0.696396

8	1	0	-1.711002	3.210179	-0.304014
9	1	0	-3.752851	1.442294	0.238938
10	1	0	1.314424	1.186119	-1.306720
11	1	0	0.769750	2.862276	-1.103086
12	1	0	1.224083	2.770639	1.301145
13	1	0	1.422401	0.999081	1.233372
14	35	0	1.766139	-1.807151	-0.069751
15	1	0	-0.068318	-0.703334	-0.335684
16	6	0	-2.793311	-1.266419	0.211279
17	6	0	-4.100058	-1.435471	0.365583
18	1	0	-2.080639	-2.080451	0.240722
19	1	0	-4.487187	-2.430145	0.537517
20	1	0	-4.816195	-0.624467	0.327875
21	7	0	2.995310	2.208878	0.373608
22	1	0	3.506468	2.460363	1.209664
23	1	0	3.420435	1.357836	0.014861

Rotational constants (GHZ): 0.8074380 0.4879127 0.3146441

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 365 symmetry adapted cartesian basis functions of A symmetry.

There are 352 symmetry adapted basis functions of A symmetry.

352 basis functions, 562 primitive gaussians, 365 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 840.0462127929 Hartrees.

NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 352 RedAO= T EigKep= 4.70D-06 NBF= 352

NBsUse= 352 1.00D-06 EigRej= -1.00D+00 NBFU= 352

Lowest energy guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999974 0.002931 0.001593 -0.006371 Ang= 0.82 deg.

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999298 -0.034375 -0.012343 0.008326 Ang= -4.29 deg.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3012.46723102 A.U. after 12 cycles

NFock= 12 Conv=0.62D-08 -V/T= 2.0017

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000207715	-0.000082723	-0.001408984
2	6	-0.000243820	-0.000107389	0.000493425
3	7	-0.000572353	-0.000409540	0.001465779
4	6	0.003208390	-0.001349192	-0.002139679
5	7	-0.001125749	0.000641320	0.002159561
6	6	0.000000414	-0.000289126	-0.000553765
7	6	0.002823560	-0.002426994	0.002688558
8	1	-0.000014895	-0.000105491	-0.000233895
9	1	-0.000088140	-0.000039137	-0.000015526
10	1	0.000018920	0.000369393	-0.000118226
11	1	-0.000468551	-0.000231391	0.000341407
12	1	-0.002506359	-0.000562980	-0.001726280
13	1	0.001426291	0.000149193	-0.000314956
14	35	0.000843636	-0.000577679	0.000153040
15	1	-0.002528539	0.002124919	-0.000341925
16	6	-0.000287579	0.000020158	0.000167700
17	6	0.000136374	-0.000335408	-0.000034003
18	1	0.000409185	0.000420426	0.000076742
19	1	0.000076771	0.000023677	-0.000005956
20	1	-0.000139367	-0.000034623	-0.000018555
21	7	-0.002794974	0.002816062	0.000901278
22	1	0.001129025	-0.000995099	-0.001476001
23	1	0.000905476	0.000981624	-0.000059738

Cartesian Forces: Max 0.003208390 RMS 0.001187865

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.002736984 RMS 0.000647102

Search for a local minimum.

Step number 20 out of a maximum of 121

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 18 20

ITU= 0 -1 0 0 0 1 1 -1 1 -1 1 1 1 1 1 1 0 1 0 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00002	0.00019	0.00434	0.00713	0.01358
Eigenvalues ---	0.01407	0.01821	0.02068	0.02170	0.02311
Eigenvalues ---	0.02391	0.02938	0.03062	0.03084	0.03479
Eigenvalues ---	0.03875	0.04275	0.04317	0.04625	0.05272
Eigenvalues ---	0.05843	0.09015	0.09462	0.10969	0.12613
Eigenvalues ---	0.12929	0.15131	0.15922	0.15988	0.16000
Eigenvalues ---	0.16017	0.16050	0.16156	0.21217	0.21732
Eigenvalues ---	0.22024	0.22955	0.23476	0.24885	0.24951
Eigenvalues ---	0.28841	0.31587	0.34012	0.34494	0.34628
Eigenvalues ---	0.34796	0.35084	0.35689	0.35858	0.35943
Eigenvalues ---	0.36438	0.36660	0.38116	0.40095	0.42198
Eigenvalues ---	0.42937	0.46802	0.47689	0.48507	0.50128
Eigenvalues ---	0.54249	0.59443	0.60358		

RFO step: Lambda=-1.46547356D-03 EMin= 2.18199694D-05

Quartic linear search produced a step of 0.95537.

Iteration 1 RMS(Cart)= 0.08979701 RMS(Int)= 0.03849667

Iteration 2 RMS(Cart)= 0.03203802 RMS(Int)= 0.00480786

Iteration 3 RMS(Cart)= 0.00479536 RMS(Int)= 0.00023918

Iteration 4 RMS(Cart)= 0.00011678 RMS(Int)= 0.00023249

Iteration 5 RMS(Cart)= 0.00000002 RMS(Int)= 0.00023249

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56657	-0.00028	-0.00002	-0.00163	-0.00165	2.56492
R2	2.61701	0.00052	-0.00082	0.00143	0.00060	2.61760
R3	2.03398	0.00008	0.00000	0.00032	0.00033	2.03430
R4	2.63098	0.00003	0.00063	-0.00025	0.00039	2.63137
R5	2.03064	0.00009	-0.00005	0.00043	0.00038	2.03103
R6	2.54349	0.00040	0.00063	0.00343	0.00407	2.54756
R7	2.68736	-0.00003	-0.00131	-0.00222	-0.00353	2.68383
R8	2.51971	-0.00007	-0.00047	-0.00139	-0.00187	2.51784
R9	2.11302	-0.00013	-0.00005	-0.00320	-0.00326	2.10976
R10	2.79047	0.00053	0.00037	0.00591	0.00627	2.79675
R11	2.90058	0.00043	-0.00050	0.00337	0.00287	2.90345
R12	2.05999	0.00018	-0.00045	-0.00091	-0.00136	2.05862
R13	2.05863	0.00039	-0.00003	0.00221	0.00218	2.06081
R14	2.06231	0.00227	-0.00047	0.01265	0.01218	2.07448
R15	2.07268	0.00007	-0.00031	-0.00178	-0.00209	2.07059
R16	2.76728	-0.00141	-0.00087	-0.01081	-0.01169	2.75560
R17	4.07689	0.00042	0.00485	0.01391	0.01875	4.09564
R18	2.50699	-0.00012	0.00015	-0.00016	-0.00001	2.50698
R19	2.04529	0.00058	-0.00109	0.00058	-0.00050	2.04478
R20	2.04301	0.00000	-0.00006	-0.00008	-0.00013	2.04288
R21	2.04580	0.00012	-0.00017	0.00015	-0.00003	2.04577

R22	1.91182	0.00204	-0.00045	0.00504	0.00459	1.91640
R23	1.92131	0.00122	0.00038	0.00077	0.00115	1.92245
A1	1.87247	0.00007	-0.00001	0.00193	0.00176	1.87424
A2	2.27789	-0.00009	-0.00009	-0.00069	-0.00071	2.27718
A3	2.13281	0.00002	0.00009	-0.00122	-0.00106	2.13175
A4	1.86291	-0.00022	0.00019	-0.00217	-0.00210	1.86081
A5	2.27718	0.00008	-0.00004	0.00035	0.00036	2.27755
A6	2.14309	0.00014	-0.00015	0.00182	0.00173	2.14482
A7	1.89658	0.00047	-0.00074	0.00269	0.00182	1.89840
A8	2.24911	-0.00014	-0.00197	-0.00363	-0.00557	2.24354
A9	2.13749	-0.00034	0.00270	0.00099	0.00372	2.14121
A10	1.88875	-0.00052	0.00017	-0.00243	-0.00272	1.88604
A11	2.25316	-0.00019	0.01635	0.01045	0.02662	2.27978
A12	2.13598	0.00077	-0.01617	-0.00397	-0.02044	2.11554
A13	1.90389	0.00021	0.00037	0.00085	0.00101	1.90489
A14	2.23071	-0.00014	0.00145	-0.00706	-0.00561	2.22510
A15	2.14504	-0.00008	-0.00240	0.00551	0.00315	2.14819
A16	1.94446	0.00151	-0.00165	0.01229	0.01064	1.95510
A17	1.86789	-0.00058	-0.00297	-0.00267	-0.00563	1.86226
A18	1.89214	-0.00073	0.00235	-0.01045	-0.00815	1.88399
A19	1.91021	-0.00036	-0.00228	-0.00573	-0.00799	1.90222
A20	1.94499	-0.00016	0.00155	0.00359	0.00515	1.95014
A21	1.90211	0.00029	0.00297	0.00259	0.00556	1.90767
A22	1.91485	-0.00095	0.00250	0.00192	0.00363	1.91848
A23	1.88881	0.00092	-0.00350	-0.00816	-0.01223	1.87658
A24	1.87366	0.00053	-0.00222	0.00836	0.00541	1.87907
A25	1.90636	-0.00030	0.00362	-0.00302	0.00123	1.90759
A26	1.88168	0.00169	-0.00153	0.05463	0.05302	1.93470
A27	1.99748	-0.00189	0.00119	-0.05235	-0.05117	1.94631
A28	2.84467	-0.00274	-0.01557	-0.03886	-0.05444	2.79023
A29	2.17620	-0.00029	0.00171	0.00027	0.00198	2.17818
A30	1.95431	0.00011	0.00132	0.00295	0.00427	1.95858
A31	2.15267	0.00018	-0.00303	-0.00322	-0.00625	2.14641
A32	2.08111	-0.00016	0.00050	-0.00068	-0.00018	2.08093
A33	2.15564	0.00017	-0.00046	0.00071	0.00024	2.15589
A34	2.04643	0.00000	-0.00004	-0.00003	-0.00007	2.04636
A35	1.92567	0.00047	-0.00032	0.02141	0.02080	1.94647
A36	1.90158	0.00039	-0.00354	0.01722	0.01339	1.91497
A37	1.86336	-0.00032	0.00130	0.01592	0.01666	1.88002
D1	-0.00327	0.00034	-0.00044	0.00780	0.00722	0.00394
D2	3.13995	0.00031	0.00178	0.00877	0.01055	-3.13269
D3	3.14129	-0.00006	-0.00016	-0.00110	-0.00131	3.13997
D4	0.00132	-0.00009	0.00206	-0.00013	0.00202	0.00334
D5	0.01311	-0.00074	0.00050	-0.03303	-0.03246	-0.01935

D6	-3.03920	-0.00056	0.00831	-0.02451	-0.01607	-3.05527
D7	-3.13115	-0.00038	0.00025	-0.02504	-0.02480	3.12724
D8	0.09973	-0.00020	0.00806	-0.01652	-0.00841	0.09132
D9	-0.00753	0.00017	0.00023	0.01973	0.02008	0.01255
D10	3.13765	0.00004	0.00370	0.00365	0.00758	-3.13796
D11	3.13259	0.00020	-0.00177	0.01886	0.01706	-3.13353
D12	-0.00542	0.00006	0.00169	0.00277	0.00457	-0.00085
D13	0.01576	-0.00064	0.00007	-0.04049	-0.04044	-0.02468
D14	3.04727	0.00008	0.00226	0.00104	0.00394	3.05121
D15	-3.12914	-0.00052	-0.00312	-0.02566	-0.02885	3.12520
D16	-0.09763	0.00020	-0.00093	0.01587	0.01553	-0.08210
D17	0.12438	-0.00007	-0.00937	-0.02635	-0.03578	0.08859
D18	-3.01404	-0.00005	-0.00985	-0.02441	-0.03432	-3.04837
D19	-3.01319	-0.00022	-0.00548	-0.04441	-0.04983	-3.06302
D20	0.13158	-0.00020	-0.00596	-0.04248	-0.04837	0.08320
D21	-0.01787	0.00086	-0.00036	0.04557	0.04509	0.02721
D22	3.03972	0.00069	-0.00750	0.03679	0.02903	3.06875
D23	-3.05833	0.00027	-0.00483	0.00632	0.00226	-3.05608
D24	-0.00074	0.00009	-0.01197	-0.00245	-0.01380	-0.01454
D25	-2.33057	-0.00076	-0.23473	-0.19359	-0.42833	-2.75890
D26	0.68714	-0.00003	-0.23092	-0.14659	-0.37750	0.30964
D27	1.64363	-0.00020	-0.05676	-0.03891	-0.09574	1.54789
D28	-2.55204	-0.00014	-0.06237	-0.04049	-0.10293	-2.65496
D29	-0.50273	-0.00049	-0.05924	-0.04428	-0.10355	-0.60629
D30	-1.39743	-0.00002	-0.04812	-0.02898	-0.07706	-1.47449
D31	0.69009	0.00005	-0.05372	-0.03056	-0.08425	0.60584
D32	2.73939	-0.00030	-0.05060	-0.03435	-0.08487	2.65452
D33	-1.27165	0.00065	-0.01619	0.05762	0.04143	-1.23022
D34	0.80690	0.00028	-0.01244	0.05023	0.03775	0.84465
D35	2.97128	-0.00114	-0.01446	-0.01299	-0.02745	2.94383
D36	2.94930	0.00067	-0.01005	0.05704	0.04701	2.99631
D37	-1.25534	0.00030	-0.00630	0.04966	0.04333	-1.21200
D38	0.90904	-0.00112	-0.00832	-0.01356	-0.02187	0.88718
D39	0.84417	0.00065	-0.01325	0.05530	0.04208	0.88625
D40	2.92272	0.00029	-0.00950	0.04792	0.03840	2.96113
D41	-1.19608	-0.00114	-0.01152	-0.01530	-0.02679	-1.22288
D42	2.92131	-0.00042	0.01842	-0.29584	-0.27747	2.64384
D43	-1.32157	-0.00030	0.01772	-0.25414	-0.23618	-1.55775
D44	0.85943	-0.00046	0.01747	-0.33128	-0.31451	0.54492
D45	2.89974	-0.00035	0.01677	-0.28958	-0.27322	2.62652
D46	-1.26528	-0.00007	0.01317	-0.33297	-0.31949	-1.58477
D47	0.77503	0.00004	0.01246	-0.29127	-0.27820	0.49683
D48	-3.12989	0.00002	-0.00045	-0.00055	-0.00100	-3.13090
D49	0.01336	-0.00001	-0.00069	-0.00289	-0.00358	0.00978

D50	0.00818	0.00000	0.00009	-0.00268	-0.00259	0.00558
D51	-3.13175	-0.00003	-0.00015	-0.00502	-0.00517	-3.13692

Item	Value	Threshold	Converged?
Maximum Force	0.002737	0.000450	NO
RMS Force	0.000647	0.000300	NO
Maximum Displacement	0.564918	0.001800	NO
RMS Displacement	0.112823	0.001200	NO

Predicted change in Energy=-1.505867D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.793780	-1.986607	0.255748
2	6	0	-2.805823	-1.114565	0.015812
3	7	0	-2.242818	0.159000	0.017267
4	6	0	-0.917582	0.047185	0.237829
5	7	0	-0.634146	-1.243897	0.405216
6	6	0	0.744761	-1.752181	0.580116
7	6	0	1.450572	-1.977784	-0.765834
8	1	0	-1.800757	-3.060060	0.336478
9	1	0	-3.853638	-1.289273	-0.147588
10	1	0	1.288651	-0.994473	1.142969
11	1	0	0.692741	-2.669480	1.167587
12	1	0	1.006055	-2.838898	-1.281572
13	1	0	1.301900	-1.076775	-1.371362
14	35	0	1.864621	1.699557	0.109585
15	1	0	-0.112497	0.820664	0.235421
16	6	0	-2.884026	1.410297	-0.183098
17	6	0	-4.193141	1.577126	-0.318542
18	1	0	-2.178907	2.230267	-0.219092
19	1	0	-4.584829	2.572089	-0.477557
20	1	0	-4.906664	0.763887	-0.279834
21	7	0	2.863632	-2.210226	-0.490924
22	1	0	3.288949	-2.797423	-1.199964
23	1	0	3.362250	-1.323513	-0.483376

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357298	0.000000			
3	N	2.205026	1.392460	0.000000		

4	C	2.214578	2.228096	1.348111	0.000000	
5	N	1.385176	2.210101	2.169436	1.332384	0.000000
6	C	2.569896	3.651253	3.590967	2.473512	1.479975
7	C	3.401401	4.412825	4.338229	3.273529	2.501199
8	H	1.076507	2.213129	3.264914	3.231826	2.159665
9	H	2.211779	1.074773	2.172421	3.248860	3.266922
10	H	3.357510	4.248485	3.881879	2.602267	2.074521
11	H	2.735060	3.998037	4.235687	3.292090	2.091440
12	H	3.305878	4.380291	4.607554	3.786612	2.842453
13	H	3.613657	4.335789	4.002556	2.962917	2.632951
14	Br	5.195485	5.453542	4.387812	3.238430	3.872357
15	H	3.272292	3.323754	2.241352	1.116439	2.136202
16	C	3.594465	2.533892	1.420224	2.429436	3.528856
17	C	4.334390	3.046579	2.434668	3.657808	4.598744
18	H	4.260966	3.411174	2.085688	2.562337	3.853033
19	H	5.395313	4.123068	3.398950	4.509504	5.563177
20	H	4.188331	2.833641	2.747768	4.085880	4.770210
21	N	4.722183	5.796549	5.652197	4.463694	3.737821
22	H	5.348893	6.438662	6.389251	5.277683	4.514500
23	H	5.250776	6.191767	5.819388	4.551473	4.094766

		6	7	8	9	10
6	C	0.000000				
7	C	1.536440	0.000000			
8	H	2.872206	3.599660	0.000000		
9	H	4.678580	5.384321	2.753966	0.000000	
10	H	1.089376	2.153287	3.802830	5.309951	0.000000
11	H	1.090534	2.188806	2.657221	4.929930	1.778022
12	H	2.171431	1.097770	3.247336	5.225310	3.059438
13	H	2.138888	1.095711	4.059139	5.303050	2.515712
14	Br	3.659232	3.802713	6.011691	6.457377	2.942349
15	H	2.733723	3.358125	4.233255	4.312152	2.466087
16	C	4.873588	5.532397	4.628987	2.868638	4.995259
17	C	6.022852	6.684980	5.258902	2.891493	6.228899
18	H	5.004645	5.583882	5.332844	3.898333	4.927283
19	H	6.944243	7.563763	6.335204	3.943809	7.060045
20	H	6.245696	6.940274	4.964783	2.311238	6.595311
21	N	2.417963	1.458199	4.812830	6.788796	2.574534
22	H	3.276294	2.059103	5.323038	7.375537	3.569475
23	H	2.857625	2.040188	5.508575	7.223777	2.655763

		11	12	13	14	15
11	H	0.000000				
12	H	2.474925	0.000000			
13	H	3.058438	1.789040	0.000000		
14	Br	4.645552	4.823902	3.196541	0.000000	

15	H	3.701141	4.116409	2.860514	2.167322	0.000000
16	C	5.591260	5.864728	5.011933	4.766443	2.864297
17	C	6.641843	6.889146	6.192503	6.074105	4.186975
18	H	5.846089	6.080237	4.937638	4.091430	2.542364
19	H	7.617958	7.821969	6.983314	6.534635	4.855675
20	H	6.725799	6.995984	6.567018	6.846709	4.822110
21	N	2.770261	2.114462	2.121058	4.079832	4.309433
22	H	3.515959	2.284728	2.634078	4.895554	5.169208
23	H	3.415200	2.912931	2.257087	3.425412	4.145845

		16	17	18	19	20
16	C	0.000000				
17	C	1.326634	0.000000			
18	H	1.082053	2.119816	0.000000		
19	H	2.080672	1.081044	2.443789	0.000000	
20	H	2.125622	1.082577	3.097518	1.847232	0.000000
21	N	6.799891	8.010730	6.724513	8.851570	8.322704
22	H	7.539532	8.711788	7.492478	9.557714	8.983186
23	H	6.824943	8.094739	6.588142	8.850526	8.530745

		21	22	23
21	N	0.000000		
22	H	1.014117	0.000000	
23	H	1.017318	1.640513	0.000000

Stoichiometry C7H12BrN3
Framework group C1[X(C7H12BrN3)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.677826	2.085206	-0.304154
2	6	0	-2.722588	1.262902	-0.031120
3	7	0	-2.212245	-0.032281	0.000454
4	6	0	-0.885528	0.018420	-0.233328
5	7	0	-0.550937	1.291344	-0.440594
6	6	0	0.846041	1.737122	-0.640751
7	6	0	1.572284	1.972329	0.692627
8	1	0	-1.641544	3.155248	-0.416230
9	1	0	-3.760894	1.485279	0.135032
10	1	0	1.353484	0.941679	-1.185280
11	1	0	0.826475	2.638395	-1.254421

12	1	0	1.167948	2.865591	1.186281
13	1	0	1.392158	1.096115	1.325389
14	35	0	1.827690	-1.742745	-0.077843
15	1	0	-0.112805	-0.787170	-0.214372
16	6	0	-2.902376	-1.249779	0.242230
17	6	0	-4.215985	-1.358553	0.392421
18	1	0	-2.231139	-2.096712	0.296875
19	1	0	-4.646680	-2.331516	0.583469
20	1	0	-4.895918	-0.518074	0.335324
21	7	0	2.991211	2.138312	0.400324
22	1	0	3.446424	2.727771	1.088620
23	1	0	3.453012	1.231967	0.414967

Rotational constants (GHZ): 0.8550459 0.4692189 0.3137792

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 365 symmetry adapted cartesian basis functions of A symmetry.

There are 352 symmetry adapted basis functions of A symmetry.

352 basis functions, 562 primitive gaussians, 365 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 841.7768513714 Hartrees.

NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 352 RedAO= T EigKep= 4.49D-06 NBF= 352

NBsUse= 352 1.00D-06 EigRej= -1.00D+00 NBFU= 352

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999973 0.006988 0.002181 -0.000970 Ang= 0.85 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3012.46691841 A.U. after 13 cycles
NFock= 13 Conv=0.83D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000151744	-0.000409815	0.000735876
2	6	0.000118023	0.000327555	0.001127038
3	7	0.000349750	0.000366064	-0.001742088
4	6	0.001203561	-0.002457641	0.002104729
5	7	0.000505630	-0.001457340	-0.002853915
6	6	-0.001167623	-0.001127129	0.001408985
7	6	-0.000645946	0.003219678	0.000750437
8	1	-0.000075122	0.000041611	0.000194251
9	1	0.000086521	0.000188327	0.000128271
10	1	0.000528511	0.000374194	-0.000239198
11	1	-0.000067650	-0.000166205	-0.000175549
12	1	0.002328821	0.001607155	0.000606355
13	1	-0.002732001	-0.000981955	-0.001897210
14	35	0.001305517	0.000283156	-0.000574139
15	1	-0.003049413	0.002950173	0.000376709
16	6	-0.000318793	0.000555754	-0.000658557
17	6	-0.000151936	-0.000313512	-0.000107837
18	1	0.000578924	0.000202029	0.000244494
19	1	0.000015468	0.000049560	0.000121275
20	1	-0.000130565	0.000047133	0.000038117
21	7	0.002440650	-0.003837554	-0.002422948
22	1	-0.000486581	0.000944079	0.000675735
23	1	-0.000787489	-0.000405318	0.002159172

Cartesian Forces: Max 0.003837554 RMS 0.001319663

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.003414141 RMS 0.000859858
Search for a local minimum.

Step number 21 out of a maximum of 121
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 20 21
DE= 3.13D-04 DEPred=-1.51D-03 R=-2.08D-01
Trust test=-2.08D-01 RLast= 9.50D-01 DXMaxT set to 3.15D-01
ITU= -1 0 -1 0 0 0 1 1 -1 1 -1 1 1 1 1 1 1 0 1 0
ITU= 0

Eigenvalues ---	0.00019	0.00043	0.00495	0.00783	0.01315
Eigenvalues ---	0.01408	0.01760	0.01904	0.02165	0.02306
Eigenvalues ---	0.02391	0.02597	0.03062	0.03077	0.03361
Eigenvalues ---	0.03478	0.03927	0.04309	0.04557	0.05260
Eigenvalues ---	0.05693	0.08931	0.09463	0.10436	0.11839
Eigenvalues ---	0.12678	0.15236	0.15919	0.15975	0.16000
Eigenvalues ---	0.16015	0.16055	0.16171	0.20091	0.21659
Eigenvalues ---	0.22035	0.22969	0.23477	0.24692	0.24936
Eigenvalues ---	0.28563	0.31087	0.33475	0.34094	0.34632
Eigenvalues ---	0.34793	0.35026	0.35689	0.35736	0.35859
Eigenvalues ---	0.36436	0.36656	0.38126	0.39865	0.42212
Eigenvalues ---	0.42923	0.46792	0.47574	0.47777	0.50127
Eigenvalues ---	0.54244	0.59538	0.60361		

En-DIIS/RFO-DIIS IScMMF= 0 using points: 21 20
RFO step: Lambda=-2.86645893D-04.
DidBck=T Rises=T RFO-DIIS coefs: 0.40734 0.59266
Iteration 1 RMS(Cart)= 0.10928500 RMS(Int)= 0.06709333
Iteration 2 RMS(Cart)= 0.04751928 RMS(Int)= 0.02128263
Iteration 3 RMS(Cart)= 0.02087175 RMS(Int)= 0.00103048
Iteration 4 RMS(Cart)= 0.00099146 RMS(Int)= 0.00024133
Iteration 5 RMS(Cart)= 0.00000210 RMS(Int)= 0.00024133
Iteration 6 RMS(Cart)= 0.00000000 RMS(Int)= 0.00024133

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56492	0.00033	0.00098	-0.00173	-0.00077	2.56415
R2	2.61760	-0.00004	-0.00035	0.00235	0.00200	2.61961
R3	2.03430	-0.00003	-0.00019	0.00031	0.00012	2.03442
R4	2.63137	-0.00029	-0.00023	-0.00024	-0.00049	2.63088
R5	2.03103	-0.00013	-0.00023	0.00056	0.00033	2.03136
R6	2.54756	-0.00045	-0.00241	0.00246	0.00004	2.54760
R7	2.68383	0.00053	0.00209	-0.00058	0.00151	2.68535
R8	2.51784	0.00163	0.00111	-0.00101	0.00013	2.51797
R9	2.10976	0.00098	0.00193	-0.00607	-0.00414	2.10562
R10	2.79675	-0.00032	-0.00372	0.00136	-0.00236	2.79439
R11	2.90345	0.00009	-0.00170	-0.00598	-0.00768	2.89577

R12	2.05862	0.00040	0.00081	0.00100	0.00181	2.06043
R13	2.06081	0.00005	-0.00129	0.00247	0.00118	2.06200
R14	2.07448	-0.00249	-0.00722	0.01444	0.00723	2.08171
R15	2.07059	0.00061	0.00124	0.00188	0.00312	2.07372
R16	2.75560	0.00173	0.00693	-0.00812	-0.00120	2.75440
R17	4.09564	0.00134	-0.01111	0.03133	0.02022	4.11586
R18	2.50698	0.00023	0.00001	-0.00054	-0.00053	2.50644
R19	2.04478	0.00052	0.00030	0.00238	0.00267	2.04746
R20	2.04288	0.00002	0.00008	-0.00003	0.00005	2.04293
R21	2.04577	0.00005	0.00002	0.00046	0.00047	2.04625
R22	1.91640	-0.00122	-0.00272	0.01353	0.01081	1.92721
R23	1.92245	-0.00072	-0.00068	0.01120	0.01052	1.93297
A1	1.87424	-0.00004	-0.00105	0.00125	0.00027	1.87451
A2	2.27718	-0.00002	0.00042	-0.00016	0.00024	2.27742
A3	2.13175	0.00006	0.00063	-0.00113	-0.00053	2.13123
A4	1.86081	0.00040	0.00125	-0.00258	-0.00130	1.85951
A5	2.27755	-0.00004	-0.00022	0.00144	0.00120	2.27875
A6	2.14482	-0.00036	-0.00103	0.00114	0.00010	2.14492
A7	1.89840	-0.00001	-0.00108	0.00317	0.00215	1.90055
A8	2.24354	0.00048	0.00330	-0.00267	0.00062	2.24416
A9	2.14121	-0.00047	-0.00220	-0.00057	-0.00278	2.13843
A10	1.88604	0.00012	0.00161	-0.00378	-0.00207	1.88397
A11	2.27978	-0.00341	-0.01578	0.00037	-0.01549	2.26429
A12	2.11554	0.00326	0.01211	0.00689	0.01899	2.13453
A13	1.90489	-0.00045	-0.00060	0.00048	-0.00003	1.90486
A14	2.22510	-0.00037	0.00332	-0.00640	-0.00314	2.22197
A15	2.14819	0.00087	-0.00187	0.00670	0.00474	2.15293
A16	1.95510	0.00014	-0.00631	0.01784	0.01153	1.96663
A17	1.86226	0.00037	0.00334	-0.00884	-0.00552	1.85674
A18	1.88399	-0.00021	0.00483	-0.01278	-0.00798	1.87602
A19	1.90222	-0.00103	0.00474	-0.00629	-0.00155	1.90067
A20	1.95014	0.00049	-0.00306	0.00751	0.00446	1.95461
A21	1.90767	0.00024	-0.00329	0.00163	-0.00169	1.90598
A22	1.91848	0.00182	-0.00215	0.00241	0.00066	1.91915
A23	1.87658	-0.00054	0.00725	0.00466	0.01223	1.88881
A24	1.87907	-0.00105	-0.00321	-0.00838	-0.01117	1.86790
A25	1.90759	-0.00107	-0.00073	0.00357	0.00245	1.91003
A26	1.93470	-0.00172	-0.03142	0.02836	-0.00305	1.93165
A27	1.94631	0.00264	0.03032	-0.03127	-0.00090	1.94541
A28	2.79023	-0.00141	0.03226	-0.05541	-0.02314	2.76709
A29	2.17818	0.00001	-0.00117	-0.00198	-0.00315	2.17503
A30	1.95858	-0.00035	-0.00253	0.00211	-0.00043	1.95816
A31	2.14641	0.00034	0.00371	-0.00012	0.00359	2.15000
A32	2.08093	-0.00013	0.00010	-0.00159	-0.00148	2.07945

A33	2.15589	0.00019	-0.00014	0.00150	0.00135	2.15724
A34	2.04636	-0.00006	0.00004	0.00009	0.00013	2.04649
A35	1.94647	0.00017	-0.01233	-0.01857	-0.03146	1.91501
A36	1.91497	0.00018	-0.00793	-0.01762	-0.02614	1.88883
A37	1.88002	0.00053	-0.00987	-0.01749	-0.02862	1.85140
D1	0.00394	0.00021	-0.00428	0.00383	-0.00027	0.00367
D2	-3.13269	-0.00001	-0.00625	0.00450	-0.00174	-3.13443
D3	3.13997	0.00005	0.00078	-0.00435	-0.00352	3.13645
D4	0.00334	-0.00018	-0.00120	-0.00368	-0.00498	-0.00164
D5	-0.01935	0.00023	0.01924	-0.03295	-0.01383	-0.03318
D6	-3.05527	-0.00031	0.00952	-0.04164	-0.03226	-3.08753
D7	3.12724	0.00038	0.01470	-0.02560	-0.01092	3.11632
D8	0.09132	-0.00016	0.00498	-0.03429	-0.02935	0.06197
D9	0.01255	-0.00056	-0.01190	0.02612	0.01411	0.02666
D10	-3.13796	-0.00028	-0.00450	0.01777	0.01303	-3.12493
D11	-3.13353	-0.00036	-0.01011	0.02552	0.01544	-3.11810
D12	-0.00085	-0.00007	-0.00271	0.01717	0.01435	0.01350
D13	-0.02468	0.00071	0.02396	-0.04678	-0.02280	-0.04747
D14	3.05121	0.00023	-0.00234	0.01600	0.01293	3.06414
D15	3.12520	0.00044	0.01710	-0.03901	-0.02181	3.10339
D16	-0.08210	-0.00004	-0.00920	0.02378	0.01391	-0.06819
D17	0.08859	-0.00014	0.02121	-0.00513	0.01615	0.10474
D18	-3.04837	-0.00030	0.02034	-0.00721	0.01320	-3.03516
D19	-3.06302	0.00019	0.02953	-0.01450	0.01496	-3.04806
D20	0.08320	0.00002	0.02867	-0.01659	0.01201	0.09522
D21	0.02721	-0.00058	-0.02672	0.04923	0.02259	0.04981
D22	3.06875	-0.00016	-0.01721	0.05653	0.03959	3.10833
D23	-3.05608	0.00014	-0.00134	-0.00623	-0.00843	-3.06451
D24	-0.01454	0.00056	0.00818	0.00106	0.00856	-0.00598
D25	-2.75890	0.00066	0.25385	-0.15594	0.09792	-2.66098
D26	0.30964	-0.00002	0.22373	-0.08651	0.13722	0.44686
D27	1.54789	0.00132	0.05674	-0.07050	-0.01370	1.53419
D28	-2.65496	0.00037	0.06100	-0.07358	-0.01254	-2.66750
D29	-0.60629	0.00075	0.06137	-0.08274	-0.02129	-0.62758
D30	-1.47449	0.00080	0.04567	-0.07981	-0.03420	-1.50870
D31	0.60584	-0.00015	0.04993	-0.08289	-0.03304	0.57280
D32	2.65452	0.00022	0.05030	-0.09205	-0.04179	2.61272
D33	-1.23022	-0.00036	-0.02455	-0.15541	-0.17997	-1.41020
D34	0.84465	-0.00095	-0.02237	-0.14703	-0.16936	0.67529
D35	2.94383	0.00130	0.01627	-0.18615	-0.16990	2.77393
D36	2.99631	-0.00024	-0.02786	-0.15123	-0.17911	2.81720
D37	-1.21200	-0.00083	-0.02568	-0.14284	-0.16849	-1.38049
D38	0.88718	0.00142	0.01296	-0.18196	-0.16904	0.71814
D39	0.88625	-0.00017	-0.02494	-0.15385	-0.17880	0.70745

D40	2.96113	-0.00076	-0.02276	-0.14547	-0.16819	2.79294
D41	-1.22288	0.00149	0.01588	-0.18459	-0.16873	-1.39161
D42	2.64384	0.00043	0.16445	0.34481	0.50885	-3.13050
D43	-1.55775	0.00131	0.13997	0.29976	0.44004	-1.11771
D44	0.54492	-0.00012	0.18640	0.33036	0.51672	1.06164
D45	2.62652	0.00077	0.16192	0.28532	0.44791	3.07442
D46	-1.58477	0.00063	0.18935	0.32761	0.51635	-1.06842
D47	0.49683	0.00151	0.16488	0.28256	0.44753	0.94436
D48	-3.13090	-0.00020	0.00059	-0.00286	-0.00227	-3.13317
D49	0.00978	-0.00004	0.00212	-0.00263	-0.00051	0.00928
D50	0.00558	-0.00002	0.00154	-0.00056	0.00098	0.00656
D51	-3.13692	0.00014	0.00306	-0.00032	0.00274	-3.13418

Item	Value	Threshold	Converged?
Maximum Force	0.003414	0.000450	NO
RMS Force	0.000860	0.000300	NO
Maximum Displacement	0.914548	0.001800	NO
RMS Displacement	0.149471	0.001200	NO

Predicted change in Energy=-1.009064D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.813845	-1.994824	0.223991
2	6	0	-2.812100	-1.104648	-0.004542
3	7	0	-2.225549	0.157958	-0.002079
4	6	0	-0.898076	0.022244	0.189917
5	7	0	-0.639221	-1.272745	0.367204
6	6	0	0.724171	-1.809472	0.566516
7	6	0	1.441499	-2.105812	-0.754773
8	1	0	-1.839052	-3.068165	0.303388
9	1	0	-3.864172	-1.259323	-0.161820
10	1	0	1.280643	-1.042779	1.106284
11	1	0	0.638170	-2.698634	1.193115
12	1	0	1.108892	-3.077336	-1.153550
13	1	0	1.187716	-1.311887	-1.468555
14	35	0	1.894103	1.649673	-0.050532
15	1	0	-0.095147	0.794793	0.185760
16	6	0	-2.846566	1.423932	-0.178021
17	6	0	-4.155991	1.614875	-0.268340
18	1	0	-2.124531	2.229868	-0.233110
19	1	0	-4.533239	2.618069	-0.409752

20	1	0	-4.883755	0.815388	-0.207556
21	7	0	2.870515	-2.128960	-0.468636
22	1	0	3.390313	-2.313465	-1.326443
23	1	0	3.150745	-1.193833	-0.163182

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.356891	0.000000			
3	N	2.203424	1.392200	0.000000		
4	C	2.215481	2.229616	1.348134	0.000000	
5	N	1.386236	2.210850	2.167883	1.332454	0.000000
6	C	2.567724	3.650767	3.590951	2.475621	1.478729
7	C	3.401112	4.433766	4.374750	3.300708	2.506437
8	H	1.076569	2.212926	3.263519	3.232482	2.160371
9	H	2.212160	1.074949	2.172392	3.250209	3.268082
10	H	3.355695	4.241263	3.868284	2.592455	2.070024
11	H	2.728907	3.984914	4.217760	3.281713	2.084950
12	H	3.407616	4.537169	4.786596	3.929405	2.936858
13	H	3.512903	4.264365	3.995168	2.980095	2.590220
14	Br	5.206400	5.453141	4.381677	3.240773	3.890085
15	H	3.276790	3.320532	2.231470	1.114247	2.145613
16	C	3.593886	2.534758	1.421024	2.428316	3.527281
17	C	4.331046	3.044904	2.433128	3.655199	4.594556
18	H	4.260692	3.412330	2.087198	2.560615	3.851600
19	H	5.392172	4.121303	3.397614	4.506919	5.559269
20	H	4.184240	2.831873	2.745996	4.083221	4.765157
21	N	4.737188	5.792815	5.605134	4.389037	3.708096
22	H	5.439544	6.455896	6.276924	5.113234	4.493181
23	H	5.043674	5.965622	5.545974	4.242226	3.827712

		6	7	8	9	10
6	C	0.000000				
7	C	1.532377	0.000000			
8	H	2.867693	3.578805	0.000000		
9	H	4.678252	5.405394	2.754894	0.000000	
10	H	1.090334	2.149290	3.805172	5.303217	0.000000
11	H	1.091161	2.188845	2.657969	4.917170	1.778248
12	H	2.171201	1.101594	3.288332	5.387028	3.045615
13	H	2.145688	1.097364	3.922451	5.218419	2.590531
14	Br	3.703400	3.847658	6.026583	6.452316	2.993970
15	H	2.756530	3.414585	4.239988	4.306479	2.473224
16	C	4.874362	5.583837	4.628798	2.869780	4.976742
17	C	6.019894	6.738844	5.256039	2.890937	6.205619
18	H	5.007073	5.637980	5.332775	3.899473	4.909115

19	H	6.942376	7.624407	6.332493	3.942498	7.035723
20	H	6.240025	6.988683	4.961175	2.312155	6.571055
21	N	2.404247	1.457565	4.863964	6.797530	2.487540
22	H	3.308415	2.041519	5.529212	7.422609	3.461721
23	H	2.607630	2.025638	5.350597	7.015224	2.265313

		11	12	13	14	15
11	H	0.000000				
12	H	2.423186	0.000000			
13	H	3.051157	1.795063	0.000000		
14	Br	4.693805	4.917094	3.358661	0.000000	
15	H	3.708983	4.270462	2.969948	2.178019	0.000000
16	C	5.569466	6.071138	5.042382	4.747753	2.845779
17	C	6.612579	7.107702	6.209803	6.054113	4.167637
18	H	5.827244	6.282408	5.004131	4.064404	2.520574
19	H	7.588148	8.051367	7.021036	6.509805	4.834835
20	H	6.693421	7.208329	6.555774	6.830816	4.804778
21	N	2.840653	2.114672	2.121145	3.925081	4.215651
22	H	3.751109	2.412109	2.423796	4.424144	4.908814
23	H	3.227538	2.949166	2.360385	3.110846	3.822592

		16	17	18	19	20
16	C	0.000000				
17	C	1.326352	0.000000			
18	H	1.083469	2.122802	0.000000		
19	H	2.079550	1.081070	2.446176	0.000000	
20	H	2.126343	1.082827	3.100762	1.847540	0.000000
21	N	6.737396	7.964182	6.633652	8.795074	8.298556
22	H	7.361092	8.573106	7.228468	9.377794	8.916379
23	H	6.543749	7.828684	6.289289	8.581084	8.282036

		21	22	23
21	N	0.000000		
22	H	1.019836	0.000000	
23	H	1.022886	1.632221	0.000000

Stoichiometry C7H12BrN3
Framework group C1[X(C7H12BrN3)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.717628	2.081612	-0.225814

2	6	0	-2.743831	1.230825	0.027607
3	7	0	-2.208132	-0.053999	0.005808
4	6	0	-0.882038	0.029751	-0.222064
5	7	0	-0.576918	1.314121	-0.402981
6	6	0	0.800769	1.797171	-0.638100
7	6	0	1.564993	2.059992	0.663847
8	1	0	-1.702373	3.155395	-0.301689
9	1	0	-3.784265	1.426456	0.214000
10	1	0	1.311477	1.011044	-1.194885
11	1	0	0.733096	2.691350	-1.259789
12	1	0	1.282180	3.042445	1.074106
13	1	0	1.299428	1.274108	1.382227
14	35	0	1.848869	-1.707843	-0.062311
15	1	0	-0.110583	-0.773997	-0.241882
16	6	0	-2.873879	-1.295030	0.195360
17	6	0	-4.186906	-1.434306	0.320955
18	1	0	-2.183163	-2.129124	0.228579
19	1	0	-4.599678	-2.422290	0.470010
20	1	0	-4.883754	-0.606408	0.282184
21	7	0	2.985482	2.027592	0.338800
22	1	0	3.535351	2.188200	1.182550
23	1	0	3.219964	1.083236	0.023356

Rotational constants (GHZ): 0.8682780 0.4704338 0.3147464

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 365 symmetry adapted cartesian basis functions of A symmetry.

There are 352 symmetry adapted basis functions of A symmetry.

352 basis functions, 562 primitive gaussians, 365 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 843.1867817912 Hartrees.

NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 352 RedAO= T EigKep= 4.41D-06 NBF= 352

NBsUse= 352 1.00D-06 EigRej= -1.00D+00 NBFU= 352

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999984 -0.003186 -0.001033 -0.004527 Ang= -0.65 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3012.46654524 A.U. after 13 cycles
NFock= 13 Conv=0.33D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000675991	-0.000444475	0.001657561
2	6	0.000293512	0.000667665	0.001513926
3	7	0.000791182	0.000945217	-0.003959766
4	6	-0.001527710	-0.001800940	0.006105588
5	7	0.000553242	-0.002281712	-0.004805177
6	6	-0.001920749	-0.000948744	0.002327148
7	6	-0.000580315	0.003225772	-0.001333214
8	1	-0.000011057	0.000092433	0.000174113
9	1	0.000232564	0.000139834	0.000199840
10	1	-0.000577491	0.000231850	0.000017403
11	1	0.000551320	0.000473077	0.000081184
12	1	0.003120981	0.004076546	0.000037113
13	1	-0.004146680	-0.000903808	-0.001193474
14	35	0.001060916	-0.000520528	0.000106228
15	1	-0.001526861	0.001706706	-0.000275833
16	6	0.000321840	0.000342253	-0.000880466
17	6	-0.000361056	0.000199139	-0.000128890
18	1	-0.000226581	-0.000414235	0.000183151
19	1	-0.000109396	0.000023411	0.000086808
20	1	0.000067243	0.000146942	0.000022169
21	7	0.005154388	-0.002680679	-0.002126723
22	1	-0.001184930	-0.000858247	0.004254836

23 1 -0.000650354 -0.001417476 -0.002063526

Cartesian Forces: Max 0.006105588 RMS 0.001856064

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.004554399 RMS 0.001251480

Search for a local minimum.

Step number 22 out of a maximum of 121

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 18 22 20

DE= 6.86D-04 DEPred=-1.01D-03 R=-6.80D-01

Trust test=-6.80D-01 RLast= 8.66D-01 DXMaxT set to 1.58D-01

ITU= -1 -1 0 -1 0 0 0 1 1 -1 1 -1 1 1 1 1 1 1 0 1

ITU= 0 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.66330.

Iteration 1 RMS(Cart)= 0.08521311 RMS(Int)= 0.00466503

Iteration 2 RMS(Cart)= 0.00938986 RMS(Int)= 0.00007387

Iteration 3 RMS(Cart)= 0.00008552 RMS(Int)= 0.00005344

Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00005344

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56415	0.00107	0.00161	0.00000	0.00161	2.56576
R2	2.61961	-0.00099	-0.00172	0.00000	-0.00171	2.61789
R3	2.03442	-0.00008	-0.00029	0.00000	-0.00029	2.03413
R4	2.63088	0.00010	0.00007	0.00000	0.00006	2.63094
R5	2.03136	-0.00028	-0.00048	0.00000	-0.00048	2.03088
R6	2.54760	-0.00078	-0.00273	0.00000	-0.00274	2.54486
R7	2.68535	0.00049	0.00134	0.00000	0.00134	2.68668
R8	2.51797	-0.00014	0.00115	0.00000	0.00115	2.51912
R9	2.10562	0.00049	0.00491	0.00000	0.00491	2.11053
R10	2.79439	-0.00065	-0.00260	0.00000	-0.00260	2.79179
R11	2.89577	0.00260	0.00319	0.00000	0.00319	2.89896
R12	2.06043	-0.00013	-0.00030	0.00000	-0.00030	2.06014
R13	2.06200	-0.00038	-0.00223	0.00000	-0.00223	2.05977
R14	2.08171	-0.00455	-0.01287	0.00000	-0.01287	2.06884
R15	2.07372	0.00108	-0.00069	0.00000	-0.00069	2.07303
R16	2.75440	0.00335	0.00855	0.00000	0.00855	2.76294
R17	4.11586	0.00075	-0.02585	0.00000	-0.02585	4.09001

R18	2.50644	0.00045	0.00036	0.00000	0.00036	2.50680
R19	2.04746	-0.00047	-0.00144	0.00000	-0.00144	2.04602
R20	2.04293	0.00005	0.00006	0.00000	0.00006	2.04298
R21	2.04625	-0.00015	-0.00030	0.00000	-0.00030	2.04595
R22	1.92721	-0.00403	-0.01021	0.00000	-0.01021	1.91700
R23	1.93297	-0.00209	-0.00774	0.00000	-0.00774	1.92523
A1	1.87451	-0.00064	-0.00135	0.00000	-0.00126	1.87325
A2	2.27742	0.00034	0.00031	0.00000	0.00028	2.27770
A3	2.13123	0.00030	0.00105	0.00000	0.00102	2.13224
A4	1.85951	0.00074	0.00226	0.00000	0.00233	1.86184
A5	2.27875	-0.00028	-0.00104	0.00000	-0.00108	2.27767
A6	2.14492	-0.00046	-0.00122	0.00000	-0.00125	2.14367
A7	1.90055	-0.00119	-0.00263	0.00000	-0.00257	1.89798
A8	2.24416	0.00079	0.00328	0.00000	0.00326	2.24742
A9	2.13843	0.00040	-0.00062	0.00000	-0.00064	2.13779
A10	1.88397	0.00122	0.00317	0.00000	0.00344	1.88741
A11	2.26429	-0.00001	-0.00738	0.00000	-0.00721	2.25708
A12	2.13453	-0.00124	0.00096	0.00000	0.00115	2.13568
A13	1.90486	-0.00001	-0.00065	0.00000	-0.00057	1.90429
A14	2.22197	0.00181	0.00580	0.00000	0.00576	2.22773
A15	2.15293	-0.00175	-0.00523	0.00000	-0.00527	2.14766
A16	1.96663	-0.00154	-0.01471	0.00000	-0.01471	1.95192
A17	1.85674	0.00009	0.00740	0.00000	0.00739	1.86413
A18	1.87602	0.00072	0.01069	0.00000	0.01073	1.88675
A19	1.90067	0.00060	0.00633	0.00000	0.00631	1.90698
A20	1.95461	0.00045	-0.00638	0.00000	-0.00639	1.94822
A21	1.90598	-0.00033	-0.00257	0.00000	-0.00255	1.90343
A22	1.91915	0.00051	-0.00285	0.00000	-0.00277	1.91638
A23	1.88881	-0.00117	0.00000	0.00000	0.00017	1.88898
A24	1.86790	0.00167	0.00382	0.00000	0.00395	1.87185
A25	1.91003	-0.00091	-0.00244	0.00000	-0.00256	1.90748
A26	1.93165	-0.00307	-0.03315	0.00000	-0.03318	1.89848
A27	1.94541	0.00307	0.03453	0.00000	0.03454	1.97996
A28	2.76709	-0.00333	0.05146	0.00000	0.05146	2.81855
A29	2.17503	0.00053	0.00078	0.00000	0.00078	2.17580
A30	1.95816	-0.00039	-0.00255	0.00000	-0.00255	1.95561
A31	2.15000	-0.00014	0.00177	0.00000	0.00177	2.15177
A32	2.07945	0.00010	0.00110	0.00000	0.00110	2.08055
A33	2.15724	0.00000	-0.00106	0.00000	-0.00106	2.15618
A34	2.04649	-0.00009	-0.00004	0.00000	-0.00004	2.04645
A35	1.91501	0.00203	0.00707	0.00000	0.00710	1.92211
A36	1.88883	-0.00087	0.00846	0.00000	0.00849	1.89732
A37	1.85140	-0.00028	0.00793	0.00000	0.00799	1.85939
D1	0.00367	0.00008	-0.00460	0.00000	-0.00459	-0.00092

D2	-3.13443	-0.00051	-0.00584	0.00000	-0.00585	-3.14028
D3	3.13645	0.00059	0.00321	0.00000	0.00322	3.13968
D4	-0.00164	0.00001	0.00197	0.00000	0.00196	0.00032
D5	-0.03318	0.00113	0.03071	0.00000	0.03072	-0.00247
D6	-3.08753	0.00075	0.03206	0.00000	0.03206	-3.05547
D7	3.11632	0.00067	0.02369	0.00000	0.02370	3.14002
D8	0.06197	0.00029	0.02505	0.00000	0.02505	0.08702
D9	0.02666	-0.00125	-0.02268	0.00000	-0.02270	0.00396
D10	-3.12493	-0.00063	-0.01367	0.00000	-0.01370	-3.13863
D11	-3.11810	-0.00072	-0.02156	0.00000	-0.02156	-3.13966
D12	0.01350	-0.00010	-0.01255	0.00000	-0.01256	0.00094
D13	-0.04747	0.00194	0.04194	0.00000	0.04194	-0.00553
D14	3.06414	0.00051	-0.01119	0.00000	-0.01124	3.05290
D15	3.10339	0.00137	0.03360	0.00000	0.03360	3.13699
D16	-0.06819	-0.00007	-0.01953	0.00000	-0.01958	-0.08777
D17	0.10474	-0.00033	0.01302	0.00000	0.01303	0.11777
D18	-3.03516	-0.00045	0.01401	0.00000	0.01402	-3.02115
D19	-3.04806	0.00036	0.02313	0.00000	0.02313	-3.02494
D20	0.09522	0.00024	0.02412	0.00000	0.02411	0.11933
D21	0.04981	-0.00186	-0.04489	0.00000	-0.04485	0.00495
D22	3.10833	-0.00128	-0.04551	0.00000	-0.04547	3.06287
D23	-3.06451	-0.00057	0.00410	0.00000	0.00403	-3.06048
D24	-0.00598	0.00001	0.00347	0.00000	0.00341	-0.00257
D25	-2.66098	0.00046	0.21916	0.00000	0.21919	-2.44179
D26	0.44686	-0.00112	0.15938	0.00000	0.15935	0.60621
D27	1.53419	0.00041	0.07259	0.00000	0.07261	1.60679
D28	-2.66750	0.00032	0.07659	0.00000	0.07661	-2.59089
D29	-0.62758	0.00034	0.08281	0.00000	0.08279	-0.54479
D30	-1.50870	-0.00014	0.07380	0.00000	0.07380	-1.43489
D31	0.57280	-0.00023	0.07780	0.00000	0.07781	0.65061
D32	2.61272	-0.00021	0.08402	0.00000	0.08399	2.69671
D33	-1.41020	-0.00030	0.09190	0.00000	0.09191	-1.31828
D34	0.67529	-0.00182	0.08730	0.00000	0.08731	0.76260
D35	2.77393	0.00212	0.13091	0.00000	0.13092	2.90485
D36	2.81720	0.00013	0.08762	0.00000	0.08762	2.90482
D37	-1.38049	-0.00139	0.08302	0.00000	0.08301	-1.29748
D38	0.71814	0.00255	0.12663	0.00000	0.12663	0.84477
D39	0.70745	-0.00015	0.09069	0.00000	0.09067	0.79812
D40	2.79294	-0.00167	0.08608	0.00000	0.08607	2.87901
D41	-1.39161	0.00226	0.12969	0.00000	0.12968	-1.26193
D42	-3.13050	-0.00156	-0.15347	0.00000	-0.15342	2.99926
D43	-1.11771	-0.00129	-0.13522	0.00000	-0.13520	-1.25291
D44	1.06164	-0.00145	-0.13413	0.00000	-0.13403	0.92761
D45	3.07442	-0.00118	-0.11587	0.00000	-0.11580	2.95862

D46	-1.06842	-0.00025	-0.13057	0.00000	-0.13068	-1.19910
D47	0.94436	0.00002	-0.11232	0.00000	-0.11245	0.83191
D48	-3.13317	-0.00015	0.00217	0.00000	0.00217	-3.13100
D49	0.00928	-0.00004	0.00271	0.00000	0.00271	0.01198
D50	0.00656	-0.00002	0.00107	0.00000	0.00107	0.00763
D51	-3.13418	0.00009	0.00161	0.00000	0.00161	-3.13257

Item	Value	Threshold	Converged?
Maximum Force	0.004554	0.000450	NO
RMS Force	0.001251	0.000300	NO
Maximum Displacement	0.380219	0.001800	NO
RMS Displacement	0.088699	0.001200	NO

Predicted change in Energy=-2.793295D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.818766	-2.007793	0.275186
2	6	0	-2.813907	-1.117759	0.028199
3	7	0	-2.225975	0.144118	0.010465
4	6	0	-0.905374	0.009510	0.237288
5	7	0	-0.642812	-1.286824	0.403530
6	6	0	0.725592	-1.816038	0.576661
7	6	0	1.441700	-1.997158	-0.767862
8	1	0	-1.847129	-3.079631	0.370185
9	1	0	-3.865435	-1.272783	-0.130639
10	1	0	1.270677	-1.089371	1.179423
11	1	0	0.658556	-2.755204	1.125780
12	1	0	1.053949	-2.884866	-1.277934
13	1	0	1.245252	-1.110683	-1.383478
14	35	0	1.797512	1.765298	-0.120099
15	1	0	-0.101763	0.784925	0.220478
16	6	0	-2.838926	1.408891	-0.203918
17	6	0	-4.146829	1.606004	-0.305179
18	1	0	-2.110236	2.206119	-0.279362
19	1	0	-4.517664	2.606609	-0.478515
20	1	0	-4.879452	0.813175	-0.222354
21	7	0	2.860289	-2.202241	-0.479341
22	1	0	3.355129	-2.460037	-1.326542
23	1	0	3.261134	-1.319345	-0.166688

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357744	0.000000			
3	N	2.206041	1.392232	0.000000		
4	C	2.214777	2.226422	1.346684	0.000000	
5	N	1.385329	2.209776	2.169908	1.333063	0.000000
6	C	2.569322	3.649172	3.588111	2.471407	1.477353
7	C	3.423259	4.417832	4.317719	3.247429	2.494378
8	H	1.076413	2.213720	3.265804	3.232238	2.160012
9	H	2.212191	1.074697	2.171485	3.246785	3.266625
10	H	3.347507	4.243813	3.887742	2.613495	2.074232
11	H	2.723831	3.992983	4.239165	3.298324	2.090776
12	H	3.381409	4.448478	4.646786	3.809496	2.874032
13	H	3.597802	4.297633	3.945506	2.916660	2.605611
14	Br	5.241177	5.440514	4.339784	3.242855	3.942692
15	H	3.278775	3.318569	2.228680	1.116844	2.149042
16	C	3.597777	2.537413	1.421731	2.427252	3.529701
17	C	4.337769	3.050690	2.434425	3.653778	4.598789
18	H	4.260227	3.411438	2.085484	2.558067	3.849717
19	H	5.398595	4.126799	3.399236	4.506211	5.563390
20	H	4.192041	2.838619	2.746412	4.080496	4.769784
21	N	4.743488	5.799155	5.622757	4.425564	3.726818
22	H	5.435002	6.457092	6.302216	5.166828	4.511442
23	H	5.145347	6.081508	5.681679	4.391906	3.945504

		6	7	8	9	10
6	C	0.000000				
7	C	1.534065	0.000000			
8	H	2.873708	3.644626	0.000000		
9	H	4.676851	5.394113	2.754829	0.000000	
10	H	1.090177	2.155283	3.786386	5.303730	0.000000
11	H	1.089981	2.184909	2.637164	4.923684	1.775548
12	H	2.165579	1.094783	3.342228	5.302399	3.051128
13	H	2.147025	1.097002	4.063854	5.264505	2.563116
14	Br	3.802691	3.834354	6.082526	6.426432	3.180479
15	H	2.752525	3.331528	4.243054	4.303798	2.513195
16	C	4.869832	5.499360	4.632503	2.872363	5.004376
17	C	6.019012	6.665472	5.263071	2.897769	6.230446
18	H	4.995242	5.524709	5.332006	3.899436	4.941546
19	H	6.940097	7.536074	6.339194	3.949191	7.064979
20	H	6.242412	6.939201	4.969911	2.321177	6.588531
21	N	2.412721	1.462087	4.863260	6.798592	2.552812
22	H	3.309286	2.046360	5.506930	7.414601	3.536033
23	H	2.688539	2.032530	5.429659	7.126813	2.413881

		11	12	13	14	15

11	H	0.000000				
12	H	2.439465	0.000000			
13	H	3.056966	1.787585	0.000000		
14	Br	4.825389	4.849484	3.189418	0.000000	
15	H	3.732314	4.128955	2.824970	2.164341	0.000000
16	C	5.598229	5.894432	4.941672	4.650872	2.839279
17	C	6.645262	6.939904	6.133324	5.949355	4.160895
18	H	5.852808	6.076787	4.845570	3.935757	2.510696
19	H	7.623389	7.863730	6.917255	6.381044	4.827764
20	H	6.724606	7.070714	6.523912	6.745283	4.798250
21	N	2.780254	2.089639	2.148792	4.123095	4.264582
22	H	3.656845	2.340571	2.505110	4.662095	4.987299
23	H	3.241231	2.925301	2.363874	3.414584	3.985841

		16	17	18	19	20
16	C	0.000000				
17	C	1.326544	0.000000			
18	H	1.082706	2.123327	0.000000		
19	H	2.080408	1.081099	2.448625	0.000000	
20	H	2.125785	1.082670	3.100338	1.847408	0.000000
21	N	6.752569	7.977015	6.646785	8.806772	8.310377
22	H	7.388857	8.593908	7.262218	9.400581	8.929808
23	H	6.682469	7.965850	6.425979	8.718948	8.415455

		21	22	23
21	N	0.000000		
22	H	1.014433	0.000000	
23	H	1.018790	1.629501	0.000000

Stoichiometry C7H12BrN3
Framework group C1[X(C7H12BrN3)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.712178	2.117786	-0.228940
2	6	0	-2.725139	1.252442	0.032901
3	7	0	-2.177112	-0.026878	-0.003391
4	6	0	-0.862196	0.073155	-0.276420
5	7	0	-0.565130	1.364774	-0.419709
6	6	0	0.811982	1.856211	-0.630953
7	6	0	1.582622	1.979781	0.689728

8	1	0	-1.710155	3.192122	-0.295742
9	1	0	-3.764661	1.435356	0.235165
10	1	0	1.311204	1.129344	-1.271989
11	1	0	0.754414	2.811149	-1.153294
12	1	0	1.242212	2.865184	1.236293
13	1	0	1.381137	1.083808	1.289768
14	35	0	1.795226	-1.773409	-0.065675
15	1	0	-0.083411	-0.726682	-0.309507
16	6	0	-2.821377	-1.277500	0.202007
17	6	0	-4.130222	-1.437064	0.347547
18	1	0	-2.115948	-2.098384	0.229771
19	1	0	-4.525828	-2.430066	0.509466
20	1	0	-4.839991	-0.620259	0.312447
21	7	0	2.995358	2.148859	0.353145
22	1	0	3.529047	2.368939	1.187300
23	1	0	3.356289	1.262656	0.003423

Rotational constants (GHZ): 0.8273919 0.4815652 0.3145402

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 365 symmetry adapted cartesian basis functions of A symmetry.

There are 352 symmetry adapted basis functions of A symmetry.

352 basis functions, 562 primitive gaussians, 365 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 840.8877429784 Hartrees.

NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 352 RedAO= T EigKep= 4.58D-06 NBF= 352

NBsUse= 352 1.00D-06 EigRej= -1.00D+00 NBFU= 352

Lowest energy guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999997 0.001229 0.000254 -0.001989 Ang= 0.27 deg.

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999989 -0.002856 -0.000668 0.003522 Ang= -0.53 deg.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3012.46744228 A.U. after 11 cycles

NFock= 11 Conv=0.26D-08 -V/T= 2.0017

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000084085	-0.000184087	-0.000370833
2	6	-0.000047524	0.000143515	0.000820988
3	7	0.000002691	-0.000035834	-0.000347880
4	6	0.001513862	-0.001458800	0.000693756
5	7	-0.000585393	-0.000269706	-0.000219275
6	6	-0.000535655	-0.000512482	0.000264127
7	6	0.001887205	-0.000222499	0.001430819
8	1	-0.000011565	-0.000038465	-0.000098714
9	1	0.000020154	0.000017105	0.000055870
10	1	-0.000126553	0.000291090	-0.000153603
11	1	-0.000090519	0.000029033	0.000296899
12	1	-0.000418108	0.000785754	-0.000902332
13	1	-0.000434111	-0.000058022	-0.000510102
14	35	0.000914400	-0.000711043	0.000195017
15	1	-0.002157274	0.001968409	-0.000422220
16	6	-0.000071060	0.000123118	-0.000170867
17	6	-0.000025002	-0.000155519	-0.000069542
18	1	0.000183415	0.000136156	0.000113377
19	1	0.000014214	0.000024334	0.000024193
20	1	-0.000069524	0.000026610	-0.000008271
21	7	-0.000476404	0.000605462	-0.000339082
22	1	0.000331608	-0.000807786	0.000443926
23	1	0.000097059	0.000303656	-0.000726250

Cartesian Forces: Max 0.002157274 RMS 0.000630962

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.003412917 RMS 0.000437332

Search for a local minimum.

Step number 23 out of a maximum of 121

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 22 20 23

ITU= 0 -1 -1 0 -1 0 0 0 1 1 -1 1 -1 1 1 1 1 1 0

ITU= 1 0 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00012	0.00085	0.00466	0.00554	0.01118
Eigenvalues ---	0.01407	0.01796	0.02015	0.02168	0.02306
Eigenvalues ---	0.02388	0.02963	0.03062	0.03117	0.03268
Eigenvalues ---	0.03556	0.04057	0.04567	0.04748	0.05249
Eigenvalues ---	0.05520	0.08253	0.08915	0.09863	0.11075
Eigenvalues ---	0.12714	0.15178	0.15946	0.15978	0.16000
Eigenvalues ---	0.16005	0.16042	0.16282	0.19822	0.21652
Eigenvalues ---	0.22039	0.22991	0.23474	0.24672	0.24917
Eigenvalues ---	0.28495	0.30921	0.34005	0.34021	0.34754
Eigenvalues ---	0.34945	0.35005	0.35651	0.35690	0.35859
Eigenvalues ---	0.36436	0.36656	0.38362	0.40268	0.42159
Eigenvalues ---	0.42997	0.46798	0.47689	0.48187	0.50240
Eigenvalues ---	0.54240	0.59417	0.60356		

RFO step: Lambda=-1.23181804D-03 EMin= 1.21352687D-04

Quartic linear search produced a step of 0.01122.

Iteration 1 RMS(Cart)= 0.08781525 RMS(Int)= 0.02580606

Iteration 2 RMS(Cart)= 0.02414819 RMS(Int)= 0.00095644

Iteration 3 RMS(Cart)= 0.00236027 RMS(Int)= 0.00009524

Iteration 4 RMS(Cart)= 0.00000781 RMS(Int)= 0.00009499

Iteration 5 RMS(Cart)= 0.00000000 RMS(Int)= 0.00009499

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56576	0.00019	-0.00001	-0.00057	-0.00059	2.56517
R2	2.61789	-0.00003	0.00001	0.00002	0.00002	2.61791
R3	2.03413	0.00003	0.00000	0.00027	0.00027	2.03439
R4	2.63094	0.00012	0.00000	0.00062	0.00063	2.63157
R5	2.03088	-0.00003	0.00000	0.00009	0.00009	2.03098
R6	2.54486	-0.00009	0.00002	0.00311	0.00314	2.54800
R7	2.68668	0.00014	-0.00001	-0.00270	-0.00271	2.68397
R8	2.51912	-0.00035	-0.00001	-0.00192	-0.00192	2.51720
R9	2.11053	-0.00002	-0.00003	-0.00129	-0.00132	2.10921
R10	2.79179	0.00005	0.00001	0.00389	0.00390	2.79570
R11	2.89896	0.00091	-0.00002	0.00533	0.00532	2.90428
R12	2.06014	0.00005	0.00000	-0.00104	-0.00104	2.05909
R13	2.05977	0.00013	0.00001	0.00170	0.00171	2.06148
R14	2.06884	-0.00007	0.00007	0.00613	0.00620	2.07504
R15	2.07303	0.00032	0.00000	-0.00050	-0.00050	2.07254
R16	2.76294	-0.00018	-0.00005	-0.00946	-0.00950	2.75344
R17	4.09001	0.00045	0.00015	0.02712	0.02727	4.11728
R18	2.50680	0.00007	0.00000	0.00024	0.00024	2.50704
R19	2.04602	0.00022	0.00001	-0.00041	-0.00040	2.04562
R20	2.04298	0.00001	0.00000	-0.00006	-0.00006	2.04293

R21	2.04595	0.00003	0.00000	-0.00006	-0.00006	2.04589
R22	1.91700	-0.00001	0.00006	0.00100	0.00106	1.91806
R23	1.92523	0.00008	0.00004	-0.00067	-0.00063	1.92461
A1	1.87325	-0.00027	0.00001	0.00005	-0.00001	1.87324
A2	2.27770	0.00010	0.00000	0.00028	0.00030	2.27799
A3	2.13224	0.00016	-0.00001	-0.00033	-0.00032	2.13192
A4	1.86184	0.00009	-0.00001	-0.00036	-0.00042	1.86142
A5	2.27767	-0.00004	0.00001	-0.00025	-0.00023	2.27745
A6	2.14367	-0.00006	0.00001	0.00062	0.00064	2.14431
A7	1.89798	-0.00015	0.00002	0.00012	0.00013	1.89810
A8	2.24742	0.00022	-0.00002	-0.00326	-0.00328	2.24414
A9	2.13779	-0.00008	0.00000	0.00314	0.00315	2.14094
A10	1.88741	0.00010	-0.00002	-0.00145	-0.00157	1.88584
A11	2.25708	0.00027	0.00004	0.02043	0.02042	2.27750
A12	2.13568	-0.00037	0.00000	-0.01728	-0.01738	2.11830
A13	1.90429	0.00022	0.00000	0.00156	0.00151	1.90580
A14	2.22773	0.00089	-0.00003	0.00053	0.00049	2.22822
A15	2.14766	-0.00111	0.00003	-0.00277	-0.00271	2.14495
A16	1.95192	0.00032	0.00008	0.00626	0.00634	1.95826
A17	1.86413	-0.00030	-0.00004	-0.00816	-0.00820	1.85593
A18	1.88675	-0.00014	-0.00006	-0.00323	-0.00333	1.88342
A19	1.90698	-0.00011	-0.00004	-0.00449	-0.00451	1.90247
A20	1.94822	0.00014	0.00004	0.00604	0.00608	1.95429
A21	1.90343	0.00006	0.00001	0.00297	0.00298	1.90641
A22	1.91638	-0.00030	0.00002	0.00042	0.00006	1.91644
A23	1.88898	0.00021	0.00000	-0.00540	-0.00545	1.88353
A24	1.87185	0.00054	-0.00002	0.00904	0.00881	1.88066
A25	1.90748	-0.00050	0.00001	-0.00777	-0.00759	1.89988
A26	1.89848	0.00020	0.00019	0.03064	0.03075	1.92923
A27	1.97996	-0.00015	-0.00020	-0.02645	-0.02657	1.95339
A28	2.81855	-0.00341	-0.00029	-0.05538	-0.05568	2.76288
A29	2.17580	0.00000	0.00000	0.00240	0.00240	2.17820
A30	1.95561	-0.00006	0.00001	0.00290	0.00292	1.95852
A31	2.15177	0.00006	-0.00001	-0.00531	-0.00532	2.14645
A32	2.08055	-0.00008	-0.00001	-0.00038	-0.00038	2.08017
A33	2.15618	0.00011	0.00001	0.00074	0.00074	2.15693
A34	2.04645	-0.00003	0.00000	-0.00036	-0.00036	2.04609
A35	1.92211	0.00098	-0.00004	0.02072	0.02050	1.94261
A36	1.89732	-0.00033	-0.00005	0.00730	0.00707	1.90438
A37	1.85939	-0.00020	-0.00004	0.01464	0.01424	1.87363
D1	-0.00092	0.00027	0.00003	0.01439	0.01435	0.01343
D2	-3.14028	0.00004	0.00003	0.00732	0.00735	-3.13293
D3	3.13968	0.00017	-0.00002	0.00694	0.00690	-3.13661
D4	0.00032	-0.00006	-0.00001	-0.00013	-0.00010	0.00022

D5	-0.00247	-0.00013	-0.00017	-0.02221	-0.02235	-0.02482
D6	-3.05547	-0.00009	-0.00018	-0.01350	-0.01359	-3.06906
D7	3.14002	-0.00004	-0.00013	-0.01551	-0.01566	3.12436
D8	0.08702	0.00000	-0.00014	-0.00680	-0.00690	0.08011
D9	0.00396	-0.00032	0.00013	-0.00193	-0.00176	0.00220
D10	-3.13863	-0.00020	0.00008	-0.00387	-0.00370	3.14085
D11	-3.13966	-0.00011	0.00012	0.00447	0.00458	-3.13508
D12	0.00094	0.00000	0.00007	0.00252	0.00264	0.00358
D13	-0.00553	0.00024	-0.00024	-0.01187	-0.01210	-0.01763
D14	3.05290	0.00016	0.00006	0.01037	0.01071	3.06361
D15	3.13699	0.00014	-0.00019	-0.01007	-0.01029	3.12669
D16	-0.08777	0.00006	0.00011	0.01217	0.01252	-0.07525
D17	0.11777	-0.00015	-0.00007	-0.03416	-0.03426	0.08351
D18	-3.02115	-0.00018	-0.00008	-0.03352	-0.03362	-3.05477
D19	-3.02494	-0.00002	-0.00013	-0.03634	-0.03644	-3.06138
D20	0.11933	-0.00005	-0.00014	-0.03570	-0.03581	0.08352
D21	0.00495	-0.00007	0.00026	0.02100	0.02122	0.02618
D22	3.06287	0.00001	0.00026	0.01296	0.01315	3.07601
D23	-3.06048	-0.00003	-0.00002	-0.00147	-0.00118	-3.06167
D24	-0.00257	0.00005	-0.00002	-0.00951	-0.00925	-0.01183
D25	-2.44179	-0.00042	-0.00125	-0.36657	-0.36783	-2.80962
D26	0.60621	-0.00049	-0.00091	-0.34055	-0.34145	0.26475
D27	1.60679	0.00009	-0.00041	-0.09099	-0.09142	1.51537
D28	-2.59089	-0.00005	-0.00044	-0.09802	-0.09849	-2.68938
D29	-0.54479	-0.00020	-0.00047	-0.10046	-0.10094	-0.64572
D30	-1.43489	0.00005	-0.00042	-0.08139	-0.08179	-1.51668
D31	0.65061	-0.00009	-0.00044	-0.08842	-0.08886	0.56175
D32	2.69671	-0.00024	-0.00048	-0.09086	-0.09130	2.60541
D33	-1.31828	0.00020	-0.00052	0.04412	0.04358	-1.27471
D34	0.76260	-0.00044	-0.00050	0.03173	0.03123	0.79383
D35	2.90485	-0.00018	-0.00075	0.00213	0.00137	2.90622
D36	2.90482	0.00045	-0.00050	0.05327	0.05277	2.95759
D37	-1.29748	-0.00020	-0.00047	0.04088	0.04041	-1.25707
D38	0.84477	0.00006	-0.00072	0.01128	0.01055	0.85532
D39	0.79812	0.00035	-0.00052	0.04867	0.04816	0.84628
D40	2.87901	-0.00029	-0.00049	0.03628	0.03581	2.91482
D41	-1.26193	-0.00003	-0.00074	0.00668	0.00595	-1.25598
D42	2.99926	-0.00070	0.00087	-0.20238	-0.20148	2.79779
D43	-1.25291	-0.00058	0.00077	-0.16897	-0.16797	-1.42088
D44	0.92761	-0.00075	0.00077	-0.22447	-0.22402	0.70359
D45	2.95862	-0.00063	0.00066	-0.19105	-0.19052	2.76810
D46	-1.19910	-0.00016	0.00074	-0.21893	-0.21819	-1.41729
D47	0.83191	-0.00004	0.00064	-0.18551	-0.18469	0.64722
D48	-3.13100	-0.00004	-0.00001	-0.00247	-0.00249	-3.13348

D49	0.01198	-0.00002	-0.00002	-0.00261	-0.00263	0.00936
D50	0.00763	-0.00001	-0.00001	-0.00317	-0.00318	0.00446
D51	-3.13257	0.00001	-0.00001	-0.00331	-0.00332	-3.13589

Item	Value	Threshold	Converged?
Maximum Force	0.003413	0.000450	NO
RMS Force	0.000437	0.000300	NO
Maximum Displacement	0.514599	0.001800	NO
RMS Displacement	0.100234	0.001200	NO

Predicted change in Energy=-9.642930D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.794647	-1.985538	0.242490
2	6	0	-2.806780	-1.110276	0.014189
3	7	0	-2.241163	0.162246	0.012630
4	6	0	-0.915891	0.047830	0.233085
5	7	0	-0.634320	-1.244091	0.394346
6	6	0	0.744218	-1.749453	0.575789
7	6	0	1.443632	-2.022944	-0.765112
8	1	0	-1.801926	-3.059562	0.315901
9	1	0	-3.855279	-1.282586	-0.147172
10	1	0	1.288945	-0.969866	1.107580
11	1	0	0.694647	-2.642756	1.199958
12	1	0	1.024157	-2.927078	-1.225901
13	1	0	1.253785	-1.167956	-1.425255
14	35	0	1.900124	1.652622	0.152215
15	1	0	-0.112525	0.822659	0.238477
16	6	0	-2.880271	1.415335	-0.183710
17	6	0	-4.189265	1.585035	-0.317082
18	1	0	-2.173412	2.234498	-0.217169
19	1	0	-4.578683	2.581778	-0.470597
20	1	0	-4.905150	0.773709	-0.280115
21	7	0	2.865079	-2.198201	-0.497173
22	1	0	3.326083	-2.687503	-1.257613
23	1	0	3.304165	-1.282984	-0.414478

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357431	0.000000			

3	N	2.205717	1.392565	0.000000		
4	C	2.215149	2.228135	1.348346	0.000000	
5	N	1.385339	2.209527	2.169201	1.332046	0.000000
6	C	2.571509	3.651511	3.589462	2.470554	1.479419
7	C	3.391624	4.416591	4.354038	3.294215	2.503765
8	H	1.076554	2.213702	3.265723	3.232306	2.159953
9	H	2.211829	1.074746	2.172199	3.248785	3.266390
10	H	3.359837	4.241483	3.865521	2.581036	2.069504
11	H	2.746864	4.001816	4.230457	3.281453	2.090796
12	H	3.314865	4.417542	4.662638	3.839597	2.864995
13	H	3.569699	4.308540	4.006446	2.989268	2.623297
14	Br	5.186106	5.459634	4.403516	3.242196	3.856550
15	H	3.273457	3.323485	2.240145	1.116148	2.137292
16	C	3.595298	2.534419	1.420296	2.429522	3.528596
17	C	4.335471	3.047246	2.434777	3.657958	4.598664
18	H	4.261861	3.412067	2.086056	2.562344	3.852705
19	H	5.396270	4.123824	3.398771	4.509114	5.562679
20	H	4.190679	2.835343	2.748894	4.087109	4.771415
21	N	4.722856	5.797850	5.648479	4.457989	3.735094
22	H	5.381908	6.458880	6.381912	5.262943	4.527383
23	H	5.188744	6.128395	5.746457	4.472055	4.020867

		6	7	8	9	10
6	C	0.000000				
7	C	1.536878	0.000000			
8	H	2.875201	3.574467	0.000000		
9	H	4.679318	5.385949	2.754694	0.000000	
10	H	1.089626	2.154037	3.814062	5.304266	0.000000
11	H	1.090887	2.192406	2.681075	4.936259	1.777719
12	H	2.170542	1.098064	3.222026	5.260885	3.057110
13	H	2.145222	1.096739	3.993391	5.267749	2.540813
14	Br	3.617963	3.815713	5.994719	6.467592	2.857220
15	H	2.731950	3.395036	4.234585	4.311495	2.435694
16	C	4.871309	5.554812	4.630026	2.868929	4.973829
17	C	6.021236	6.704310	5.260450	2.892000	6.210311
18	H	5.001322	5.613294	5.333783	3.899162	4.900084
19	H	6.941741	7.586731	6.336693	3.944772	7.038031
20	H	6.246141	6.954389	4.967817	2.312629	6.582747
21	N	2.418817	1.457058	4.814974	6.791470	2.562857
22	H	3.302624	2.056165	5.376881	7.401272	3.562913
23	H	2.784160	2.032748	5.455442	7.164432	2.544762

		11	12	13	14	15
11	H	0.000000				
12	H	2.464591	0.000000			
13	H	3.062583	1.785212	0.000000		

14	Br	4.582708	4.862117	3.295729	0.000000	
15	H	3.685794	4.182938	2.932124	2.178769	0.000000
16	C	5.582355	5.931886	5.030432	4.798054	2.861805
17	C	6.635376	6.954487	6.199500	6.107819	4.184456
18	H	5.832806	6.154987	4.978137	4.131430	2.539323
19	H	7.608845	7.893656	6.999255	6.574660	4.852201
20	H	6.724625	7.053157	6.558498	6.875402	4.820849
21	N	2.790817	2.109810	2.125796	4.022647	4.304985
22	H	3.600849	2.314576	2.575178	4.780969	5.136491
23	H	3.356332	2.925728	2.288877	3.303068	4.066183

		16	17	18	19	20
16	C	0.000000				
17	C	1.326669	0.000000			
18	H	1.082496	2.120247	0.000000		
19	H	2.080264	1.081069	2.443391	0.000000	
20	H	2.126291	1.082639	3.098429	1.847154	0.000000
21	N	6.794480	8.006814	6.716667	8.846384	8.322008
22	H	7.517006	8.695954	7.453393	9.532578	8.982688
23	H	6.751402	8.024120	6.512715	8.779455	8.464094

		21	22	23
21	N	0.000000		
22	H	1.014993	0.000000	
23	H	1.018458	1.638301	0.000000

Stoichiometry C7H12BrN3
Framework group C1[X(C7H12BrN3)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.682149	2.072302	-0.313572
2	6	0	-2.731296	1.252783	-0.048433
3	7	0	-2.222518	-0.042439	0.004330
4	6	0	-0.894172	0.004054	-0.222323
5	7	0	-0.556231	1.274587	-0.436539
6	6	0	0.842743	1.710545	-0.640237
7	6	0	1.557721	2.007135	0.687481
8	1	0	-1.642141	3.141713	-0.430745
9	1	0	-3.770642	1.477822	0.107116
10	1	0	1.350802	0.886575	-1.140471

11	1	0	0.830801	2.579012	-1.300279
12	1	0	1.180079	2.946983	1.111528
13	1	0	1.332287	1.188989	1.382213
14	35	0	1.848338	-1.719351	-0.079662
15	1	0	-0.125885	-0.805197	-0.197125
16	6	0	-2.915818	-1.256936	0.252473
17	6	0	-4.230617	-1.362879	0.394350
18	1	0	-2.245784	-2.104582	0.318423
19	1	0	-4.663266	-2.334305	0.588919
20	1	0	-4.910025	-0.522799	0.325227
21	7	0	2.984692	2.108162	0.410777
22	1	0	3.469241	2.607105	1.150018
23	1	0	3.382606	1.171776	0.364936

Rotational constants (GHZ): 0.8678660 0.4654617 0.3138679

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 365 symmetry adapted cartesian basis functions of A symmetry.

There are 352 symmetry adapted basis functions of A symmetry.

352 basis functions, 562 primitive gaussians, 365 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 842.4337522124 Hartrees.

NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 352 RedAO= T EigKep= 4.37D-06 NBF= 352

NBsUse= 352 1.00D-06 EigRej= -1.00D+00 NBFU= 352

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999972 0.007142 0.002212 -0.000733 Ang= 0.86 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3012.46741221 A.U. after 12 cycles
NFock= 12 Conv=0.98D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000218577	0.000068536	0.001459467
2	6	0.000247381	0.000273252	-0.000115121
3	7	0.000366069	0.000342282	-0.000769686
4	6	0.000686363	-0.001774765	0.001511826
5	7	0.001044774	-0.001390060	-0.003223220
6	6	-0.000515002	-0.001416337	0.001565851
7	6	-0.001676042	0.002320366	-0.000216800
8	1	-0.000107467	0.000107224	0.000351626
9	1	0.000074704	0.000160972	0.000055958
10	1	0.000736104	0.000510184	-0.000203335
11	1	0.000125962	-0.000251387	-0.000626971
12	1	0.002507255	0.001563780	0.000388161
13	1	-0.002888083	-0.000546553	-0.001144730
14	35	0.001198494	0.000317157	-0.000590218
15	1	-0.002913857	0.002084447	0.000349593
16	6	-0.000297376	0.000548877	-0.000457201
17	6	-0.000132083	-0.000142168	-0.000042473
18	1	0.000312107	-0.000035821	0.000221355
19	1	-0.000013540	0.000024936	0.000038057
20	1	-0.000022315	0.000039593	0.000017749
21	7	0.002532143	-0.002867894	-0.001252541
22	1	-0.000994348	0.000482656	0.000958812
23	1	-0.000489822	-0.000419279	0.001723842

Cartesian Forces: Max 0.003223220 RMS 0.001161925

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.003128493 RMS 0.000855886

Search for a local minimum.
Step number 24 out of a maximum of 121
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 21 23 24
DE= 3.01D-05 DEPred=-9.64D-04 R=-3.12D-02
Trust test=-3.12D-02 RLast= 7.52D-01 DXMaxT set to 7.88D-02
ITU= -1 0 -1 -1 0 -1 0 0 0 1 1 -1 1 -1 1 1 1 1 1 1
ITU= 0 1 0 0
Eigenvalues --- 0.00026 0.00201 0.00461 0.00691 0.01009
Eigenvalues --- 0.01407 0.01738 0.01981 0.02171 0.02308
Eigenvalues --- 0.02391 0.02668 0.03061 0.03079 0.03274
Eigenvalues --- 0.03456 0.04083 0.04519 0.04850 0.05242
Eigenvalues --- 0.05436 0.08222 0.09053 0.10047 0.11754
Eigenvalues --- 0.12738 0.15283 0.15945 0.15962 0.16000
Eigenvalues --- 0.16007 0.16041 0.16244 0.19007 0.21660
Eigenvalues --- 0.22044 0.23114 0.23484 0.24919 0.24955
Eigenvalues --- 0.28800 0.29997 0.33986 0.34163 0.34767
Eigenvalues --- 0.34888 0.35060 0.35685 0.35691 0.35859
Eigenvalues --- 0.36437 0.36657 0.38243 0.40209 0.42164
Eigenvalues --- 0.42960 0.46751 0.47709 0.48167 0.50163
Eigenvalues --- 0.54251 0.59481 0.60360
En-DIIS/RFO-DIIS IScMMF= 0 using points: 24 23
RFO step: Lambda=-2.63125840D-04.
DidBck=T Rises=F RFO-DIIS coefs: 0.45080 0.54920
Iteration 1 RMS(Cart)= 0.13487521 RMS(Int)= 0.04667269
Iteration 2 RMS(Cart)= 0.02837099 RMS(Int)= 0.01905847
Iteration 3 RMS(Cart)= 0.01910302 RMS(Int)= 0.00063028
Iteration 4 RMS(Cart)= 0.00143883 RMS(Int)= 0.00015719
Iteration 5 RMS(Cart)= 0.00000289 RMS(Int)= 0.00015717
Iteration 6 RMS(Cart)= 0.00000000 RMS(Int)= 0.00015717

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56517	0.00026	0.00033	-0.00044	-0.00014	2.56503
R2	2.61791	-0.00028	-0.00001	0.00415	0.00424	2.62215
R3	2.03439	-0.00008	-0.00015	0.00022	0.00007	2.03446
R4	2.63157	-0.00048	-0.00035	-0.00337	-0.00383	2.62774
R5	2.03098	-0.00011	-0.00005	0.00004	-0.00001	2.03097
R6	2.54800	-0.00048	-0.00172	0.00218	0.00041	2.54841
R7	2.68397	0.00048	0.00149	0.00327	0.00475	2.68873
R8	2.51720	0.00167	0.00106	0.00066	0.00180	2.51900
R9	2.10921	0.00043	0.00072	-0.00250	-0.00178	2.10744
R10	2.79570	-0.00026	-0.00214	0.00108	-0.00106	2.79463

R11	2.90428	-0.00095	-0.00292	0.00704	0.00412	2.90840
R12	2.05909	0.00063	0.00057	0.00212	0.00269	2.06178
R13	2.06148	-0.00016	-0.00094	0.00278	0.00184	2.06332
R14	2.07504	-0.00241	-0.00340	0.00473	0.00132	2.07636
R15	2.07254	0.00076	0.00027	0.00354	0.00381	2.07635
R16	2.75344	0.00163	0.00522	-0.00705	-0.00183	2.75161
R17	4.11728	0.00125	-0.01497	0.06845	0.05347	4.17075
R18	2.50704	0.00015	-0.00013	-0.00016	-0.00029	2.50675
R19	2.04562	0.00017	0.00022	0.00525	0.00547	2.05109
R20	2.04293	0.00002	0.00003	0.00028	0.00031	2.04324
R21	2.04589	-0.00001	0.00003	0.00076	0.00079	2.04669
R22	1.91806	-0.00140	-0.00058	0.00150	0.00092	1.91898
R23	1.92461	-0.00045	0.00034	-0.00247	-0.00213	1.92248
A1	1.87324	0.00023	0.00000	-0.00017	-0.00001	1.87323
A2	2.27799	-0.00016	-0.00016	0.00204	0.00179	2.27978
A3	2.13192	-0.00006	0.00018	-0.00198	-0.00190	2.13002
A4	1.86142	0.00030	0.00023	-0.00056	-0.00042	1.86100
A5	2.27745	-0.00001	0.00013	-0.00008	-0.00001	2.27743
A6	2.14431	-0.00029	-0.00035	0.00053	0.00012	2.14443
A7	1.89810	-0.00005	-0.00007	0.00313	0.00302	1.90113
A8	2.24414	0.00030	0.00180	0.00622	0.00803	2.25217
A9	2.14094	-0.00025	-0.00173	-0.00938	-0.01110	2.12984
A10	1.88584	0.00026	0.00086	-0.00255	-0.00150	1.88434
A11	2.27750	-0.00307	-0.01121	-0.07232	-0.08358	2.19392
A12	2.11830	0.00278	0.00955	0.07576	0.08530	2.20360
A13	1.90580	-0.00072	-0.00083	-0.00041	-0.00150	1.90430
A14	2.22822	-0.00060	-0.00027	-0.01019	-0.01115	2.21708
A15	2.14495	0.00136	0.00149	0.01542	0.01626	2.16121
A16	1.95826	-0.00047	-0.00348	0.01446	0.01095	1.96921
A17	1.85593	0.00061	0.00450	-0.00122	0.00322	1.85915
A18	1.88342	0.00023	0.00183	-0.01182	-0.00998	1.87344
A19	1.90247	-0.00090	0.00248	-0.00046	0.00196	1.90443
A20	1.95429	0.00029	-0.00334	0.00632	0.00301	1.95731
A21	1.90641	0.00029	-0.00164	-0.00822	-0.00985	1.89656
A22	1.91644	0.00226	-0.00003	-0.00432	-0.00418	1.91226
A23	1.88353	-0.00072	0.00300	0.01374	0.01661	1.90014
A24	1.88066	-0.00211	-0.00484	0.01892	0.01401	1.89467
A25	1.89988	-0.00095	0.00417	-0.03913	-0.03499	1.86489
A26	1.92923	-0.00154	-0.01689	0.02239	0.00554	1.93477
A27	1.95339	0.00313	0.01459	-0.01106	0.00319	1.95658
A28	2.76288	-0.00092	0.03058	-0.03722	-0.00664	2.75623
A29	2.17820	0.00008	-0.00132	-0.00403	-0.00534	2.17286
A30	1.95852	-0.00034	-0.00160	-0.00330	-0.00491	1.95362
A31	2.14645	0.00026	0.00292	0.00733	0.01025	2.15671

A32	2.08017	-0.00002	0.00021	-0.00355	-0.00334	2.07683
A33	2.15693	0.00005	-0.00041	0.00430	0.00389	2.16081
A34	2.04609	-0.00003	0.00020	-0.00075	-0.00056	2.04554
A35	1.94261	-0.00038	-0.01126	0.02298	0.01166	1.95427
A36	1.90438	0.00041	-0.00388	0.01932	0.01538	1.91976
A37	1.87363	0.00066	-0.00782	0.01716	0.00922	1.88285
D1	0.01343	-0.00024	-0.00788	0.02596	0.01822	0.03165
D2	-3.13293	-0.00012	-0.00404	-0.00008	-0.00415	-3.13708
D3	-3.13661	-0.00019	-0.00379	0.01109	0.00748	-3.12912
D4	0.00022	-0.00007	0.00006	-0.01496	-0.01488	-0.01467
D5	-0.02482	0.00050	0.01228	-0.02599	-0.01381	-0.03863
D6	-3.06906	-0.00008	0.00747	-0.08244	-0.07453	3.13959
D7	3.12436	0.00046	0.00860	-0.01266	-0.00422	3.12014
D8	0.08011	-0.00012	0.00379	-0.06911	-0.06494	0.01517
D9	0.00220	-0.00007	0.00097	-0.01742	-0.01658	-0.01438
D10	3.14085	0.00000	0.00203	-0.02622	-0.02438	3.11647
D11	-3.13508	-0.00018	-0.00251	0.00616	0.00367	-3.13141
D12	0.00358	-0.00011	-0.00145	-0.00264	-0.00413	-0.00055
D13	-0.01763	0.00037	0.00664	0.00143	0.00811	-0.00951
D14	3.06361	-0.00007	-0.00588	0.02214	0.01603	3.07964
D15	3.12669	0.00031	0.00565	0.00957	0.01523	-3.14126
D16	-0.07525	-0.00014	-0.00688	0.03028	0.02314	-0.05211
D17	0.08351	-0.00006	0.01881	-0.01745	0.00136	0.08487
D18	-3.05477	-0.00017	0.01846	-0.01894	-0.00047	-3.05524
D19	-3.06138	0.00002	0.02002	-0.02733	-0.00732	-3.06870
D20	0.08352	-0.00009	0.01967	-0.02882	-0.00915	0.07437
D21	0.02618	-0.00054	-0.01165	0.01498	0.00336	0.02954
D22	3.07601	-0.00011	-0.00722	0.06652	0.05993	3.13594
D23	-3.06167	0.00009	0.00065	0.00234	0.00242	-3.05924
D24	-0.01183	0.00051	0.00508	0.05389	0.05899	0.04716
D25	-2.80962	0.00069	0.20201	0.32254	0.52460	-2.28503
D26	0.26475	0.00009	0.18753	0.34245	0.52994	0.79469
D27	1.51537	0.00125	0.05021	0.14057	0.19082	1.70619
D28	-2.68938	0.00027	0.05409	0.14737	0.20154	-2.48784
D29	-0.64572	0.00103	0.05543	0.13135	0.18687	-0.45886
D30	-1.51668	0.00072	0.04492	0.07811	0.12294	-1.39374
D31	0.56175	-0.00026	0.04880	0.08491	0.13366	0.69541
D32	2.60541	0.00050	0.05014	0.06889	0.11899	2.72439
D33	-1.27471	-0.00052	-0.02393	0.12077	0.09686	-1.17784
D34	0.79383	-0.00081	-0.01715	0.07930	0.06206	0.85589
D35	2.90622	0.00131	-0.00075	0.08468	0.08402	2.99024
D36	2.95759	-0.00041	-0.02898	0.11389	0.08491	3.04250
D37	-1.25707	-0.00070	-0.02220	0.07242	0.05011	-1.20695
D38	0.85532	0.00142	-0.00580	0.07780	0.07208	0.92740

D39	0.84628	-0.00035	-0.02645	0.12046	0.09403	0.94031
D40	2.91482	-0.00064	-0.01967	0.07899	0.05923	2.97404
D41	-1.25598	0.00148	-0.00327	0.08437	0.08119	-1.17479
D42	2.79779	0.00038	0.11065	-0.25244	-0.14188	2.65591
D43	-1.42088	0.00122	0.09225	-0.20528	-0.11306	-1.53394
D44	0.70359	-0.00017	0.12303	-0.27197	-0.14888	0.55471
D45	2.76810	0.00068	0.10463	-0.22481	-0.12005	2.64805
D46	-1.41729	-0.00002	0.11983	-0.23009	-0.11033	-1.52762
D47	0.64722	0.00082	0.10143	-0.18293	-0.08150	0.56572
D48	-3.13348	-0.00010	0.00137	-0.00616	-0.00479	-3.13828
D49	0.00936	-0.00004	0.00144	-0.00218	-0.00074	0.00862
D50	0.00446	0.00002	0.00174	-0.00454	-0.00279	0.00167
D51	-3.13589	0.00008	0.00182	-0.00056	0.00127	-3.13462

Item	Value	Threshold	Converged?
Maximum Force	0.003128	0.000450	NO
RMS Force	0.000856	0.000300	NO
Maximum Displacement	1.017532	0.001800	NO
RMS Displacement	0.166466	0.001200	NO

Predicted change in Energy=-7.047748D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.824653	-2.010501	0.228372
2	6	0	-2.832219	-1.118794	0.049249
3	7	0	-2.247648	0.142683	0.025693
4	6	0	-0.917570	0.011852	0.205683
5	7	0	-0.648272	-1.285295	0.353221
6	6	0	0.712195	-1.824712	0.565758
7	6	0	1.521963	-1.933250	-0.738540
8	1	0	-1.842824	-3.084997	0.293016
9	1	0	-3.887309	-1.275247	-0.082571
10	1	0	1.217174	-1.134702	1.243452
11	1	0	0.605290	-2.789667	1.065352
12	1	0	1.076372	-2.701546	-1.385418
13	1	0	1.451540	-0.980271	-1.280886
14	35	0	1.667672	1.920423	-0.386239
15	1	0	-0.172588	0.841314	0.179539
16	6	0	-2.862309	1.411844	-0.163563
17	6	0	-4.170680	1.605176	-0.265731
18	1	0	-2.131346	2.212418	-0.216909

19	1	0	-4.542142	2.610040	-0.411784
20	1	0	-4.903714	0.810059	-0.206841
21	7	0	2.897690	-2.272339	-0.402996
22	1	0	3.355678	-2.785187	-1.150281
23	1	0	3.433225	-1.424385	-0.232291

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357356	0.000000			
3	N	2.203680	1.390540	0.000000		
4	C	2.216580	2.229061	1.348563	0.000000	
5	N	1.387581	2.211276	2.168963	1.332996	0.000000
6	C	2.565920	3.650749	3.594855	2.481683	1.478855
7	C	3.484355	4.499205	4.370757	3.259800	2.514301
8	H	1.076592	2.214560	3.263933	3.233294	2.160903
9	H	2.211748	1.074741	2.170422	3.249471	3.268237
10	H	3.324172	4.221842	3.888398	2.636035	2.072457
11	H	2.685565	3.954839	4.221235	3.302520	2.083671
12	H	3.390842	4.454262	4.596736	3.724236	2.828963
13	H	3.751357	4.487654	4.080707	2.967638	2.678163
14	Br	5.293982	5.447523	4.319696	3.267490	4.023310
15	H	3.296142	3.306454	2.194910	1.115208	2.186072
16	C	3.597609	2.539749	1.422813	2.424528	3.527547
17	C	4.338329	3.051345	2.433488	3.652895	4.598400
18	H	4.257392	3.414534	2.087148	2.548398	3.841687
19	H	5.398514	4.128026	3.397638	4.502152	5.560674
20	H	4.198283	2.842032	2.748481	4.086154	4.776291
21	N	4.771552	5.862341	5.700053	4.488231	3.757654
22	H	5.416332	6.519647	6.430599	5.284194	4.532307
23	H	5.310464	6.279206	5.898693	4.602609	4.125626

		6	7	8	9	10
6	C	0.000000				
7	C	1.539058	0.000000			
8	H	2.861962	3.703029	0.000000		
9	H	4.677357	5.488487	2.756116	0.000000	
10	H	1.091048	2.158441	3.751075	5.275778	0.000000
11	H	1.091862	2.197218	2.583986	4.877975	1.773423
12	H	2.169920	1.098764	3.389083	5.326337	3.063622
13	H	2.160973	1.098757	4.214247	5.479624	2.539893
14	Br	3.980611	3.872485	6.151357	6.415787	3.491794
15	H	2.835436	3.378251	4.268311	4.283420	2.639694
16	C	4.876913	5.544556	4.633508	2.877089	5.010666
17	C	6.024779	6.719389	5.265817	2.900118	6.230051

18	H	4.999671	5.550255	5.329716	3.907078	4.954640
19	H	6.944830	7.584301	6.341649	3.953814	7.066302
20	H	6.251188	7.006980	4.978992	2.323150	6.584126
21	N	2.432127	1.456089	4.859765	6.865352	2.613262
22	H	3.294739	2.063453	5.403463	7.475345	3.609329
23	H	2.863765	2.041606	5.556102	7.323583	2.678174

		11	12	13	14	15
11	H	0.000000				
12	H	2.497190	0.000000			
13	H	3.081377	1.764785	0.000000		
14	Br	5.041896	4.765563	3.043210	0.000000	
15	H	3.817562	4.069502	2.844082	2.207065	0.000000
16	C	5.584548	5.824613	5.057660	4.563876	2.770889
17	C	6.625430	6.879906	6.270920	5.848098	4.094691
18	H	5.844162	5.983470	4.915525	3.813983	2.423599
19	H	7.604922	7.792856	7.040589	6.248041	4.750901
20	H	6.702658	7.034332	6.689402	6.666948	4.746980
21	N	2.771059	2.113426	2.128727	4.369494	4.411438
22	H	3.531810	2.292929	2.626884	5.057261	5.231500
23	H	3.397806	2.918150	2.285577	3.785316	4.278420

		16	17	18	19	20
16	C	0.000000				
17	C	1.326517	0.000000			
18	H	1.085391	2.128382	0.000000		
19	H	2.078251	1.081234	2.451126	0.000000	
20	H	2.128697	1.083060	3.106885	1.847341	0.000000
21	N	6.841646	8.063238	6.740836	8.898809	8.390563
22	H	7.566508	8.758069	7.480286	9.593196	9.057230
23	H	6.905264	8.185275	6.647633	8.939535	8.631218

		21	22	23
21	N	0.000000		
22	H	1.015481	0.000000	
23	H	1.017332	1.643321	0.000000

Stoichiometry C7H12BrN3
Framework group C1[X(C7H12BrN3)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-1.667291	2.188375	-0.089005
2	6	0	-2.695482	1.320751	0.091179
3	7	0	-2.162106	0.041901	-0.025673
4	6	0	-0.843215	0.140437	-0.289185
5	7	0	-0.532432	1.435093	-0.353664
6	6	0	0.831036	1.942201	-0.619761
7	6	0	1.731651	1.916700	0.628015
8	1	0	-1.646409	3.264559	-0.067983
9	1	0	-3.731932	1.502698	0.309661
10	1	0	1.260301	1.292046	-1.383578
11	1	0	0.729356	2.947512	-1.033491
12	1	0	1.362646	2.645259	1.363079
13	1	0	1.659964	0.926041	1.097826
14	35	0	1.697178	-1.898624	-0.033990
15	1	0	-0.132303	-0.713872	-0.381115
16	6	0	-2.813186	-1.216219	0.107084
17	6	0	-4.118274	-1.371481	0.286777
18	1	0	-2.113226	-2.043462	0.045460
19	1	0	-4.519193	-2.371310	0.379911
20	1	0	-4.820897	-0.549154	0.342609
21	7	0	3.093843	2.233667	0.222851
22	1	0	3.622105	2.668178	0.973412
23	1	0	3.581787	1.384143	-0.051348

Rotational constants (GHZ): 0.7747664 0.4909512 0.3085018

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 365 symmetry adapted cartesian basis functions of A symmetry.

There are 352 symmetry adapted basis functions of A symmetry.

352 basis functions, 562 primitive gaussians, 365 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 834.6621990632 Hartrees.

NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 352 RedAO= T EigKep= 4.40D-06 NBF= 352

NBsUse= 352 1.00D-06 EigRej= -1.00D+00 NBFU= 352

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999838 -0.009096 -0.004687 0.014814 Ang= -2.06 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3012.46637664 A.U. after 14 cycles
NFock= 14 Conv=0.21D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000617099	0.001060061	0.003164148
2	6	0.000156293	-0.000092269	-0.003041284
3	7	0.000832036	0.000424085	-0.000488515
4	6	-0.004568202	0.002882599	0.003019537
5	7	0.002017091	-0.000327129	-0.003483484
6	6	0.001753427	0.001753053	0.000665270
7	6	-0.005205456	0.002451276	-0.006481670
8	1	-0.000062299	0.000217709	0.000616565
9	1	0.000067080	-0.000045842	-0.000116099
10	1	0.000361718	-0.000750017	-0.000259002
11	1	0.001263443	0.000512982	-0.001266629
12	1	0.002917043	-0.000732531	0.002934824
13	1	-0.001819472	0.000214567	0.002607622
14	35	-0.000856687	-0.001148059	0.000658502
15	1	0.002457838	-0.003580635	-0.000609620
16	6	0.000447152	-0.000150903	0.000308161
17	6	-0.000078135	0.000783688	0.000154194
18	1	-0.001170314	-0.000979417	-0.000161462
19	1	-0.000157980	-0.000072986	-0.000136794
20	1	0.000370094	0.000046638	-0.000069771
21	7	0.002983775	-0.003311673	0.000653160

22	1	-0.001585406	0.002085696	0.001630870
23	1	-0.000740140	-0.001240893	-0.000298524

Cartesian Forces: Max 0.006481670 RMS 0.001895608

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.006515747 RMS 0.001362705
Search for a local minimum.
Step number 25 out of a maximum of 121
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 22 20 25 23
DE= 1.07D-03 DEPred=-7.05D-04 R=-1.51D+00
Trust test=-1.51D+00 RLast= 9.33D-01 DXMaxT set to 5.00D-02
ITU= -1 -1 0 -1 -1 0 -1 0 0 0 1 1 -1 1 -1 1 1 1 1 1
ITU= 1 0 1 0 0
Use linear search instead of GDIIS.
Energy rises -- skip Quadratic/GDIIS search.
Quartic linear search produced a step of -0.77304.
Iteration 1 RMS(Cart)= 0.09152467 RMS(Int)= 0.01354061
Iteration 2 RMS(Cart)= 0.01407635 RMS(Int)= 0.00040144
Iteration 3 RMS(Cart)= 0.00038762 RMS(Int)= 0.00005583
Iteration 4 RMS(Cart)= 0.00000027 RMS(Int)= 0.00005583

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56503	0.00069	0.00057	0.00000	0.00058	2.56561
R2	2.62215	-0.00126	-0.00329	0.00000	-0.00329	2.61886
R3	2.03446	-0.00018	-0.00026	0.00000	-0.00026	2.03420
R4	2.62774	0.00023	0.00247	0.00000	0.00248	2.63022
R5	2.03097	-0.00004	-0.00006	0.00000	-0.00006	2.03090
R6	2.54841	-0.00054	-0.00275	0.00000	-0.00275	2.54567
R7	2.68873	-0.00009	-0.00158	0.00000	-0.00158	2.68715
R8	2.51900	-0.00196	0.00010	0.00000	0.00009	2.51908
R9	2.10744	-0.00245	0.00239	0.00000	0.00239	2.10983
R10	2.79463	-0.00039	-0.00219	0.00000	-0.00219	2.79244
R11	2.90840	-0.00267	-0.00729	0.00000	-0.00729	2.90110
R12	2.06178	-0.00047	-0.00127	0.00000	-0.00127	2.06051
R13	2.06332	-0.00116	-0.00275	0.00000	-0.00275	2.06057
R14	2.07636	-0.00240	-0.00581	0.00000	-0.00581	2.07055
R15	2.07635	-0.00098	-0.00256	0.00000	-0.00256	2.07379
R16	2.75161	0.00166	0.00876	0.00000	0.00876	2.76037

R17	4.17075	-0.00144	-0.06241	0.00000	-0.06241	4.10834
R18	2.50675	-0.00002	0.00004	0.00000	0.00004	2.50679
R19	2.05109	-0.00150	-0.00392	0.00000	-0.00392	2.04717
R20	2.04324	0.00000	-0.00020	0.00000	-0.00020	2.04304
R21	2.04669	-0.00029	-0.00057	0.00000	-0.00057	2.04612
R22	1.91898	-0.00297	-0.00153	0.00000	-0.00153	1.91745
R23	1.92248	-0.00147	0.00213	0.00000	0.00213	1.92461
A1	1.87323	0.00003	0.00001	0.00000	0.00003	1.87326
A2	2.27978	0.00002	-0.00161	0.00000	-0.00160	2.27817
A3	2.13002	-0.00004	0.00172	0.00000	0.00172	2.13174
A4	1.86100	-0.00001	0.00065	0.00000	0.00068	1.86169
A5	2.27743	-0.00004	0.00019	0.00000	0.00020	2.27763
A6	2.14443	0.00006	-0.00059	0.00000	-0.00057	2.14386
A7	1.90113	-0.00132	-0.00244	0.00000	-0.00243	1.89870
A8	2.25217	0.00002	-0.00367	0.00000	-0.00367	2.24850
A9	2.12984	0.00130	0.00615	0.00000	0.00614	2.13598
A10	1.88434	0.00160	0.00237	0.00000	0.00238	1.88672
A11	2.19392	0.00486	0.04882	0.00000	0.04887	2.24279
A12	2.20360	-0.00652	-0.05251	0.00000	-0.05250	2.15110
A13	1.90430	-0.00023	0.00000	0.00000	0.00006	1.90435
A14	2.21708	0.00232	0.00824	0.00000	0.00831	2.22539
A15	2.16121	-0.00208	-0.01047	0.00000	-0.01040	2.15081
A16	1.96921	-0.00370	-0.01336	0.00000	-0.01336	1.95585
A17	1.85915	0.00139	0.00385	0.00000	0.00386	1.86301
A18	1.87344	0.00230	0.01029	0.00000	0.01031	1.88375
A19	1.90443	0.00077	0.00197	0.00000	0.00197	1.90640
A20	1.95731	-0.00023	-0.00703	0.00000	-0.00703	1.95027
A21	1.89656	-0.00037	0.00532	0.00000	0.00533	1.90188
A22	1.91226	0.00143	0.00318	0.00000	0.00332	1.91558
A23	1.90014	-0.00207	-0.00862	0.00000	-0.00865	1.89149
A24	1.89467	-0.00165	-0.01764	0.00000	-0.01758	1.87709
A25	1.86489	0.00118	0.03292	0.00000	0.03289	1.89778
A26	1.93477	-0.00157	-0.02806	0.00000	-0.02801	1.90676
A27	1.95658	0.00271	0.01807	0.00000	0.01807	1.97465
A28	2.75623	-0.00114	0.04817	0.00000	0.04817	2.80441
A29	2.17286	0.00056	0.00228	0.00000	0.00228	2.17514
A30	1.95362	-0.00004	0.00154	0.00000	0.00154	1.95516
A31	2.15671	-0.00052	-0.00382	0.00000	-0.00382	2.15289
A32	2.07683	0.00040	0.00288	0.00000	0.00288	2.07971
A33	2.16081	-0.00044	-0.00358	0.00000	-0.00358	2.15723
A34	2.04554	0.00004	0.00071	0.00000	0.00071	2.04624
A35	1.95427	-0.00098	-0.02486	0.00000	-0.02475	1.92952
A36	1.91976	0.00010	-0.01735	0.00000	-0.01723	1.90253
A37	1.88285	0.00009	-0.01814	0.00000	-0.01790	1.86495

D1	0.03165	-0.00137	-0.02518	0.00000	-0.02522	0.00643
D2	-3.13708	-0.00077	-0.00247	0.00000	-0.00247	-3.13955
D3	-3.12912	-0.00015	-0.01112	0.00000	-0.01114	-3.14026
D4	-0.01467	0.00045	0.01159	0.00000	0.01161	-0.00306
D5	-0.03863	0.00178	0.02795	0.00000	0.02799	-0.01063
D6	3.13959	0.00181	0.06813	0.00000	0.06812	-3.07548
D7	3.12014	0.00069	0.01537	0.00000	0.01540	3.13554
D8	0.01517	0.00072	0.05554	0.00000	0.05552	0.07069
D9	-0.01438	0.00053	0.01418	0.00000	0.01422	-0.00017
D10	3.11647	0.00042	0.02171	0.00000	0.02178	3.13825
D11	-3.13141	-0.00001	-0.00638	0.00000	-0.00638	-3.13779
D12	-0.00055	-0.00013	0.00116	0.00000	0.00119	0.00063
D13	-0.00951	0.00057	0.00308	0.00000	0.00307	-0.00644
D14	3.07964	-0.00063	-0.02067	0.00000	-0.02049	3.05915
D15	-3.14126	0.00068	-0.00381	0.00000	-0.00384	3.13808
D16	-0.05211	-0.00052	-0.02756	0.00000	-0.02740	-0.07951
D17	0.08487	0.00008	0.02543	0.00000	0.02542	0.11029
D18	-3.05524	0.00021	0.02635	0.00000	0.02634	-3.02890
D19	-3.06870	-0.00006	0.03383	0.00000	0.03385	-3.03486
D20	0.07437	0.00008	0.03475	0.00000	0.03477	0.10914
D21	0.02954	-0.00143	-0.01901	0.00000	-0.01902	0.01052
D22	3.13594	-0.00135	-0.05649	0.00000	-0.05660	3.07934
D23	-3.05924	-0.00065	-0.00096	0.00000	-0.00072	-3.05996
D24	0.04716	-0.00057	-0.03844	0.00000	-0.03831	0.00885
D25	-2.28503	0.00010	-0.12119	0.00000	-0.12119	-2.40621
D26	0.79469	-0.00099	-0.14571	0.00000	-0.14571	0.64898
D27	1.70619	-0.00021	-0.07684	0.00000	-0.07685	1.62934
D28	-2.48784	-0.00050	-0.07966	0.00000	-0.07967	-2.56751
D29	-0.45886	0.00087	-0.06643	0.00000	-0.06646	-0.52532
D30	-1.39374	-0.00024	-0.03181	0.00000	-0.03179	-1.42553
D31	0.69541	-0.00053	-0.03464	0.00000	-0.03461	0.66080
D32	2.72439	0.00085	-0.02140	0.00000	-0.02140	2.70300
D33	-1.17784	-0.00121	-0.10857	0.00000	-0.10856	-1.28640
D34	0.85589	-0.00017	-0.07212	0.00000	-0.07210	0.78379
D35	2.99024	0.00086	-0.06601	0.00000	-0.06601	2.92423
D36	3.04250	-0.00117	-0.10643	0.00000	-0.10643	2.93607
D37	-1.20695	-0.00013	-0.06998	0.00000	-0.06997	-1.27692
D38	0.92740	0.00090	-0.06388	0.00000	-0.06388	0.86351
D39	0.94031	-0.00108	-0.10992	0.00000	-0.10992	0.83038
D40	2.97404	-0.00004	-0.07347	0.00000	-0.07347	2.90058
D41	-1.17479	0.00099	-0.06736	0.00000	-0.06738	-1.24217
D42	2.65591	0.00098	0.26543	0.00000	0.26542	2.92133
D43	-1.53394	0.00052	0.21725	0.00000	0.21711	-1.31683
D44	0.55471	0.00124	0.28827	0.00000	0.28840	0.84312

D45	2.64805	0.00077	0.24008	0.00000	0.24009	2.88814
D46	-1.52762	-0.00100	0.25396	0.00000	0.25403	-1.27359
D47	0.56572	-0.00146	0.20578	0.00000	0.20571	0.77143
D48	-3.13828	0.00020	0.00563	0.00000	0.00563	-3.13265
D49	0.00862	0.00000	0.00260	0.00000	0.00260	0.01122
D50	0.00167	0.00005	0.00461	0.00000	0.00461	0.00628
D51	-3.13462	-0.00015	0.00158	0.00000	0.00158	-3.13304

Item	Value	Threshold	Converged?
Maximum Force	0.006516	0.000450	NO
RMS Force	0.001363	0.000300	NO
Maximum Displacement	0.469552	0.001800	NO
RMS Displacement	0.097454	0.001200	NO

Predicted change in Energy=-6.036102D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.820846	-2.008603	0.263575
2	6	0	-2.818906	-1.117697	0.032482
3	7	0	-2.231519	0.144011	0.014533
4	6	0	-0.908674	0.009837	0.230822
5	7	0	-0.644754	-1.286861	0.391823
6	6	0	0.721891	-1.818657	0.573628
7	6	0	1.459507	-1.982230	-0.762785
8	1	0	-1.846933	-3.081192	0.350891
9	1	0	-3.871310	-1.272747	-0.120494
10	1	0	1.258400	-1.100486	1.194358
11	1	0	0.645404	-2.764279	1.111159
12	1	0	1.056477	-2.844790	-1.305082
13	1	0	1.292211	-1.078926	-1.363068
14	35	0	1.772822	1.798085	-0.176418
15	1	0	-0.117894	0.797764	0.212154
16	6	0	-2.844690	1.410070	-0.193153
17	6	0	-4.152670	1.606549	-0.294583
18	1	0	-2.115383	2.208085	-0.262835
19	1	0	-4.523508	2.608371	-0.460934
20	1	0	-4.885489	0.813160	-0.217940
21	7	0	2.869224	-2.218451	-0.461758
22	1	0	3.361828	-2.536711	-1.289774
23	1	0	3.300335	-1.339387	-0.181315

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357661	0.000000			
3	N	2.205543	1.391853	0.000000		
4	C	2.215227	2.227029	1.347108	0.000000	
5	N	1.385839	2.210131	2.169692	1.333042	0.000000
6	C	2.568604	3.649854	3.589886	2.473793	1.477694
7	C	3.437270	4.436743	4.329988	3.250210	2.498914
8	H	1.076454	2.213917	3.265422	3.232524	2.160216
9	H	2.212102	1.074707	2.171256	3.247407	3.267006
10	H	3.342572	4.239656	3.888482	2.618670	2.073836
11	H	2.715112	3.984497	4.235259	3.299374	2.089190
12	H	3.382142	4.448655	4.635217	3.790741	2.863707
13	H	3.633372	4.341699	3.976183	2.927420	2.621968
14	Br	5.253467	5.443289	4.336723	3.248707	3.960362
15	H	3.283045	3.316133	2.221228	1.116473	2.157667
16	C	3.597803	2.537948	1.421977	2.426636	3.529214
17	C	4.338003	3.050805	2.434213	3.653634	4.598744
18	H	4.259615	3.412182	2.085862	2.555805	3.847853
19	H	5.398680	4.127071	3.398876	4.505322	5.562802
20	H	4.193595	2.839310	2.746882	4.081883	4.771345
21	N	4.750463	5.814702	5.641424	4.440434	3.734234
22	H	5.436165	6.477919	6.338218	5.199452	4.521348
23	H	5.183847	6.126987	5.730639	4.439146	3.986850

		6	7	8	9	10
6	C	0.000000				
7	C	1.535198	0.000000			
8	H	2.870970	3.657942	0.000000		
9	H	4.677320	5.416042	2.755136	0.000000	
10	H	1.090375	2.155997	3.778589	5.298343	0.000000
11	H	1.090408	2.187699	2.624916	4.913485	1.775076
12	H	2.166668	1.095687	3.350810	5.306378	3.054598
13	H	2.150177	1.097400	4.098897	5.314462	2.557740
14	Br	3.840292	3.838329	6.098199	6.425680	3.247363
15	H	2.771563	3.341716	4.249133	4.299512	2.542099
16	C	4.871667	5.509836	4.632811	2.873454	5.006339
17	C	6.020562	6.677955	5.263837	2.898244	6.230944
18	H	4.996443	5.530690	5.331527	3.901248	4.944944
19	H	6.941406	7.547265	6.339893	3.950234	7.065839
20	H	6.244658	6.954857	4.972159	2.321436	6.588172
21	N	2.417209	1.460726	4.862804	6.815102	2.566578
22	H	3.310156	2.050363	5.488117	7.435260	3.557817
23	H	2.729104	2.034699	5.459991	7.172212	2.473671

		11	12	13	14	15
11	H	0.000000				
12	H	2.452282	0.000000			
13	H	3.062772	1.782473	0.000000		
14	Br	4.872790	4.831492	3.149018	0.000000	
15	H	3.752197	4.116959	2.826957	2.174037	0.000000
16	C	5.595281	5.878718	4.967671	4.633816	2.823935
17	C	6.640915	6.926091	6.164427	5.929764	4.146122
18	H	5.851000	6.056280	4.860725	3.910717	2.490899
19	H	7.619350	7.847662	6.944969	6.354627	4.810486
20	H	6.719773	7.061830	6.561653	6.730892	4.786980
21	N	2.778016	2.095124	2.144259	4.173258	4.298208
22	H	3.632523	2.325895	2.532552	4.749206	5.048067
23	H	3.278637	2.926429	2.344555	3.489562	4.050497

		16	17	18	19	20
16	C	0.000000				
17	C	1.326538	0.000000			
18	H	1.083315	2.124474	0.000000		
19	H	2.079919	1.081130	2.449192	0.000000	
20	H	2.126447	1.082758	3.101826	1.847393	0.000000
21	N	6.774004	7.997848	6.669340	8.828970	8.329807
22	H	7.436432	8.638558	7.318984	9.451845	8.965974
23	H	6.732086	8.014901	6.474658	8.767867	8.464190

		21	22	23
21	N	0.000000		
22	H	1.014671	0.000000	
23	H	1.018459	1.632803	0.000000

Stoichiometry C7H12BrN3
Framework group C1[X(C7H12BrN3)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.705286	2.132771	-0.197677
2	6	0	-2.721020	1.265502	0.045984
3	7	0	-2.175322	-0.013765	-0.008273
4	6	0	-0.859588	0.086951	-0.279200
5	7	0	-0.560417	1.379882	-0.405007
6	6	0	0.813678	1.875075	-0.629118

7	6	0	1.614447	1.965133	0.677592
8	1	0	-1.699824	3.208174	-0.244900
9	1	0	-3.759978	1.447575	0.251922
10	1	0	1.298353	1.164289	-1.299036
11	1	0	0.744795	2.842160	-1.128109
12	1	0	1.264353	2.818902	1.268389
13	1	0	1.444076	1.045591	1.251789
14	35	0	1.776841	-1.798433	-0.058596
15	1	0	-0.095156	-0.725499	-0.324819
16	6	0	-2.820148	-1.266911	0.181047
17	6	0	-4.128154	-1.426006	0.334383
18	1	0	-2.115181	-2.089428	0.188774
19	1	0	-4.524125	-2.421267	0.481025
20	1	0	-4.837087	-0.607737	0.319700
21	7	0	3.016553	2.168237	0.321827
22	1	0	3.555381	2.439573	1.137669
23	1	0	3.405678	1.287263	-0.009422

Rotational constants (GHZ): 0.8165299 0.4831827 0.3131493

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 365 symmetry adapted cartesian basis functions of A symmetry.

There are 352 symmetry adapted basis functions of A symmetry.

352 basis functions, 562 primitive gaussians, 365 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 839.4775430351 Hartrees.

NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 352 RedAO= T EigKep= 4.53D-06 NBF= 352

NBsUse= 352 1.00D-06 EigRej= -1.00D+00 NBFU= 352

Lowest energy guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999996 -0.000538 -0.000651 0.002654 Ang= -0.32 deg.

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999932 0.001914 0.001993 -0.011363 Ang= 1.34 deg.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3012.46756715 A.U. after 10 cycles

NFock= 10 Conv=0.65D-08 -V/T= 2.0017

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000199015	0.000145244	0.000438394
2	6	0.000035901	0.000082483	-0.000055311
3	7	0.000197027	0.000066300	-0.000374284
4	6	0.000148355	-0.000451882	0.001161793
5	7	0.000035365	-0.000278787	-0.000988674
6	6	0.000126245	0.000089751	0.000273046
7	6	0.000148885	0.000329113	-0.000429826
8	1	-0.000022924	0.000024425	0.000060201
9	1	0.000034063	-0.000000718	0.000020379
10	1	0.000008490	0.000067228	-0.000174984
11	1	0.000215904	0.000130141	-0.000093127
12	1	0.000526895	0.000495682	0.000053768
13	1	-0.000764702	0.000013028	0.000214267
14	35	0.000479403	-0.000835423	0.000288589
15	1	-0.001116599	0.000624253	-0.000422430
16	6	0.000051809	0.000056834	-0.000068453
17	6	-0.000034943	0.000062533	-0.000024635
18	1	-0.000129455	-0.000123357	0.000067131
19	1	-0.000025970	0.000001033	-0.000011590
20	1	0.000030751	0.000033167	-0.000020940
21	7	0.000264392	-0.000374913	-0.000047925
22	1	-0.000250374	-0.000145751	0.000721667
23	1	-0.000157532	-0.000010386	-0.000587055

Cartesian Forces: Max 0.001161793 RMS 0.000357801

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.002929263 RMS 0.000477081

Search for a local minimum.

Step number 26 out of a maximum of 121

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 18 20 23 26

ITU= 0 -1 -1 0 -1 -1 0 -1 0 0 0 1 1 -1 1 -1 1 1 1 1

ITU= 1 1 0 1 0 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00032	0.00246	0.00449	0.00624	0.01219
Eigenvalues ---	0.01407	0.01820	0.02031	0.02167	0.02309
Eigenvalues ---	0.02390	0.03051	0.03060	0.03229	0.03308
Eigenvalues ---	0.03783	0.04119	0.04516	0.04894	0.05234
Eigenvalues ---	0.05443	0.08980	0.09228	0.10158	0.11680
Eigenvalues ---	0.12798	0.15240	0.15926	0.15974	0.16000
Eigenvalues ---	0.16010	0.16023	0.16267	0.19073	0.21734
Eigenvalues ---	0.22043	0.23121	0.23495	0.24846	0.24938
Eigenvalues ---	0.28303	0.30126	0.34078	0.34369	0.34733
Eigenvalues ---	0.34892	0.35108	0.35689	0.35739	0.35859
Eigenvalues ---	0.36437	0.36659	0.38695	0.40239	0.42160
Eigenvalues ---	0.43038	0.46711	0.47711	0.48452	0.50257
Eigenvalues ---	0.54244	0.59603	0.60363		

RFO step: Lambda=-8.52232711D-04 EMin= 3.15935603D-04

Quartic linear search produced a step of 0.00675.

Maximum step size (0.050) exceeded in Quadratic search.

-- Step size scaled by 0.410

Iteration 1 RMS(Cart)= 0.04240533 RMS(Int)= 0.00269743

Iteration 2 RMS(Cart)= 0.00294266 RMS(Int)= 0.00002823

Iteration 3 RMS(Cart)= 0.00004136 RMS(Int)= 0.00001003

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001003

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56561	0.00032	0.00000	-0.00007	-0.00008	2.56553
R2	2.61886	-0.00035	0.00001	-0.00047	-0.00046	2.61839
R3	2.03420	-0.00002	0.00000	0.00001	0.00001	2.03421
R4	2.63022	0.00015	0.00000	0.00006	0.00005	2.63027
R5	2.03090	-0.00004	0.00000	-0.00003	-0.00003	2.03087
R6	2.54567	-0.00022	0.00001	0.00097	0.00098	2.54664
R7	2.68715	0.00008	0.00000	-0.00080	-0.00080	2.68634
R8	2.51908	-0.00083	0.00000	-0.00038	-0.00038	2.51870
R9	2.10983	-0.00060	0.00000	-0.00147	-0.00148	2.10835
R10	2.79244	-0.00011	0.00000	0.00089	0.00089	2.79333
R11	2.90110	-0.00009	0.00001	-0.00100	-0.00098	2.90012
R12	2.06051	-0.00005	0.00000	0.00010	0.00010	2.06061
R13	2.06057	-0.00017	0.00001	0.00025	0.00026	2.06083
R14	2.07055	-0.00061	0.00001	0.00048	0.00049	2.07104
R15	2.07379	0.00001	0.00001	0.00012	0.00013	2.07391
R16	2.76037	-0.00003	-0.00002	-0.00242	-0.00244	2.75793
R17	4.10834	-0.00002	0.00012	0.02194	0.02206	4.13040
R18	2.50679	0.00005	0.00000	0.00012	0.00012	2.50691

R19	2.04717	-0.00018	0.00001	-0.00043	-0.00042	2.04675
R20	2.04304	0.00001	0.00000	-0.00001	-0.00001	2.04303
R21	2.04612	-0.00005	0.00000	-0.00010	-0.00010	2.04601
R22	1.91745	-0.00067	0.00000	0.00002	0.00003	1.91748
R23	1.92461	-0.00024	0.00000	0.00059	0.00058	1.92519
A1	1.87326	-0.00023	0.00000	0.00032	0.00032	1.87358
A2	2.27817	0.00010	0.00000	-0.00011	-0.00010	2.27807
A3	2.13174	0.00013	0.00000	-0.00022	-0.00022	2.13152
A4	1.86169	0.00006	0.00000	0.00001	0.00001	1.86170
A5	2.27763	-0.00004	0.00000	0.00007	0.00007	2.27770
A6	2.14386	-0.00002	0.00000	-0.00007	-0.00007	2.14379
A7	1.89870	-0.00044	0.00000	-0.00044	-0.00043	1.89827
A8	2.24850	0.00020	0.00001	-0.00139	-0.00138	2.24711
A9	2.13598	0.00025	-0.00001	0.00184	0.00182	2.13780
A10	1.88672	0.00047	0.00000	0.00010	0.00009	1.88681
A11	2.24279	0.00143	-0.00010	0.00849	0.00838	2.25118
A12	2.15110	-0.00192	0.00010	-0.00795	-0.00787	2.14323
A13	1.90435	0.00014	0.00000	0.00000	0.00000	1.90435
A14	2.22539	0.00133	-0.00002	0.00004	0.00002	2.22540
A15	2.15081	-0.00147	0.00002	0.00011	0.00013	2.15094
A16	1.95585	-0.00076	0.00003	0.00011	0.00013	1.95597
A17	1.86301	0.00011	-0.00001	-0.00289	-0.00291	1.86010
A18	1.88375	0.00051	-0.00002	0.00118	0.00116	1.88491
A19	1.90640	0.00012	0.00000	-0.00471	-0.00471	1.90168
A20	1.95027	0.00008	0.00001	0.00237	0.00238	1.95265
A21	1.90188	-0.00005	-0.00001	0.00390	0.00389	1.90578
A22	1.91558	0.00020	-0.00001	0.00459	0.00459	1.92017
A23	1.89149	-0.00032	0.00002	-0.00362	-0.00361	1.88788
A24	1.87709	-0.00014	0.00004	-0.00223	-0.00220	1.87489
A25	1.89778	-0.00009	-0.00007	-0.00125	-0.00131	1.89647
A26	1.90676	-0.00024	0.00006	0.00253	0.00258	1.90934
A27	1.97465	0.00060	-0.00004	0.00014	0.00009	1.97474
A28	2.80441	-0.00293	-0.00010	-0.02856	-0.02866	2.77575
A29	2.17514	0.00013	0.00000	0.00130	0.00130	2.17643
A30	1.95516	-0.00006	0.00000	0.00090	0.00089	1.95605
A31	2.15289	-0.00007	0.00001	-0.00220	-0.00219	2.15070
A32	2.07971	0.00003	-0.00001	0.00006	0.00005	2.07976
A33	2.15723	-0.00001	0.00001	0.00008	0.00009	2.15732
A34	2.04624	-0.00002	0.00000	-0.00014	-0.00014	2.04610
A35	1.92952	0.00033	0.00005	0.00154	0.00159	1.93111
A36	1.90253	-0.00041	0.00004	-0.00161	-0.00158	1.90095
A37	1.86495	-0.00003	0.00004	0.00440	0.00444	1.86939
D1	0.00643	-0.00010	0.00005	-0.00071	-0.00067	0.00576
D2	-3.13955	-0.00015	0.00000	0.00182	0.00183	-3.13772

D3	-3.14026	0.00011	0.00002	-0.00169	-0.00167	3.14125
D4	-0.00306	0.00006	-0.00002	0.00084	0.00083	-0.00223
D5	-0.01063	0.00030	-0.00006	-0.00022	-0.00026	-0.01090
D6	-3.07548	0.00037	-0.00014	-0.00233	-0.00245	-3.07793
D7	3.13554	0.00012	-0.00003	0.00066	0.00063	3.13617
D8	0.07069	0.00018	-0.00011	-0.00145	-0.00155	0.06914
D9	-0.00017	-0.00013	-0.00003	0.00140	0.00137	0.00121
D10	3.13825	-0.00007	-0.00004	0.00405	0.00401	-3.14092
D11	-3.13779	-0.00009	0.00001	-0.00090	-0.00089	-3.13867
D12	0.00063	-0.00003	0.00000	0.00175	0.00175	0.00239
D13	-0.00644	0.00032	-0.00001	-0.00154	-0.00155	-0.00799
D14	3.05915	-0.00004	0.00004	0.00751	0.00761	3.06676
D15	3.13808	0.00026	0.00001	-0.00398	-0.00398	3.13409
D16	-0.07951	-0.00010	0.00006	0.00508	0.00517	-0.07434
D17	0.11029	-0.00010	-0.00005	-0.01566	-0.01571	0.09458
D18	-3.02890	-0.00010	-0.00005	-0.01699	-0.01704	-3.04594
D19	-3.03486	-0.00003	-0.00007	-0.01269	-0.01275	-3.04761
D20	0.10914	-0.00003	-0.00007	-0.01402	-0.01408	0.09505
D21	0.01052	-0.00038	0.00004	0.00109	0.00113	0.01165
D22	3.07934	-0.00029	0.00011	0.00309	0.00319	3.08253
D23	-3.05996	-0.00022	0.00000	-0.00823	-0.00818	-3.06814
D24	0.00885	-0.00013	0.00008	-0.00623	-0.00611	0.00274
D25	-2.40621	-0.00034	0.00024	-0.20077	-0.20053	-2.60674
D26	0.64898	-0.00063	0.00029	-0.19002	-0.18973	0.45926
D27	1.62934	0.00001	0.00015	-0.03851	-0.03836	1.59098
D28	-2.56751	-0.00020	0.00016	-0.04604	-0.04588	-2.61339
D29	-0.52532	0.00005	0.00013	-0.04239	-0.04226	-0.56758
D30	-1.42553	-0.00001	0.00006	-0.04089	-0.04082	-1.46635
D31	0.66080	-0.00022	0.00007	-0.04841	-0.04834	0.61246
D32	2.70300	0.00003	0.00004	-0.04477	-0.04472	2.65827
D33	-1.28640	-0.00022	0.00022	-0.01318	-0.01296	-1.29937
D34	0.78379	-0.00041	0.00014	-0.01419	-0.01405	0.76974
D35	2.92423	0.00004	0.00013	-0.01748	-0.01734	2.90688
D36	2.93607	0.00002	0.00021	-0.00663	-0.00642	2.92965
D37	-1.27692	-0.00017	0.00014	-0.00764	-0.00750	-1.28443
D38	0.86351	0.00028	0.00013	-0.01093	-0.01080	0.85271
D39	0.83038	-0.00005	0.00022	-0.00988	-0.00966	0.82072
D40	2.90058	-0.00024	0.00015	-0.01089	-0.01075	2.88983
D41	-1.24217	0.00022	0.00013	-0.01418	-0.01404	-1.25621
D42	2.92133	-0.00017	-0.00053	-0.01392	-0.01445	2.90688
D43	-1.31683	-0.00026	-0.00043	-0.00864	-0.00908	-1.32591
D44	0.84312	-0.00019	-0.00057	-0.01954	-0.02011	0.82301
D45	2.88814	-0.00028	-0.00048	-0.01426	-0.01474	2.87340
D46	-1.27359	-0.00030	-0.00050	-0.01984	-0.02035	-1.29394

D47	0.77143	-0.00039	-0.00041	-0.01457	-0.01497	0.75646
D48	-3.13265	0.00001	-0.00001	-0.00115	-0.00116	-3.13381
D49	0.01122	-0.00002	-0.00001	-0.00170	-0.00171	0.00951
D50	0.00628	0.00001	-0.00001	0.00033	0.00032	0.00659
D51	-3.13304	-0.00002	0.00000	-0.00023	-0.00023	-3.13327

Item	Value	Threshold	Converged?
Maximum Force	0.002929	0.000450	NO
RMS Force	0.000477	0.000300	NO
Maximum Displacement	0.251783	0.001800	NO
RMS Displacement	0.043406	0.001200	NO

Predicted change in Energy=-3.175029D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.811417	-1.998979	0.256541
2	6	0	-2.814954	-1.113969	0.026751
3	7	0	-2.235627	0.151533	0.012090
4	6	0	-0.911392	0.024563	0.227430
5	7	0	-0.639893	-1.270606	0.386450
6	6	0	0.729932	-1.794661	0.570615
7	6	0	1.451443	-2.005334	-0.767398
8	1	0	-1.831035	-3.071801	0.342732
9	1	0	-3.866547	-1.275157	-0.125338
10	1	0	1.272728	-1.048911	1.152222
11	1	0	0.662692	-2.718646	1.145956
12	1	0	1.055179	-2.894169	-1.271425
13	1	0	1.261713	-1.128965	-1.400182
14	35	0	1.848602	1.723299	-0.043180
15	1	0	-0.120349	0.811295	0.219153
16	6	0	-2.858985	1.413210	-0.188928
17	6	0	-4.167495	1.599480	-0.302840
18	1	0	-2.137961	2.219746	-0.240996
19	1	0	-4.545348	2.599908	-0.461592
20	1	0	-4.894083	0.798921	-0.244325
21	7	0	2.866999	-2.205252	-0.473828
22	1	0	3.353895	-2.565029	-1.288126
23	1	0	3.287427	-1.305560	-0.246498

Distance matrix (angstroms):

	1	2	3	4	5

1	C	0.000000				
2	C	1.357620	0.000000			
3	N	2.205542	1.391880	0.000000		
4	C	2.214863	2.227124	1.347625	0.000000	
5	N	1.385595	2.210161	2.170021	1.332840	0.000000
6	C	2.568822	3.650390	3.590845	2.474125	1.478165
7	C	3.419758	4.430277	4.342138	3.270039	2.498975
8	H	1.076457	2.213831	3.265410	3.232106	2.159869
9	H	2.212082	1.074690	2.171227	3.247562	3.266993
10	H	3.349153	4.240290	3.879372	2.603453	2.072118
11	H	2.725838	3.990192	4.233655	3.293422	2.090550
12	H	3.369483	4.453348	4.664024	3.825306	2.873635
13	H	3.598025	4.319211	3.983162	2.949938	2.613087
14	Br	5.228855	5.459280	4.376577	3.252152	3.916715
15	H	3.280054	3.317312	2.225435	1.115690	2.152261
16	C	3.597065	2.536748	1.421553	2.427924	3.529631
17	C	4.337386	3.049722	2.434716	3.655648	4.599618
18	H	4.260496	3.412282	2.085928	2.557875	3.849735
19	H	5.398135	4.126212	3.399077	4.506971	5.563509
20	H	4.193083	2.838205	2.748135	4.084607	4.772730
21	N	4.739574	5.807415	5.641573	4.442980	3.729870
22	H	5.420964	6.472184	6.349254	5.214937	4.519964
23	H	5.170308	6.111499	5.717877	4.429888	3.978151

		6	7	8	9	10
6	C	0.000000				
7	C	1.534679	0.000000			
8	H	2.870813	3.625521	0.000000		
9	H	4.677804	5.406146	2.755055	0.000000	
10	H	1.090429	2.152120	3.792189	5.300518	0.000000
11	H	1.090545	2.189033	2.643588	4.920757	1.777695
12	H	2.169750	1.095946	3.311690	5.306421	3.053910
13	H	2.147087	1.097468	4.046907	5.286365	2.553682
14	Br	3.742220	3.819022	6.056537	6.454487	3.073397
15	H	2.763605	3.373013	4.245015	4.301854	2.504326
16	C	4.873158	5.531804	4.631918	2.871679	4.993173
17	C	6.022284	6.692008	5.262763	2.895792	6.223119
18	H	4.999899	5.568862	5.332487	3.900735	4.925239
19	H	6.943073	7.567250	6.338984	3.948413	7.054664
20	H	6.246626	6.957237	4.970854	2.317712	6.587441
21	N	2.413815	1.459434	4.846565	6.806406	2.553989
22	H	3.306594	2.050302	5.458938	7.426346	3.547557
23	H	2.729042	2.032697	5.446600	7.155064	2.466028

		11	12	13	14	15
11	H	0.000000				

12	H	2.455318	0.000000			
13	H	3.060838	1.781904	0.000000		
14	Br	4.748822	4.843461	3.212678	0.000000	
15	H	3.732640	4.163431	2.880443	2.185712	0.000000
16	C	5.590739	5.919966	4.990986	4.720039	2.833541
17	C	6.638970	6.957540	6.174535	6.022971	4.156092
18	H	5.844229	6.116377	4.910740	4.022222	2.503244
19	H	7.615439	7.887117	6.964726	6.467310	4.821116
20	H	6.721897	7.077257	6.553364	6.808724	4.796196
21	N	2.783207	2.096057	2.143237	4.081190	4.301631
22	H	3.631931	2.322220	2.540090	4.712277	5.073640
23	H	3.290133	2.925249	2.337881	3.359396	4.038668

		16	17	18	19	20
16	C	0.000000				
17	C	1.326602	0.000000			
18	H	1.083091	2.123103	0.000000		
19	H	2.080004	1.081125	2.447181	0.000000	
20	H	2.126510	1.082704	3.100800	1.847261	0.000000
21	N	6.779478	7.999333	6.684643	8.833606	8.325390
22	H	7.458853	8.653625	7.358739	9.474057	8.968546
23	H	6.721116	8.001143	6.470135	8.755073	8.447836

		21	22	23
21	N	0.000000		
22	H	1.014685	0.000000	
23	H	1.018767	1.635747	0.000000

Stoichiometry C7H12BrN3
Framework group C1[X(C7H12BrN3)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.707334	2.101011	-0.247171
2	6	0	-2.735224	1.250909	0.005618
3	7	0	-2.201358	-0.034492	-0.002258
4	6	0	-0.879818	0.046553	-0.253374
5	7	0	-0.566613	1.332185	-0.413109
6	6	0	0.815529	1.808239	-0.632263
7	6	0	1.580471	1.984830	0.686417
8	1	0	-1.690910	3.174361	-0.327231

9	1	0	-3.775819	1.448512	0.187482
10	1	0	1.315173	1.047226	-1.232472
11	1	0	0.765663	2.737561	-1.200737
12	1	0	1.230206	2.884094	1.205778
13	1	0	1.376904	1.111893	1.319645
14	35	0	1.824007	-1.751050	-0.067782
15	1	0	-0.117498	-0.767893	-0.270990
16	6	0	-2.863717	-1.274379	0.209336
17	6	0	-4.174444	-1.414620	0.358322
18	1	0	-2.170854	-2.106392	0.237322
19	1	0	-4.583359	-2.401914	0.522249
20	1	0	-4.873256	-0.588343	0.324015
21	7	0	2.993706	2.136005	0.354962
22	1	0	3.515270	2.473186	1.157375
23	1	0	3.375297	1.223326	0.111467

Rotational constants (GHZ): 0.8434647 0.4733027 0.3132212

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 365 symmetry adapted cartesian basis functions of A symmetry.

There are 352 symmetry adapted basis functions of A symmetry.

352 basis functions, 562 primitive gaussians, 365 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 840.7343888881 Hartrees.

NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 352 RedAO= T EigKep= 4.44D-06 NBF= 352

NBsUse= 352 1.00D-06 EigRej= -1.00D+00 NBFU= 352

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999989 0.002826 0.001198 -0.003578 Ang= 0.54 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0

NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3012.46786164 A.U. after 12 cycles
NFock= 12 Conv=0.50D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000251432	0.000176215	0.000458210
2	6	-0.000019187	0.000110159	0.000091020
3	7	0.000229618	0.000072435	-0.000423348
4	6	0.000258643	-0.000464415	0.000855465
5	7	-0.000047664	-0.000377434	-0.000927629
6	6	-0.000070941	0.000122503	0.000665824
7	6	-0.000027488	0.000479295	-0.000403333
8	1	-0.000029312	0.000025433	0.000054122
9	1	0.000033953	0.000018010	0.000026840
10	1	0.000023409	-0.000064410	-0.000169826
11	1	0.000087087	0.000108670	-0.000196726
12	1	0.000546269	0.000620894	0.000215650
13	1	-0.000756901	-0.000022674	-0.000157231
14	35	0.000475954	-0.000669544	0.000091959
15	1	-0.001248148	0.000481838	-0.000134547
16	6	0.000018779	0.000117152	-0.000082881
17	6	-0.000016774	0.000029124	-0.000055112
18	1	-0.000080742	-0.000126795	0.000055576
19	1	-0.000021643	0.000001258	0.000010071
20	1	0.000024755	0.000027729	-0.000020017
21	7	0.000655452	-0.000605220	-0.000588067
22	1	-0.000172730	0.000052320	0.000809277
23	1	-0.000113823	-0.000112544	-0.000175296

Cartesian Forces: Max 0.001248148 RMS 0.000367035

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.003052066 RMS 0.000437795
Search for a local minimum.
Step number 27 out of a maximum of 121
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 20 24 23 26 27
DE= -2.94D-04 DEPred=-3.18D-04 R= 9.28D-01
TightC=F SS= 1.41D+00 RLast= 3.05D-01 DXNew= 8.4090D-02 9.1567D-01
Trust test= 9.28D-01 RLast= 3.05D-01 DXMaxT set to 8.41D-02
ITU= 1 0 -1 -1 0 -1 -1 0 -1 0 0 0 1 1 -1 1 -1 1 1 1
ITU= 1 1 1 0 1 0 0
Eigenvalues --- 0.00078 0.00276 0.00427 0.00508 0.01190
Eigenvalues --- 0.01412 0.01825 0.01988 0.02158 0.02304
Eigenvalues --- 0.02389 0.03054 0.03055 0.03167 0.03274
Eigenvalues --- 0.03645 0.04012 0.04506 0.04734 0.05247
Eigenvalues --- 0.05394 0.08831 0.09435 0.10077 0.10821
Eigenvalues --- 0.12748 0.15278 0.15900 0.15960 0.16000
Eigenvalues --- 0.16008 0.16024 0.16203 0.18557 0.21812
Eigenvalues --- 0.22040 0.23100 0.23510 0.24736 0.24961
Eigenvalues --- 0.27883 0.29679 0.34102 0.34329 0.34663
Eigenvalues --- 0.34903 0.35196 0.35689 0.35776 0.35859
Eigenvalues --- 0.36437 0.36659 0.38617 0.40602 0.42152
Eigenvalues --- 0.43080 0.46671 0.47719 0.48449 0.50267
Eigenvalues --- 0.54242 0.59920 0.60374
En-DIIS/RFO-DIIS IScMMF= 0 using points: 27 26
RFO step: Lambda=-5.34860504D-05.
DidBck=F Rises=F RFO-DIIS coefs: 2.28363 -1.28363
Maximum step size (0.084) exceeded in Quadratic search.
-- Step size scaled by 0.653
Iteration 1 RMS(Cart)= 0.04786752 RMS(Int)= 0.00937015
Iteration 2 RMS(Cart)= 0.01012612 RMS(Int)= 0.00017605
Iteration 3 RMS(Cart)= 0.00038566 RMS(Int)= 0.00001756
Iteration 4 RMS(Cart)= 0.00000022 RMS(Int)= 0.00001756

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56553	0.00032	-0.00006	0.00029	0.00022	2.56575
R2	2.61839	-0.00035	-0.00039	-0.00042	-0.00080	2.61759
R3	2.03421	-0.00002	0.00001	-0.00003	-0.00003	2.03418
R4	2.63027	0.00007	0.00004	-0.00047	-0.00043	2.62984
R5	2.03087	-0.00004	-0.00003	-0.00010	-0.00013	2.03074
R6	2.54664	-0.00027	0.00082	0.00026	0.00108	2.54773
R7	2.68634	0.00009	-0.00067	0.00019	-0.00048	2.68586

R8	2.51870	-0.00069	-0.00032	-0.00019	-0.00050	2.51820
R9	2.10835	-0.00068	-0.00124	-0.00283	-0.00407	2.10428
R10	2.79333	-0.00004	0.00075	0.00026	0.00100	2.79433
R11	2.90012	0.00025	-0.00082	0.00076	-0.00006	2.90006
R12	2.06061	-0.00012	0.00009	0.00014	0.00022	2.06084
R13	2.06083	-0.00020	0.00022	-0.00014	0.00007	2.06090
R14	2.07104	-0.00080	0.00041	-0.00134	-0.00093	2.07010
R15	2.07391	0.00020	0.00011	0.00155	0.00166	2.07557
R16	2.75793	0.00046	-0.00205	-0.00032	-0.00236	2.75557
R17	4.13040	0.00014	0.01849	0.03180	0.05029	4.18069
R18	2.50691	0.00003	0.00010	0.00001	0.00011	2.50702
R19	2.04675	-0.00015	-0.00035	0.00004	-0.00032	2.04643
R20	2.04303	0.00001	-0.00001	0.00003	0.00003	2.04306
R21	2.04601	-0.00004	-0.00009	-0.00005	-0.00013	2.04588
R22	1.91748	-0.00075	0.00002	-0.00073	-0.00071	1.91677
R23	1.92519	-0.00018	0.00049	0.00078	0.00127	1.92646
A1	1.87358	-0.00017	0.00027	0.00033	0.00060	1.87418
A2	2.27807	0.00006	-0.00009	-0.00008	-0.00017	2.27790
A3	2.13152	0.00010	-0.00018	-0.00026	-0.00045	2.13107
A4	1.86170	0.00004	0.00001	0.00010	0.00011	1.86180
A5	2.27770	-0.00001	0.00005	0.00013	0.00018	2.27788
A6	2.14379	-0.00003	-0.00006	-0.00023	-0.00029	2.14350
A7	1.89827	-0.00039	-0.00036	-0.00054	-0.00089	1.89738
A8	2.24711	0.00021	-0.00116	0.00032	-0.00085	2.24627
A9	2.13780	0.00017	0.00153	0.00021	0.00173	2.13954
A10	1.88681	0.00047	0.00008	0.00072	0.00078	1.88760
A11	2.25118	0.00098	0.00703	-0.00369	0.00328	2.25446
A12	2.14323	-0.00147	-0.00660	0.00334	-0.00332	2.13992
A13	1.90435	0.00005	0.00000	-0.00058	-0.00058	1.90377
A14	2.22540	0.00117	0.00001	0.00028	0.00025	2.22565
A15	2.15094	-0.00122	0.00011	0.00111	0.00118	2.15212
A16	1.95597	-0.00042	0.00011	0.00144	0.00153	1.95750
A17	1.86010	0.00014	-0.00244	-0.00180	-0.00426	1.85584
A18	1.88491	0.00025	0.00097	-0.00004	0.00092	1.88583
A19	1.90168	-0.00011	-0.00395	-0.00376	-0.00772	1.89396
A20	1.95265	0.00014	0.00199	0.00190	0.00389	1.95655
A21	1.90578	0.00001	0.00326	0.00217	0.00545	1.91123
A22	1.92017	0.00018	0.00384	0.00198	0.00582	1.92599
A23	1.88788	-0.00021	-0.00302	0.00218	-0.00084	1.88704
A24	1.87489	-0.00012	-0.00184	-0.00141	-0.00325	1.87164
A25	1.89647	-0.00015	-0.00109	-0.00609	-0.00718	1.88930
A26	1.90934	-0.00029	0.00217	-0.00324	-0.00107	1.90827
A27	1.97474	0.00059	0.00008	0.00676	0.00684	1.98158
A28	2.77575	-0.00305	-0.02402	-0.02819	-0.05221	2.72354

A29	2.17643	0.00011	0.00109	0.00048	0.00156	2.17800
A30	1.95605	-0.00008	0.00075	-0.00027	0.00048	1.95653
A31	2.15070	-0.00002	-0.00184	-0.00021	-0.00204	2.14866
A32	2.07976	0.00002	0.00004	-0.00022	-0.00018	2.07958
A33	2.15732	-0.00001	0.00008	0.00041	0.00049	2.15781
A34	2.04610	-0.00002	-0.00012	-0.00019	-0.00031	2.04579
A35	1.93111	0.00049	0.00133	0.00229	0.00361	1.93472
A36	1.90095	-0.00018	-0.00132	-0.00075	-0.00208	1.89887
A37	1.86939	-0.00007	0.00372	0.00296	0.00667	1.87606
D1	0.00576	-0.00003	-0.00056	0.00114	0.00057	0.00633
D2	-3.13772	-0.00011	0.00153	0.00019	0.00172	-3.13601
D3	3.14125	0.00010	-0.00140	-0.00067	-0.00207	3.13919
D4	-0.00223	0.00002	0.00069	-0.00162	-0.00092	-0.00315
D5	-0.01090	0.00022	-0.00022	0.00146	0.00125	-0.00964
D6	-3.07793	0.00024	-0.00205	-0.01067	-0.01269	-3.09062
D7	3.13617	0.00011	0.00053	0.00309	0.00362	3.13979
D8	0.06914	0.00012	-0.00130	-0.00904	-0.01033	0.05881
D9	0.00121	-0.00017	0.00115	-0.00334	-0.00218	-0.00097
D10	-3.14092	-0.00011	0.00337	-0.00087	0.00250	-3.13841
D11	-3.13867	-0.00010	-0.00074	-0.00248	-0.00322	3.14130
D12	0.00239	-0.00004	0.00147	-0.00001	0.00147	0.00385
D13	-0.00799	0.00031	-0.00130	0.00427	0.00297	-0.00502
D14	3.06676	-0.00004	0.00638	0.01064	0.01709	3.08385
D15	3.13409	0.00026	-0.00334	0.00200	-0.00136	3.13273
D16	-0.07434	-0.00009	0.00433	0.00836	0.01275	-0.06158
D17	0.09458	-0.00010	-0.01317	-0.01394	-0.02712	0.06746
D18	-3.04594	-0.00009	-0.01429	-0.01427	-0.02856	-3.07451
D19	-3.04761	-0.00004	-0.01069	-0.01118	-0.02186	-3.06947
D20	0.09505	-0.00003	-0.01181	-0.01150	-0.02330	0.07175
D21	0.01165	-0.00032	0.00094	-0.00356	-0.00262	0.00903
D22	3.08253	-0.00022	0.00267	0.00791	0.01057	3.09310
D23	-3.06814	-0.00011	-0.00685	-0.00912	-0.01590	-3.08404
D24	0.00274	-0.00001	-0.00512	0.00234	-0.00271	0.00003
D25	-2.60674	-0.00010	-0.16808	-0.08200	-0.25008	-2.85682
D26	0.45926	-0.00041	-0.15902	-0.07495	-0.23397	0.22529
D27	1.59098	0.00025	-0.03215	0.00114	-0.03102	1.55997
D28	-2.61339	-0.00003	-0.03845	-0.00376	-0.04221	-2.65560
D29	-0.56758	0.00018	-0.03542	-0.00219	-0.03762	-0.60520
D30	-1.46635	0.00020	-0.03421	-0.01250	-0.04672	-1.51307
D31	0.61246	-0.00008	-0.04052	-0.01740	-0.05791	0.55455
D32	2.65827	0.00013	-0.03749	-0.01583	-0.05332	2.60495
D33	-1.29937	-0.00017	-0.01087	-0.01816	-0.02902	-1.32839
D34	0.76974	-0.00037	-0.01178	-0.02310	-0.03487	0.73487
D35	2.90688	0.00015	-0.01454	-0.01453	-0.02906	2.87782

D36	2.92965	-0.00001	-0.00538	-0.01440	-0.01979	2.90986
D37	-1.28443	-0.00022	-0.00629	-0.01934	-0.02564	-1.31007
D38	0.85271	0.00030	-0.00905	-0.01077	-0.01983	0.83288
D39	0.82072	-0.00004	-0.00810	-0.01581	-0.02390	0.79683
D40	2.88983	-0.00024	-0.00901	-0.02074	-0.02975	2.86009
D41	-1.25621	0.00028	-0.01177	-0.01218	-0.02394	-1.28015
D42	2.90688	-0.00017	-0.01211	0.02432	0.01221	2.91909
D43	-1.32591	-0.00007	-0.00761	0.02880	0.02119	-1.30471
D44	0.82301	-0.00015	-0.01685	0.02458	0.00773	0.83073
D45	2.87340	-0.00005	-0.01235	0.02906	0.01671	2.89011
D46	-1.29394	-0.00015	-0.01705	0.03014	0.01309	-1.28085
D47	0.75646	-0.00005	-0.01255	0.03462	0.02207	0.77853
D48	-3.13381	0.00000	-0.00098	-0.00111	-0.00209	-3.13590
D49	0.00951	-0.00001	-0.00143	-0.00103	-0.00246	0.00705
D50	0.00659	-0.00001	0.00026	-0.00075	-0.00049	0.00611
D51	-3.13327	-0.00002	-0.00019	-0.00067	-0.00086	-3.13413

Item	Value	Threshold	Converged?
Maximum Force	0.003052	0.000450	NO
RMS Force	0.000438	0.000300	NO
Maximum Displacement	0.337773	0.001800	NO
RMS Displacement	0.053875	0.001200	NO

Predicted change in Energy=-1.955865D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.802969	-1.987643	0.253624
2	6	0	-2.813178	-1.108169	0.031262
3	7	0	-2.240718	0.160085	0.008623
4	6	0	-0.913864	0.039446	0.214893
5	7	0	-0.634076	-1.253912	0.372040
6	6	0	0.738566	-1.770775	0.559785
7	6	0	1.444490	-2.037281	-0.776547
8	1	0	-1.816728	-3.060209	0.343846
9	1	0	-3.865388	-1.274750	-0.109868
10	1	0	1.288303	-0.994451	1.093082
11	1	0	0.680563	-2.666619	1.179034
12	1	0	1.067408	-2.960893	-1.229052
13	1	0	1.217118	-1.204080	-1.455103
14	35	0	1.934076	1.626893	0.135561
15	1	0	-0.127378	0.827733	0.213925

16	6	0	-2.873826	1.417525	-0.186583
17	6	0	-4.182359	1.594341	-0.315053
18	1	0	-2.160816	2.231925	-0.219603
19	1	0	-4.566467	2.593647	-0.465753
20	1	0	-4.903112	0.787410	-0.276724
21	7	0	2.866985	-2.184865	-0.491895
22	1	0	3.357909	-2.566175	-1.293407
23	1	0	3.260985	-1.264266	-0.300802

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357734	0.000000			
3	N	2.205535	1.391651	0.000000		
4	C	2.213842	2.226687	1.348199	0.000000	
5	N	1.385169	2.210397	2.170888	1.332573	0.000000
6	C	2.569080	3.651476	3.592789	2.475152	1.478696
7	C	3.407302	4.432104	4.361841	3.295084	2.500671
8	H	1.076441	2.213839	3.265338	3.231045	2.159205
9	H	2.212219	1.074622	2.170794	3.247164	3.267116
10	H	3.353667	4.238224	3.868202	2.586445	2.069484
11	H	2.735933	3.994043	4.230130	3.285507	2.091712
12	H	3.374109	4.481063	4.713389	3.874591	2.893498
13	H	3.557337	4.296716	3.995006	2.979317	2.601510
14	Br	5.200416	5.479769	4.426799	3.261449	3.866571
15	H	3.276512	3.315812	2.225783	1.113535	2.148254
16	C	3.596622	2.535797	1.421298	2.429349	3.530598
17	C	4.337684	3.049287	2.435534	3.658087	4.601625
18	H	4.261075	3.412439	2.085904	2.559422	3.851239
19	H	5.398393	4.126074	3.399466	4.508740	5.565008
20	H	4.194410	2.838291	2.750146	4.088427	4.776249
21	N	4.733199	5.804931	5.642512	4.443189	3.724310
22	H	5.418734	6.477874	6.361792	5.226115	4.520144
23	H	5.145318	6.085235	5.691506	4.403972	3.952761

		6	7	8	9	10
6	C	0.000000				
7	C	1.534645	0.000000			
8	H	2.870331	3.596833	0.000000		
9	H	4.678768	5.405619	2.755127	0.000000	
10	H	1.090548	2.146486	3.803936	5.299640	0.000000
11	H	1.090583	2.191791	2.662502	4.925875	1.781258
12	H	2.173582	1.095451	3.286657	5.331803	3.050901
13	H	2.147074	1.098344	3.985681	5.257996	2.557784
14	Br	3.626756	3.807599	6.006733	6.489496	2.864492

15	H	2.760747	3.414690	4.241094	4.300930	2.469296
16	C	4.875624	5.561618	4.631297	2.870091	4.977800
17	C	6.025351	6.712904	5.262622	2.893830	6.213922
18	H	5.003546	5.615562	5.333156	3.900561	4.901945
19	H	6.945739	7.594320	6.338975	3.947488	7.041502
20	H	6.250808	6.965684	4.971423	2.314566	6.586730
21	N	2.409910	1.458184	4.837547	6.804344	2.534063
22	H	3.305744	2.051353	5.449912	7.432669	3.528303
23	H	2.712887	2.030649	5.424403	7.128938	2.430471

		11	12	13	14	15
11	H	0.000000				
12	H	2.456649	0.000000			
13	H	3.060325	1.777612	0.000000		
14	Br	4.592862	4.864265	3.325456	0.000000	
15	H	3.714122	4.226510	2.953234	2.212327	0.000000
16	C	5.583801	5.982526	5.021731	4.823229	2.837471
17	C	6.635969	7.010393	6.187506	6.133098	4.160574
18	H	5.833126	6.197240	4.974237	4.154557	2.508899
19	H	7.609669	7.948339	6.989378	6.599489	4.825550
20	H	6.725101	7.113636	6.543075	6.900860	4.801042
21	N	2.793659	2.093824	2.147503	3.974107	4.305826
22	H	3.645715	2.325154	2.542525	4.653072	5.092926
23	H	3.288629	2.924375	2.348068	3.210904	4.015271

		16	17	18	19	20
16	C	0.000000				
17	C	1.326659	0.000000			
18	H	1.082923	2.121853	0.000000		
19	H	2.079960	1.081140	2.445116	0.000000	
20	H	2.126775	1.082633	3.100013	1.847040	0.000000
21	N	6.784346	8.000433	6.697833	8.836916	8.321967
22	H	7.478600	8.667336	7.391289	9.492340	8.973553
23	H	6.696339	7.973406	6.451811	8.728099	8.417983

		21	22	23
21	N	0.000000		
22	H	1.014311	0.000000	
23	H	1.019439	1.640008	0.000000

Stoichiometry C7H12BrN3
Framework group C1[X(C7H12BrN3)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.708265	2.061461	-0.318272
2	6	0	-2.752588	1.233116	-0.060052
3	7	0	-2.232670	-0.056043	0.006635
4	6	0	-0.903105	0.002120	-0.209039
5	7	0	-0.571198	1.276260	-0.414361
6	6	0	0.820515	1.728827	-0.626158
7	6	0	1.543978	2.014281	0.696813
8	1	0	-1.678375	3.129697	-0.447519
9	1	0	-3.796280	1.448030	0.078981
10	1	0	1.334976	0.911612	-1.132897
11	1	0	0.796086	2.603232	-1.277457
12	1	0	1.207648	2.968499	1.116770
13	1	0	1.286174	1.216366	1.406198
14	35	0	1.877507	-1.697681	-0.082865
15	1	0	-0.149719	-0.817426	-0.182352
16	6	0	-2.915912	-1.278343	0.250049
17	6	0	-4.229901	-1.396178	0.389953
18	1	0	-2.236840	-2.119764	0.310003
19	1	0	-4.653977	-2.372636	0.578507
20	1	0	-4.917045	-0.562088	0.324997
21	7	0	2.969790	2.092553	0.401456
22	1	0	3.480286	2.482104	1.186612
23	1	0	3.324552	1.150135	0.242560

Rotational constants (GHZ): 0.8758733 0.4616777 0.3129937
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 365 symmetry adapted cartesian basis functions of A symmetry.
There are 352 symmetry adapted basis functions of A symmetry.
352 basis functions, 562 primitive gaussians, 365 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 842.0869441426 Hartrees.
NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 352 RedAO= T EigKep= 4.32D-06 NBF= 352
NBsUse= 352 1.00D-06 EigRej= -1.00D+00 NBFU= 352
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"
B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999986 0.003540 0.001484 -0.003665 Ang= 0.61 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3012.46798035 A.U. after 12 cycles
NFock= 12 Conv=0.60D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000168979	0.000251801	0.000476802
2	6	-0.000063189	0.000023360	-0.000065622
3	7	0.000226597	0.000051347	-0.000039581
4	6	0.000358978	-0.000028759	-0.000213257
5	7	-0.000141340	-0.000342794	-0.000414528
6	6	-0.000144126	0.000002614	0.000613248
7	6	-0.000299645	0.000175273	-0.000429506
8	1	-0.000022668	0.000022331	0.000034825
9	1	0.000001619	0.000000547	0.000020855
10	1	0.000041867	0.000140412	0.000252685
11	1	-0.000025489	-0.000013651	-0.000396074
12	1	0.000191214	0.000243122	0.000181152
13	1	-0.000253345	0.000092306	-0.000116049
14	35	0.000308782	-0.000174632	-0.000293416
15	1	-0.000947710	-0.000163228	0.000416959
16	6	0.000041789	0.000087618	-0.000043985
17	6	0.000014141	0.000037308	-0.000071303
18	1	-0.000085249	-0.000123625	0.000025327

19	1	-0.000014562	-0.000007968	0.000027037
20	1	0.000048077	-0.000005831	-0.000023173
21	7	0.000578659	-0.000026999	-0.000575780
22	1	-0.000075721	0.000151157	0.000544629
23	1	0.000092344	-0.000391711	0.000088754

Cartesian Forces: Max 0.000947710 RMS 0.000256741

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.001238902 RMS 0.000225837
Search for a local minimum.
Step number 28 out of a maximum of 121
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 24 27 28
DE= -1.19D-04 DEPred=-1.96D-04 R= 6.07D-01
TightC=F SS= 1.41D+00 RLast= 3.84D-01 DXNew= 1.4142D-01 1.1510D+00
Trust test= 6.07D-01 RLast= 3.84D-01 DXMaxT set to 1.41D-01
ITU= 1 1 0 -1 -1 0 -1 -1 0 -1 0 0 0 1 1 -1 1 -1 1 1
ITU= 1 1 1 1 0 1 0 0
Eigenvalues --- 0.00182 0.00234 0.00437 0.00708 0.01086
Eigenvalues --- 0.01416 0.01817 0.02009 0.02160 0.02303
Eigenvalues --- 0.02393 0.02770 0.03061 0.03070 0.03328
Eigenvalues --- 0.03587 0.04035 0.04456 0.04961 0.05272
Eigenvalues --- 0.05363 0.08962 0.09498 0.10060 0.12620
Eigenvalues --- 0.12743 0.15210 0.15789 0.15960 0.16000
Eigenvalues --- 0.16005 0.16017 0.16242 0.18025 0.21930
Eigenvalues --- 0.22072 0.23076 0.23535 0.24889 0.25066
Eigenvalues --- 0.27513 0.29793 0.34089 0.34420 0.34510
Eigenvalues --- 0.34939 0.35200 0.35689 0.35802 0.35858
Eigenvalues --- 0.36437 0.36663 0.37975 0.39750 0.42186
Eigenvalues --- 0.43032 0.46694 0.47696 0.48325 0.49923
Eigenvalues --- 0.54252 0.60211 0.60504
En-DIIS/RFO-DIIS IScMMF= 0 using points: 28 27 26
RFO step: Lambda=-1.93383240D-05.
DidBck=F Rises=F RFO-DIIS coefs: 0.94572 -0.64304 0.69732
Iteration 1 RMS(Cart)= 0.04430836 RMS(Int)= 0.00141184
Iteration 2 RMS(Cart)= 0.00241085 RMS(Int)= 0.00001562
Iteration 3 RMS(Cart)= 0.00000733 RMS(Int)= 0.00001464
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001464

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56575	0.00011	0.00004	0.00027	0.00032	2.56606
R2	2.61759	-0.00023	0.00037	-0.00064	-0.00028	2.61731
R3	2.03418	-0.00002	0.00000	-0.00002	-0.00003	2.03415
R4	2.62984	-0.00001	-0.00001	-0.00007	-0.00008	2.62976
R5	2.03074	0.00000	0.00003	-0.00003	-0.00001	2.03074
R6	2.54773	-0.00025	-0.00074	-0.00039	-0.00114	2.54659
R7	2.68586	0.00000	0.00059	0.00018	0.00076	2.68663
R8	2.51820	-0.00030	0.00029	-0.00013	0.00016	2.51836
R9	2.10428	-0.00069	0.00125	-0.00220	-0.00095	2.10333
R10	2.79433	-0.00001	-0.00067	0.00063	-0.00004	2.79429
R11	2.90006	0.00033	0.00069	0.00088	0.00157	2.90163
R12	2.06084	0.00024	-0.00008	0.00080	0.00072	2.06155
R13	2.06090	-0.00021	-0.00018	-0.00062	-0.00080	2.06010
R14	2.07010	-0.00035	-0.00029	-0.00073	-0.00102	2.06908
R15	2.07557	0.00020	-0.00018	-0.00002	-0.00020	2.07536
R16	2.75557	0.00062	0.00183	0.00000	0.00183	2.75740
R17	4.18069	0.00023	-0.01811	0.01471	-0.00341	4.17728
R18	2.50702	-0.00004	-0.00009	-0.00003	-0.00012	2.50690
R19	2.04643	-0.00015	0.00031	-0.00029	0.00002	2.04645
R20	2.04306	0.00000	0.00000	0.00001	0.00001	2.04307
R21	2.04588	-0.00003	0.00008	-0.00009	-0.00001	2.04587
R22	1.91677	-0.00052	0.00002	-0.00151	-0.00149	1.91528
R23	1.92646	-0.00030	-0.00047	-0.00109	-0.00156	1.92490
A1	1.87418	0.00000	-0.00026	0.00024	-0.00002	1.87416
A2	2.27790	-0.00002	0.00008	-0.00046	-0.00037	2.27753
A3	2.13107	0.00002	0.00018	0.00023	0.00041	2.13148
A4	1.86180	-0.00006	-0.00001	-0.00005	-0.00006	1.86174
A5	2.27788	0.00003	-0.00006	-0.00007	-0.00012	2.27776
A6	2.14350	0.00003	0.00006	0.00012	0.00018	2.14368
A7	1.89738	-0.00012	0.00035	-0.00040	-0.00006	1.89732
A8	2.24627	0.00008	0.00101	0.00038	0.00140	2.24766
A9	2.13954	0.00004	-0.00136	0.00002	-0.00133	2.13820
A10	1.88760	0.00023	-0.00011	0.00063	0.00053	1.88812
A11	2.25446	0.00016	-0.00602	-0.00047	-0.00646	2.24800
A12	2.13992	-0.00040	0.00567	-0.00027	0.00543	2.14535
A13	1.90377	-0.00004	0.00003	-0.00038	-0.00035	1.90342
A14	2.22565	0.00050	-0.00002	0.00168	0.00167	2.22732
A15	2.15212	-0.00046	-0.00016	-0.00109	-0.00123	2.15089
A16	1.95750	-0.00006	-0.00017	-0.00076	-0.00092	1.95659
A17	1.85584	0.00006	0.00226	0.00014	0.00242	1.85826
A18	1.88583	-0.00002	-0.00086	0.00099	0.00013	1.88596
A19	1.89396	-0.00008	0.00371	-0.00029	0.00342	1.89738

A20	1.95655	0.00004	-0.00187	-0.00186	-0.00373	1.95282
A21	1.91123	0.00005	-0.00301	0.00196	-0.00106	1.91016
A22	1.92599	0.00005	-0.00351	0.00064	-0.00288	1.92311
A23	1.88704	-0.00009	0.00256	-0.00142	0.00113	1.88818
A24	1.87164	-0.00005	0.00171	-0.00028	0.00143	1.87306
A25	1.88930	-0.00001	0.00130	-0.00220	-0.00090	1.88839
A26	1.90827	-0.00016	-0.00174	0.00082	-0.00093	1.90734
A27	1.98158	0.00026	-0.00044	0.00246	0.00203	1.98360
A28	2.72354	-0.00124	0.02282	-0.00817	0.01465	2.73819
A29	2.17800	0.00002	-0.00099	0.00013	-0.00086	2.17714
A30	1.95653	-0.00003	-0.00065	-0.00027	-0.00092	1.95561
A31	2.14866	0.00001	0.00164	0.00014	0.00178	2.15043
A32	2.07958	0.00004	-0.00003	0.00014	0.00011	2.07969
A33	2.15781	-0.00006	-0.00009	-0.00016	-0.00025	2.15756
A34	2.04579	0.00002	0.00012	0.00002	0.00013	2.04593
A35	1.93472	0.00033	-0.00130	0.00527	0.00395	1.93867
A36	1.89887	0.00040	0.00121	0.00545	0.00665	1.90552
A37	1.87606	-0.00019	-0.00346	0.00344	-0.00004	1.87602
D1	0.00633	-0.00002	0.00044	-0.00201	-0.00156	0.00477
D2	-3.13601	-0.00003	-0.00137	0.00013	-0.00124	-3.13724
D3	3.13919	0.00000	0.00128	-0.00161	-0.00033	3.13886
D4	-0.00315	-0.00001	-0.00053	0.00053	0.00000	-0.00315
D5	-0.00964	0.00005	0.00012	0.00390	0.00400	-0.00564
D6	-3.09062	0.00003	0.00240	0.00010	0.00248	-3.08814
D7	3.13979	0.00003	-0.00064	0.00354	0.00290	-3.14050
D8	0.05881	0.00001	0.00164	-0.00026	0.00137	0.06018
D9	-0.00097	-0.00002	-0.00084	-0.00051	-0.00136	-0.00232
D10	-3.13841	-0.00007	-0.00294	-0.00113	-0.00408	3.14069
D11	3.14130	-0.00001	0.00079	-0.00244	-0.00165	3.13964
D12	0.00385	-0.00006	-0.00130	-0.00307	-0.00438	-0.00053
D13	-0.00502	0.00005	0.00092	0.00293	0.00386	-0.00116
D14	3.08385	-0.00016	-0.00623	0.00049	-0.00581	3.07804
D15	3.13273	0.00009	0.00285	0.00351	0.00638	3.13912
D16	-0.06158	-0.00011	-0.00430	0.00107	-0.00328	-0.06487
D17	0.06746	-0.00004	0.01243	-0.00965	0.00278	0.07024
D18	-3.07451	-0.00003	0.01344	-0.00951	0.00393	-3.07058
D19	-3.06947	-0.00009	0.01008	-0.01036	-0.00029	-3.06976
D20	0.07175	-0.00009	0.01109	-0.01022	0.00086	0.07261
D21	0.00903	-0.00006	-0.00064	-0.00421	-0.00485	0.00418
D22	3.09310	0.00000	-0.00280	-0.00050	-0.00329	3.08981
D23	-3.08404	0.00011	0.00656	-0.00195	0.00455	-3.07950
D24	0.00003	0.00017	0.00441	0.00176	0.00611	0.00614
D25	-2.85682	0.00032	0.15341	0.01987	0.17328	-2.68355
D26	0.22529	0.00011	0.14500	0.01713	0.16213	0.38742

D27	1.55997	0.00037	0.02843	0.02092	0.04936	1.60933
D28	-2.65560	0.00028	0.03428	0.02023	0.05452	-2.60109
D29	-0.60520	0.00037	0.03151	0.02309	0.05461	-0.55059
D30	-1.51307	0.00033	0.03100	0.01659	0.04759	-1.46548
D31	0.55455	0.00024	0.03685	0.01590	0.05275	0.60729
D32	2.60495	0.00032	0.03408	0.01876	0.05284	2.65779
D33	-1.32839	0.00000	0.01062	0.00993	0.02054	-1.30785
D34	0.73487	-0.00004	0.01169	0.00679	0.01848	0.75335
D35	2.87782	0.00019	0.01367	0.00876	0.02242	2.90024
D36	2.90986	0.00002	0.00555	0.01039	0.01594	2.92580
D37	-1.31007	-0.00003	0.00662	0.00725	0.01389	-1.29618
D38	0.83288	0.00021	0.00861	0.00921	0.01782	0.85071
D39	0.79683	-0.00003	0.00803	0.00931	0.01734	0.81416
D40	2.86009	-0.00007	0.00911	0.00617	0.01528	2.87536
D41	-1.28015	0.00016	0.01109	0.00813	0.01922	-1.26093
D42	2.91909	-0.00011	0.00941	-0.04329	-0.03389	2.88520
D43	-1.30471	0.00010	0.00518	-0.03266	-0.02748	-1.33219
D44	0.83073	-0.00005	0.01360	-0.04435	-0.03076	0.79998
D45	2.89011	0.00016	0.00937	-0.03371	-0.02434	2.86577
D46	-1.28085	-0.00010	0.01348	-0.04377	-0.03029	-1.31114
D47	0.77853	0.00011	0.00924	-0.03313	-0.02388	0.75466
D48	-3.13590	-0.00002	0.00093	-0.00034	0.00058	-3.13532
D49	0.00705	-0.00002	0.00133	-0.00116	0.00017	0.00722
D50	0.00611	-0.00003	-0.00019	-0.00050	-0.00069	0.00541
D51	-3.13413	-0.00003	0.00021	-0.00131	-0.00111	-3.13523

Item	Value	Threshold	Converged?
Maximum Force	0.001239	0.000450	NO
RMS Force	0.000226	0.000300	YES
Maximum Displacement	0.293711	0.001800	NO
RMS Displacement	0.044654	0.001200	NO

Predicted change in Energy=-3.955261D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.815341	-1.997504	0.266193
2	6	0	-2.820762	-1.112636	0.042504
3	7	0	-2.240946	0.152156	0.016344
4	6	0	-0.915500	0.024401	0.223444
5	7	0	-0.641967	-1.270476	0.379823
6	6	0	0.729096	-1.792709	0.564039

7	6	0	1.453655	-1.998434	-0.774011
8	1	0	-1.835658	-3.069712	0.359227
9	1	0	-3.874051	-1.273578	-0.097083
10	1	0	1.270244	-1.043359	1.143483
11	1	0	0.664207	-2.717591	1.137473
12	1	0	1.068301	-2.890150	-1.279152
13	1	0	1.249557	-1.127892	-1.411682
14	35	0	1.900765	1.655507	-0.019864
15	1	0	-0.129033	0.811946	0.214103
16	6	0	-2.864639	1.413668	-0.185721
17	6	0	-4.171840	1.598542	-0.315711
18	1	0	-2.144656	2.221716	-0.223512
19	1	0	-4.549270	2.599489	-0.472327
20	1	0	-4.897797	0.796501	-0.273340
21	7	0	2.869673	-2.187148	-0.476677
22	1	0	3.363579	-2.562381	-1.278231
23	1	0	3.287908	-1.285438	-0.254040

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357903	0.000000			
3	N	2.205584	1.391607	0.000000		
4	C	2.213513	2.226121	1.347597	0.000000	
5	N	1.385023	2.210394	2.170882	1.332659	0.000000
6	C	2.569983	3.651847	3.592160	2.474387	1.478674
7	C	3.430505	4.440944	4.347387	3.271036	2.500578
8	H	1.076428	2.213795	3.265311	3.230891	2.159299
9	H	2.212313	1.074619	2.170856	3.246615	3.267081
10	H	3.346770	4.237132	3.876616	2.600781	2.071548
11	H	2.725034	3.989968	4.234653	3.293849	2.091474
12	H	3.391209	4.475617	4.678146	3.832476	2.881070
13	H	3.600707	4.322313	3.982636	2.947693	2.609154
14	Br	5.218789	5.473511	4.406262	3.263596	3.897000
15	H	3.277096	3.313437	2.221397	1.113034	2.151057
16	C	3.597409	2.536972	1.421702	2.428296	3.530544
17	C	4.338577	3.050282	2.435292	3.656823	4.601634
18	H	4.260291	3.412592	2.085637	2.557105	3.849349
19	H	5.399271	4.127064	3.399500	4.507710	5.565051
20	H	4.195127	2.838773	2.749174	4.086761	4.776097
21	N	4.747334	5.814222	5.642148	4.439444	3.729008
22	H	5.433741	6.487848	6.360450	5.220822	4.523556
23	H	5.178884	6.118305	5.719091	4.428579	3.980694

	6	7	8	9	10

6	C	0.000000				
7	C	1.535476	0.000000			
8	H	2.872394	3.640254	0.000000		
9	H	4.679268	5.419235	2.754879	0.000000	
10	H	1.090927	2.150021	3.790487	5.296771	0.000000
11	H	1.090158	2.189563	2.641776	4.919866	1.780553
12	H	2.171818	1.094909	3.339088	5.332676	3.052963
13	H	2.148565	1.098236	4.052818	5.291574	2.556647
14	Br	3.688352	3.757649	6.035914	6.475647	3.005796
15	H	2.764610	3.373353	4.242746	4.297838	2.502775
16	C	4.874210	5.534997	4.632112	2.871944	4.990093
17	C	6.024427	6.692867	5.263637	2.895782	6.222955
18	H	4.999429	5.573199	5.332379	3.901778	4.918428
19	H	6.944537	7.567497	6.339953	3.949351	7.053221
20	H	6.250371	6.957246	4.972367	2.316106	6.590690
21	N	2.412622	1.459153	4.859815	6.815902	2.547812
22	H	3.305579	2.054284	5.474552	7.445765	3.543187
23	H	2.733879	2.035489	5.459914	7.163689	2.466301

		11	12	13	14	15
11	H	0.000000				
12	H	2.456247	0.000000			
13	H	3.060713	1.776505	0.000000		
14	Br	4.689615	4.789760	3.179393	0.000000	
15	H	3.733560	4.167606	2.882128	2.210524	0.000000
16	C	5.592038	5.931818	4.988900	4.774418	2.829393
17	C	6.642898	6.966754	6.166534	6.080074	4.152556
18	H	5.842836	6.129326	4.914499	4.089926	2.498338
19	H	7.618604	7.895835	6.957165	6.534430	4.817155
20	H	6.728678	7.085011	6.541336	6.857302	4.793636
21	N	2.784050	2.093591	2.149659	3.989168	4.296974
22	H	3.625786	2.318563	2.558252	4.638307	5.080500
23	H	3.297147	2.924486	2.349432	3.260086	4.036541

		16	17	18	19	20
16	C	0.000000				
17	C	1.326594	0.000000			
18	H	1.082933	2.122810	0.000000		
19	H	2.079974	1.081145	2.446791	0.000000	
20	H	2.126571	1.082626	3.100565	1.847115	0.000000
21	N	6.777380	7.996266	6.681742	8.829079	8.323287
22	H	7.469487	8.661539	7.371612	9.481959	8.974532
23	H	6.718905	7.998062	6.466360	8.749952	8.446337

		21	22	23
21	N	0.000000		
22	H	1.013524	0.000000	

23 H 1.018612 1.638682 0.000000

Stoichiometry C7H12BrN3

Framework group C1[X(C7H12BrN3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.722149	2.083160	-0.262506
2	6	0	-2.754399	1.236322	-0.015068
3	7	0	-2.222242	-0.049475	-0.004868
4	6	0	-0.898447	0.028693	-0.244602
5	7	0	-0.580207	1.312680	-0.406096
6	6	0	0.804608	1.783276	-0.623590
7	6	0	1.569274	1.958629	0.696343
8	1	0	-1.704295	3.155572	-0.353668
9	1	0	-3.797093	1.436537	0.150788
10	1	0	1.302609	1.015333	-1.217206
11	1	0	0.760499	2.711196	-1.194084
12	1	0	1.230442	2.863129	1.211996
13	1	0	1.348307	1.095007	1.337790
14	35	0	1.859432	-1.707910	-0.073219
15	1	0	-0.142260	-0.787949	-0.255743
16	6	0	-2.887897	-1.287027	0.211019
17	6	0	-4.197528	-1.422792	0.373142
18	1	0	-2.198197	-2.121712	0.229941
19	1	0	-4.608464	-2.409144	0.537816
20	1	0	-4.893536	-0.593873	0.349782
21	7	0	2.983619	2.094497	0.364235
22	1	0	3.510995	2.449100	1.153767
23	1	0	3.361905	1.178155	0.130172

Rotational constants (GHZ): 0.8689218 0.4659695 0.3134919

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 365 symmetry adapted cartesian basis functions of A symmetry.

There are 352 symmetry adapted basis functions of A symmetry.

352 basis functions, 562 primitive gaussians, 365 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 841.9842684942 Hartrees.

NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F

Big=F
 Integral buffers will be 131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis= 352 RedAO= T EigKep= 4.37D-06 NBF= 352
 NBsUse= 352 1.00D-06 EigRej= -1.00D+00 NBFU= 352
 Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"
 B after Tr= 0.000000 0.000000 0.000000
 Rot= 0.999990 -0.004152 -0.001205 0.000577 Ang= -0.50 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
 Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
 HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
 FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
 NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
 wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
 NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on energy=1.00D-06.
 No special actions if energy rises.
 SCF Done: E(RB3LYP) = -3012.46799466 A.U. after 12 cycles
 NFock= 12 Conv=0.48D-08 -V/T= 2.0017
 Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****

 Center Atomic Forces (Hartrees/Bohr)
 Number Number X Y Z

1	6	0.000026871	0.000130581	0.000150932
2	6	-0.000026615	-0.000022199	-0.000106479
3	7	-0.000005190	0.000007588	0.000038037
4	6	0.000239344	0.000082766	-0.000058534
5	7	-0.000050932	0.000034040	0.000070328
6	6	0.000387198	0.000595698	0.000151253
7	6	0.000035709	0.000277097	-0.000754035
8	1	0.000020506	0.000004939	-0.000026615
9	1	0.000002946	-0.000023174	-0.000000942

10	1	-0.000066807	-0.000512406	-0.000183117
11	1	-0.000036288	0.000019879	-0.000011923
12	1	0.000108749	-0.000283415	0.000347113
13	1	0.000339045	0.000090194	0.000486678
14	35	0.000050514	-0.000331782	0.000171210
15	1	-0.000393977	0.000059529	-0.000146939
16	6	0.000055378	-0.000127052	0.000086814
17	6	0.000020076	0.000079317	-0.000053882
18	1	-0.000111232	-0.000049040	-0.000022400
19	1	-0.000011842	-0.000010279	0.000008874
20	1	0.000018535	-0.000005747	-0.000016433
21	7	-0.000104990	-0.000333929	0.000251751
22	1	-0.000145817	0.000115866	-0.000015998
23	1	-0.000351183	0.000201529	-0.000365695

Cartesian Forces: Max 0.000754035 RMS 0.000211114

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.001174129 RMS 0.000219973
Search for a local minimum.
Step number 29 out of a maximum of 121
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 20 24 23 26 27
28 29
DE= -1.43D-05 DEPred=-3.96D-05 R= 3.62D-01
Trust test= 3.62D-01 RLast= 2.85D-01 DXMaxT set to 1.41D-01
ITU= 0 1 1 0 -1 -1 0 -1 -1 0 -1 0 0 0 1 1 -1 1 -1 1
ITU= 1 1 1 1 1 0 1 0 0

Eigenvalues ---	0.00178	0.00224	0.00380	0.00720	0.00973
Eigenvalues ---	0.01413	0.01813	0.02020	0.02161	0.02305
Eigenvalues ---	0.02393	0.02743	0.03060	0.03070	0.03291
Eigenvalues ---	0.04043	0.04193	0.04468	0.05070	0.05271
Eigenvalues ---	0.05722	0.08977	0.09442	0.09814	0.12500
Eigenvalues ---	0.12983	0.15523	0.15764	0.15974	0.16000
Eigenvalues ---	0.16006	0.16018	0.16454	0.18217	0.22029
Eigenvalues ---	0.22636	0.23104	0.23539	0.24920	0.25116
Eigenvalues ---	0.27042	0.29806	0.34134	0.34465	0.34711
Eigenvalues ---	0.35069	0.35431	0.35690	0.35847	0.35859
Eigenvalues ---	0.36436	0.36664	0.37839	0.40678	0.42214

Eigenvalues --- 0.43032 0.46680 0.47712 0.48449 0.49933
Eigenvalues --- 0.54246 0.60056 0.60420
En-DIIS/RFO-DIIS IScMMF= 0 using points: 29 28 27 26
RFO step: Lambda=-1.41604123D-05.
DidBck=F Rises=F RFO-DIIS coefs: 0.90908 0.45424 -0.45056 0.08724
Iteration 1 RMS(Cart)= 0.01908767 RMS(Int)= 0.00071743
Iteration 2 RMS(Cart)= 0.00082699 RMS(Int)= 0.00000608
Iteration 3 RMS(Cart)= 0.00000261 RMS(Int)= 0.00000587
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000587

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56606	0.00001	0.00006	-0.00013	-0.00007	2.56599
R2	2.61731	-0.00010	-0.00023	-0.00022	-0.00045	2.61687
R3	2.03415	-0.00001	-0.00001	-0.00002	-0.00003	2.03412
R4	2.62976	0.00004	-0.00015	-0.00019	-0.00034	2.62941
R5	2.03074	0.00000	-0.00004	0.00000	-0.00004	2.03070
R6	2.54659	0.00003	0.00041	0.00000	0.00041	2.54700
R7	2.68663	-0.00008	-0.00017	-0.00004	-0.00022	2.68641
R8	2.51836	-0.00028	-0.00016	0.00012	-0.00004	2.51832
R9	2.10333	-0.00044	-0.00126	-0.00204	-0.00330	2.10003
R10	2.79429	0.00008	0.00029	0.00049	0.00079	2.79508
R11	2.90163	-0.00003	-0.00008	0.00001	-0.00007	2.90155
R12	2.06155	-0.00048	0.00001	-0.00061	-0.00061	2.06095
R13	2.06010	-0.00002	0.00008	-0.00009	-0.00001	2.06009
R14	2.06908	0.00003	-0.00029	0.00023	-0.00006	2.06902
R15	2.07536	-0.00028	0.00061	-0.00059	0.00002	2.07539
R16	2.75740	-0.00061	-0.00081	-0.00074	-0.00155	2.75585
R17	4.17728	-0.00010	0.01666	0.00710	0.02376	4.20104
R18	2.50690	-0.00001	0.00004	-0.00006	-0.00002	2.50688
R19	2.04645	-0.00011	-0.00008	-0.00020	-0.00028	2.04616
R20	2.04307	0.00000	0.00001	-0.00002	-0.00001	2.04306
R21	2.04587	-0.00001	-0.00004	-0.00004	-0.00007	2.04579
R22	1.91528	-0.00010	-0.00012	-0.00014	-0.00027	1.91502
R23	1.92490	-0.00005	0.00055	-0.00021	0.00034	1.92524
A1	1.87416	0.00001	0.00019	0.00047	0.00067	1.87483
A2	2.27753	0.00001	-0.00002	-0.00020	-0.00022	2.27730
A3	2.13148	-0.00002	-0.00018	-0.00026	-0.00045	2.13103
A4	1.86174	-0.00004	0.00004	-0.00027	-0.00023	1.86151
A5	2.27776	0.00000	0.00007	0.00004	0.00011	2.27787
A6	2.14368	0.00004	-0.00012	0.00024	0.00012	2.14380
A7	1.89732	-0.00009	-0.00028	0.00010	-0.00018	1.89713
A8	2.24766	-0.00002	-0.00031	-0.00017	-0.00048	2.24718
A9	2.13820	0.00011	0.00059	0.00007	0.00066	2.13887
A10	1.88812	0.00008	0.00023	0.00009	0.00032	1.88845

A11	2.24800	0.00064	0.00105	-0.00108	-0.00003	2.24796
A12	2.14535	-0.00072	-0.00101	0.00115	0.00013	2.14548
A13	1.90342	0.00003	-0.00018	-0.00039	-0.00057	1.90285
A14	2.22732	0.00020	-0.00006	-0.00137	-0.00145	2.22587
A15	2.15089	-0.00024	0.00053	0.00173	0.00224	2.15312
A16	1.95659	-0.00044	0.00063	-0.00046	0.00017	1.95676
A17	1.85826	0.00025	-0.00151	0.00247	0.00096	1.85922
A18	1.88596	0.00013	0.00022	-0.00157	-0.00135	1.88461
A19	1.89738	0.00008	-0.00270	0.00018	-0.00253	1.89486
A20	1.95282	0.00009	0.00155	-0.00086	0.00068	1.95350
A21	1.91016	-0.00010	0.00174	0.00044	0.00217	1.91234
A22	1.92311	-0.00024	0.00198	-0.00055	0.00143	1.92454
A23	1.88818	-0.00007	-0.00009	-0.00071	-0.00081	1.88736
A24	1.87306	0.00026	-0.00112	-0.00051	-0.00163	1.87143
A25	1.88839	0.00034	-0.00241	0.00374	0.00133	1.88972
A26	1.90734	-0.00003	-0.00053	0.00014	-0.00039	1.90695
A27	1.98360	-0.00028	0.00229	-0.00217	0.00012	1.98372
A28	2.73819	-0.00117	-0.01780	-0.00542	-0.02322	2.71498
A29	2.17714	0.00007	0.00053	0.00008	0.00062	2.17776
A30	1.95561	0.00002	0.00018	0.00013	0.00031	1.95592
A31	2.15043	-0.00009	-0.00071	-0.00021	-0.00093	2.14951
A32	2.07969	0.00002	-0.00008	0.00016	0.00008	2.07978
A33	2.15756	-0.00003	0.00019	-0.00023	-0.00004	2.15752
A34	2.04593	0.00000	-0.00011	0.00007	-0.00004	2.04589
A35	1.93867	-0.00016	0.00082	-0.00143	-0.00062	1.93805
A36	1.90552	-0.00077	-0.00122	-0.00296	-0.00419	1.90132
A37	1.87602	0.00019	0.00204	-0.00056	0.00147	1.87749
D1	0.00477	-0.00006	0.00041	-0.00093	-0.00052	0.00425
D2	-3.13724	-0.00006	0.00058	-0.00031	0.00027	-3.13697
D3	3.13886	0.00005	-0.00057	0.00039	-0.00019	3.13867
D4	-0.00315	0.00005	-0.00041	0.00101	0.00060	-0.00255
D5	-0.00564	0.00009	0.00011	0.00074	0.00085	-0.00479
D6	-3.08814	0.00018	-0.00462	0.00116	-0.00347	-3.09161
D7	-3.14050	-0.00001	0.00100	-0.00044	0.00056	-3.13994
D8	0.06018	0.00008	-0.00374	-0.00002	-0.00377	0.05642
D9	-0.00232	0.00001	-0.00079	0.00081	0.00002	-0.00231
D10	3.14069	0.00000	0.00093	0.00016	0.00108	-3.14141
D11	3.13964	0.00001	-0.00094	0.00024	-0.00070	3.13895
D12	-0.00053	0.00000	0.00078	-0.00041	0.00037	-0.00016
D13	-0.00116	0.00004	0.00086	-0.00035	0.00052	-0.00065
D14	3.07804	0.00001	0.00607	0.00265	0.00870	3.08674
D15	3.13912	0.00005	-0.00073	0.00025	-0.00047	3.13864
D16	-0.06487	0.00002	0.00448	0.00325	0.00771	-0.05716
D17	0.07024	-0.00004	-0.00874	-0.00528	-0.01401	0.05623

D18	-3.07058	-0.00001	-0.00925	-0.00489	-0.01413	-3.08471
D19	-3.06976	-0.00006	-0.00680	-0.00601	-0.01281	-3.08257
D20	0.07261	-0.00002	-0.00732	-0.00561	-0.01293	0.05968
D21	0.00418	-0.00008	-0.00061	-0.00024	-0.00085	0.00333
D22	3.08981	-0.00015	0.00386	-0.00075	0.00311	3.09293
D23	-3.07950	-0.00011	-0.00548	-0.00293	-0.00843	-3.08793
D24	0.00614	-0.00018	-0.00101	-0.00344	-0.00447	0.00167
D25	-2.68355	-0.00020	-0.08912	0.00117	-0.08794	-2.77149
D26	0.38742	-0.00019	-0.08320	0.00452	-0.07868	0.30874
D27	1.60933	-0.00011	-0.01241	0.00863	-0.00378	1.60555
D28	-2.60109	-0.00010	-0.01629	0.01013	-0.00616	-2.60724
D29	-0.55059	-0.00003	-0.01495	0.01114	-0.00380	-0.55440
D30	-1.46548	-0.00002	-0.01774	0.00918	-0.00856	-1.47404
D31	0.60729	-0.00001	-0.02162	0.01068	-0.01094	0.59635
D32	2.65779	0.00007	-0.02027	0.01169	-0.00859	2.64920
D33	-1.30785	-0.00007	-0.01128	-0.00384	-0.01512	-1.32297
D34	0.75335	0.00016	-0.01312	-0.00006	-0.01319	0.74016
D35	2.90024	-0.00006	-0.01108	-0.00340	-0.01448	2.88576
D36	2.92580	-0.00017	-0.00808	-0.00673	-0.01481	2.91099
D37	-1.29618	0.00006	-0.00992	-0.00295	-0.01287	-1.30905
D38	0.85071	-0.00016	-0.00788	-0.00629	-0.01417	0.83654
D39	0.81416	-0.00016	-0.00942	-0.00684	-0.01626	0.79791
D40	2.87536	0.00008	-0.01126	-0.00306	-0.01432	2.86104
D41	-1.26093	-0.00015	-0.00922	-0.00640	-0.01562	-1.27655
D42	2.88520	0.00008	0.00878	-0.00835	0.00042	2.88563
D43	-1.33219	-0.00026	0.01099	-0.01175	-0.00076	-1.33295
D44	0.79998	0.00023	0.00736	-0.00748	-0.00013	0.79985
D45	2.86577	-0.00011	0.00957	-0.01088	-0.00131	2.86446
D46	-1.31114	0.00000	0.00928	-0.01091	-0.00162	-1.31276
D47	0.75466	-0.00034	0.01150	-0.01431	-0.00281	0.75184
D48	-3.13532	0.00001	-0.00071	-0.00040	-0.00111	-3.13643
D49	0.00722	0.00000	-0.00076	-0.00065	-0.00141	0.00581
D50	0.00541	-0.00002	-0.00014	-0.00084	-0.00098	0.00443
D51	-3.13523	-0.00004	-0.00019	-0.00109	-0.00128	-3.13651

Item	Value	Threshold	Converged?
Maximum Force	0.001174	0.000450	NO
RMS Force	0.000220	0.000300	YES
Maximum Displacement	0.116461	0.001800	NO
RMS Displacement	0.019401	0.001200	NO

Predicted change in Energy=-4.071927D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.813034	-1.993014	0.270292
2	6	0	-2.820569	-1.110191	0.048273
3	7	0	-2.242440	0.155043	0.016442
4	6	0	-0.915837	0.029131	0.218614
5	7	0	-0.639873	-1.265002	0.376699
6	6	0	0.731474	-1.787758	0.560657
7	6	0	1.450883	-2.007035	-0.777975
8	1	0	-1.831717	-3.064964	0.366404
9	1	0	-3.874268	-1.272812	-0.086024
10	1	0	1.277318	-1.033644	1.128800
11	1	0	0.665893	-2.707037	1.142944
12	1	0	1.074165	-2.911093	-1.267384
13	1	0	1.234178	-1.148202	-1.427277
14	35	0	1.936363	1.613091	0.041765
15	1	0	-0.132484	0.817335	0.211459
16	6	0	-2.869156	1.414971	-0.185336
17	6	0	-4.175894	1.596434	-0.324377
18	1	0	-2.152218	2.225874	-0.214585
19	1	0	-4.555346	2.596944	-0.478845
20	1	0	-4.899543	0.791905	-0.291844
21	7	0	2.869284	-2.174892	-0.483543
22	1	0	3.363724	-2.557229	-1.281223
23	1	0	3.274622	-1.262940	-0.278653

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357864	0.000000			
3	N	2.205216	1.391425	0.000000		
4	C	2.212849	2.226000	1.347814	0.000000	
5	N	1.384785	2.210716	2.171297	1.332639	0.000000
6	C	2.569234	3.652211	3.593718	2.476230	1.479090
7	C	3.428150	4.442107	4.352736	3.277274	2.501028
8	H	1.076413	2.213633	3.264906	3.230186	2.158810
9	H	2.212314	1.074598	2.170744	3.246563	3.267335
10	H	3.347791	4.238642	3.878017	2.601511	2.072391
11	H	2.723313	3.987937	4.233073	3.292852	2.090843
12	H	3.397535	4.488113	4.695665	3.848794	2.889732
13	H	3.589004	4.315052	3.983672	2.952564	2.603850
14	Br	5.207129	5.481306	4.425940	3.267300	3.877189
15	H	3.275023	3.311766	2.220040	1.111287	2.149622

16	C	3.596853	2.536411	1.421586	2.428824	3.530983
17	C	4.338303	3.049852	2.435572	3.657765	4.602474
18	H	4.260184	3.412495	2.085630	2.557729	3.850067
19	H	5.399000	4.126761	3.399666	4.508452	5.565744
20	H	4.195034	2.838271	2.749697	4.088069	4.777301
21	N	4.746099	5.812990	5.639885	4.435976	3.725869
22	H	5.433632	6.488988	6.361558	5.220480	4.521874
23	H	5.169004	6.105864	5.704010	4.413238	3.968975

		6	7	8	9	10
6	C	0.000000				
7	C	1.535437	0.000000			
8	H	2.870355	3.633769	0.000000		
9	H	4.679340	5.419881	2.754726	0.000000	
10	H	1.090606	2.147884	3.791254	5.298286	0.000000
11	H	1.090152	2.190009	2.639921	4.917360	1.781653
12	H	2.172799	1.094879	3.337228	5.344770	3.050867
13	H	2.147935	1.098248	4.036209	5.283058	2.559006
14	Br	3.645104	3.743391	6.015648	6.489083	2.936186
15	H	2.766745	3.385720	4.240713	4.296295	2.501036
16	C	4.876322	5.542931	4.631471	2.871287	4.991585
17	C	6.026467	6.697115	5.263172	2.894886	6.226279
18	H	5.002592	5.587241	5.332282	3.901639	4.918420
19	H	6.946701	7.573697	6.339543	3.948821	7.055896
20	H	6.252182	6.956889	4.971950	2.314435	6.595793
21	N	2.410489	1.458331	4.859429	6.815223	2.537016
22	H	3.303535	2.053030	5.474036	7.447600	3.533074
23	H	2.729007	2.032000	5.453264	7.151491	2.454123

		11	12	13	14	15
11	H	0.000000				
12	H	2.453163	0.000000			
13	H	3.059240	1.777345	0.000000		
14	Br	4.635752	4.788058	3.205602	0.000000	
15	H	3.731792	4.188575	2.901131	2.223095	0.000000
16	C	5.590336	5.952768	4.994960	4.814960	2.829132
17	C	6.641972	6.983566	6.165898	6.123236	4.152502
18	H	5.841083	6.156815	4.931804	4.142187	2.498964
19	H	7.617333	7.915281	6.960189	6.586447	4.817181
20	H	6.728692	7.095708	6.532669	6.893131	4.793622
21	N	2.789905	2.092571	2.149022	3.936382	4.295005
22	H	3.630057	2.316784	2.557666	4.602089	5.083233
23	H	3.303304	2.921645	2.344337	3.188284	4.021956

		16	17	18	19	20
16	C	0.000000				
17	C	1.326584	0.000000			

18	H	1.082783	2.122148	0.000000		
19	H	2.080011	1.081141	2.445925	0.000000	
20	H	2.126506	1.082587	3.100005	1.847054	0.000000
21	N	6.775378	7.992670	6.682407	8.825847	8.318252
22	H	7.471823	8.661080	7.378442	9.482667	8.970906
23	H	6.702681	7.980495	6.451862	8.731963	8.428496

		21	22	23
21	N	0.000000		
22	H	1.013383	0.000000	
23	H	1.018791	1.639595	0.000000

Stoichiometry C7H12BrN3
Framework group C1[X(C7H12BrN3)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.724632	2.067055	-0.289962
2	6	0	-2.762516	1.227832	-0.040371
3	7	0	-2.234697	-0.059045	-0.002722
4	6	0	-0.907804	0.011399	-0.228538
5	7	0	-0.583349	1.291554	-0.407027
6	6	0	0.804341	1.756921	-0.620235
7	6	0	1.554778	1.962724	0.703417
8	1	0	-1.702318	3.137713	-0.398854
9	1	0	-3.806453	1.433979	0.109500
10	1	0	1.309929	0.975077	-1.188145
11	1	0	0.765381	2.671296	-1.212547
12	1	0	1.222769	2.886712	1.187953
13	1	0	1.315272	1.120800	1.366703
14	35	0	1.881767	-1.683144	-0.079971
15	1	0	-0.156408	-0.807350	-0.224822
16	6	0	-2.907465	-1.290502	0.224887
17	6	0	-4.217805	-1.417973	0.387934
18	1	0	-2.222944	-2.129019	0.252080
19	1	0	-4.634036	-2.400665	0.560942
20	1	0	-4.909340	-0.585593	0.357649
21	7	0	2.973468	2.070342	0.383316
22	1	0	3.496344	2.441805	1.167892
23	1	0	3.338642	1.140611	0.182857

```
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.8841794           0.4613289           0.3136201
 Standard basis: 6-311++G(d,p) (5D, 7F)
 There are     365 symmetry adapted cartesian basis functions of A      symmetry.
 There are     352 symmetry adapted basis functions of A      symmetry.
    352 basis functions,      562 primitive gaussians,      365 cartesian basis functions
     55 alpha electrons              55 beta electrons
          nuclear repulsion energy              842.7709813770 Hartrees.
 NAtoms=       23 NActive=       23 NUniq=       23 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      352 RedAO= T EigKep=    4.32D-06    NBF=      352
 NBsUse=      352 1.00D-06 EigRej= -1.00D+00 NBFU=      352
 Initial guess from the checkpoint file:    "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"
 B after Tr=          0.000000        0.000000        0.000000
             Rot=        0.999998        0.000869        0.000524      -0.001658 Ang=      0.22 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn=                5 AccDes=
0.00D+00
 Harris functional with IExCor=    402 and IRadAn=             5 diagonalized for initial guess.
 HarFok:    IExCor=    402 AccDes= 0.00D+00 IRadAn=                5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=    3500011 ScaDFX=    1.000000    1.000000    1.000000    1.000000
 FoFCou: FMM=F IPFlag=                  0 FMFlag=           100000 FMFlg1=                  0
             NFxFlg=                    0 DoJE=T BraDBF=F KetDBF=T FulRan=T
             wScrn=      0.000000  ICntrl=             500  IOpCl=      0  I1Cent=        200000004  NGrid=
0
             NMat0=         1 NMatS0=            1 NMatT0=         0 NMatD0=         1 NMtDS0=         0
NMtDT0=        0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                       energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3012.46804499          A.U. after      12 cycles
                   NFock= 12    Conv=0.22D-08         -V/T= 2.0017
 Calling FoFJK, ICntrl=             2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 ---------------------------------------------------------------------
 Center         Atomic                             Forces (Hartrees/Bohr)
 Number          Number                       X                       Y                       Z
 ---------------------------------------------------------------------
```

1	6	0.000003351	0.000007391	0.000060940
2	6	-0.000039049	-0.000035075	-0.000113271
3	7	-0.000041299	0.000047147	0.000097717
4	6	0.000024520	0.000030537	-0.000249493
5	7	-0.000072018	0.000141822	0.000286192
6	6	0.000088789	0.000311469	0.000072847
7	6	-0.000170630	0.000039433	-0.000551423
8	1	0.000020033	-0.000004718	-0.000016329
9	1	-0.000002741	-0.000018624	0.000012348
10	1	-0.000141334	-0.000231488	0.000030595
11	1	-0.000003347	-0.000000059	0.000010761
12	1	-0.000080677	-0.000138330	0.000219758
13	1	0.000257660	0.000037996	0.000205086
14	35	0.000041419	-0.000101588	0.000028480
15	1	0.000032553	-0.000051749	-0.000023645
16	6	0.000069565	-0.000137860	0.000082903
17	6	0.000002452	0.000051291	-0.000050562
18	1	-0.000062669	-0.000009029	-0.000022654
19	1	-0.000005071	-0.000010305	0.000006044
20	1	0.000004676	-0.000011693	-0.000005658
21	7	0.000067193	-0.000144737	0.000071100
22	1	0.000029667	0.000064253	-0.000102336
23	1	-0.000023042	0.000163914	-0.000049401

Cartesian Forces: Max 0.000551423 RMS 0.000122900

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000438907 RMS 0.000107680
Search for a local minimum.
Step number 30 out of a maximum of 121
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 24 23 26 27 28
29 30
DE= -5.03D-05 DEPred=-4.07D-05 R= 1.24D+00
TightC=F SS= 1.41D+00 RLast= 1.35D-01 DXNew= 2.3784D-01 4.0643D-01
Trust test= 1.24D+00 RLast= 1.35D-01 DXMaxT set to 2.38D-01
ITU= 1 0 1 1 0 -1 -1 0 -1 -1 0 -1 0 0 0 1 1 -1 1 -1
ITU= 1 1 1 1 1 1 0 1 0 0
Eigenvalues --- 0.00161 0.00235 0.00361 0.00811 0.00968

Eigenvalues --- 0.01416 0.01807 0.01991 0.02156 0.02300
Eigenvalues --- 0.02390 0.02691 0.03060 0.03069 0.03309
Eigenvalues --- 0.04052 0.04142 0.04478 0.05082 0.05284
Eigenvalues --- 0.05691 0.08965 0.09560 0.09986 0.12750
Eigenvalues --- 0.13118 0.15557 0.15665 0.15985 0.16000
Eigenvalues --- 0.16007 0.16015 0.16282 0.18326 0.21990
Eigenvalues --- 0.22190 0.23113 0.23555 0.24813 0.25102
Eigenvalues --- 0.26313 0.29946 0.34079 0.34642 0.34684
Eigenvalues --- 0.34939 0.35286 0.35690 0.35779 0.35859
Eigenvalues --- 0.36437 0.36661 0.37809 0.40538 0.42215
Eigenvalues --- 0.42968 0.46682 0.47698 0.48644 0.49926
Eigenvalues --- 0.54257 0.59940 0.60402

En-DIIS/RFO-DIIS IScMMF= 0 using points: 30 29 28 27 26

RFO step: Lambda=-3.16322444D-06.

DidBck=F Rises=F RFO-DIIS coefs: 1.24014 -0.25602 0.07102 -0.18867 0.13353

Iteration 1 RMS(Cart)= 0.00689672 RMS(Int)= 0.00003220

Iteration 2 RMS(Cart)= 0.00003739 RMS(Int)= 0.00000289

Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00000289

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56599	0.00001	0.00000	-0.00002	-0.00002	2.56597
R2	2.61687	-0.00003	-0.00009	-0.00013	-0.00022	2.61665
R3	2.03412	0.00000	-0.00001	0.00002	0.00001	2.03414
R4	2.62941	0.00007	-0.00011	0.00018	0.00007	2.62949
R5	2.03070	0.00000	-0.00001	0.00000	-0.00002	2.03068
R6	2.54700	0.00006	0.00005	0.00001	0.00005	2.54705
R7	2.68641	-0.00011	0.00002	-0.00025	-0.00024	2.68617
R8	2.51832	-0.00022	0.00001	0.00004	0.00005	2.51837
R9	2.10003	-0.00006	-0.00080	0.00032	-0.00049	2.09954
R10	2.79508	-0.00003	0.00013	-0.00005	0.00007	2.79515
R11	2.90155	0.00021	0.00008	0.00103	0.00112	2.90267
R12	2.06095	-0.00022	-0.00016	-0.00029	-0.00045	2.06050
R13	2.06009	0.00001	-0.00002	0.00003	0.00001	2.06010
R14	2.06902	0.00004	-0.00011	-0.00007	-0.00018	2.06884
R15	2.07539	-0.00014	0.00008	-0.00041	-0.00033	2.07506
R16	2.75585	0.00005	-0.00021	0.00065	0.00044	2.75628
R17	4.20104	0.00000	0.00559	0.00263	0.00822	4.20926
R18	2.50688	0.00000	-0.00001	0.00003	0.00002	2.50690
R19	2.04616	-0.00005	-0.00003	-0.00009	-0.00012	2.04604
R20	2.04306	-0.00001	0.00000	-0.00003	-0.00003	2.04303
R21	2.04579	0.00000	-0.00001	0.00001	0.00000	2.04579
R22	1.91502	0.00007	-0.00008	0.00012	0.00004	1.91506
R23	1.92524	0.00013	0.00010	0.00029	0.00039	1.92562

A1	1.87483	-0.00003	0.00015	-0.00008	0.00007	1.87490
A2	2.27730	0.00003	-0.00004	0.00001	-0.00003	2.27727
A3	2.13103	0.00000	-0.00011	0.00007	-0.00004	2.13100
A4	1.86151	-0.00004	-0.00005	-0.00005	-0.00010	1.86141
A5	2.27787	0.00000	0.00003	-0.00006	-0.00003	2.27784
A6	2.14380	0.00004	0.00002	0.00011	0.00013	2.14393
A7	1.89713	-0.00003	-0.00003	0.00011	0.00008	1.89721
A8	2.24718	-0.00004	0.00000	-0.00027	-0.00027	2.24691
A9	2.13887	0.00007	0.00003	0.00016	0.00020	2.13906
A10	1.88845	-0.00001	0.00010	-0.00025	-0.00015	1.88829
A11	2.24796	0.00041	-0.00084	0.00146	0.00062	2.24858
A12	2.14548	-0.00041	0.00081	-0.00118	-0.00036	2.14512
A13	1.90285	0.00009	-0.00016	0.00027	0.00010	1.90295
A14	2.22587	0.00010	-0.00036	-0.00014	-0.00051	2.22536
A15	2.15312	-0.00020	0.00060	-0.00039	0.00021	2.15334
A16	1.95676	-0.00024	0.00012	-0.00099	-0.00086	1.95589
A17	1.85922	0.00005	0.00035	-0.00039	-0.00005	1.85918
A18	1.88461	0.00007	-0.00043	0.00034	-0.00009	1.88452
A19	1.89486	0.00013	-0.00046	0.00144	0.00098	1.89584
A20	1.95350	0.00007	0.00012	-0.00019	-0.00007	1.95343
A21	1.91234	-0.00009	0.00032	-0.00022	0.00010	1.91243
A22	1.92454	-0.00023	0.00010	-0.00130	-0.00121	1.92334
A23	1.88736	-0.00002	0.00022	-0.00019	0.00003	1.88739
A24	1.87143	0.00024	-0.00030	0.00054	0.00024	1.87167
A25	1.88972	0.00019	0.00011	0.00113	0.00124	1.89097
A26	1.90695	0.00005	-0.00048	0.00092	0.00044	1.90738
A27	1.98372	-0.00024	0.00036	-0.00118	-0.00082	1.98290
A28	2.71498	-0.00044	-0.00486	0.00039	-0.00447	2.71050
A29	2.17776	0.00002	0.00007	0.00010	0.00018	2.17793
A30	1.95592	0.00003	0.00000	0.00020	0.00020	1.95612
A31	2.14951	-0.00005	-0.00007	-0.00031	-0.00038	2.14913
A32	2.07978	0.00001	0.00000	0.00007	0.00007	2.07985
A33	2.15752	-0.00002	0.00001	-0.00009	-0.00008	2.15744
A34	2.04589	0.00000	-0.00001	0.00002	0.00001	2.04589
A35	1.93805	-0.00004	-0.00022	0.00028	0.00005	1.93811
A36	1.90132	-0.00018	-0.00102	-0.00006	-0.00108	1.90024
A37	1.87749	0.00002	0.00013	-0.00034	-0.00021	1.87728
D1	0.00425	-0.00002	0.00002	-0.00011	-0.00009	0.00416
D2	-3.13697	-0.00001	-0.00006	0.00042	0.00036	-3.13661
D3	3.13867	0.00002	0.00007	0.00061	0.00068	3.13935
D4	-0.00255	0.00003	-0.00002	0.00115	0.00113	-0.00142
D5	-0.00479	0.00000	0.00025	-0.00093	-0.00069	-0.00548
D6	-3.09161	0.00009	-0.00125	0.00429	0.00304	-3.08857
D7	-3.13994	-0.00004	0.00020	-0.00158	-0.00138	-3.14132

D8	0.05642	0.00005	-0.00129	0.00364	0.00235	0.05877
D9	-0.00231	0.00003	-0.00028	0.00110	0.00082	-0.00148
D10	-3.14141	0.00000	-0.00007	-0.00026	-0.00034	3.14143
D11	3.13895	0.00002	-0.00020	0.00062	0.00042	3.13937
D12	-0.00016	-0.00001	0.00000	-0.00075	-0.00074	-0.00090
D13	-0.00065	-0.00003	0.00043	-0.00169	-0.00126	-0.00191
D14	3.08674	-0.00004	0.00211	-0.00120	0.00089	3.08763
D15	3.13864	0.00000	0.00024	-0.00043	-0.00018	3.13846
D16	-0.05716	-0.00001	0.00192	0.00007	0.00197	-0.05519
D17	0.05623	-0.00002	-0.00281	-0.00176	-0.00457	0.05166
D18	-3.08471	0.00001	-0.00275	-0.00103	-0.00378	-3.08849
D19	-3.08257	-0.00005	-0.00257	-0.00330	-0.00587	-3.08844
D20	0.05968	-0.00003	-0.00252	-0.00256	-0.00509	0.05459
D21	0.00333	0.00002	-0.00042	0.00163	0.00121	0.00454
D22	3.09293	-0.00005	0.00096	-0.00332	-0.00236	3.09057
D23	-3.08793	0.00000	-0.00188	0.00107	-0.00083	-3.08876
D24	0.00167	-0.00007	-0.00050	-0.00388	-0.00440	-0.00273
D25	-2.77149	-0.00005	-0.01088	-0.00631	-0.01719	-2.78869
D26	0.30874	-0.00004	-0.00904	-0.00571	-0.01474	0.29400
D27	1.60555	-0.00003	0.00172	0.00238	0.00411	1.60965
D28	-2.60724	0.00003	0.00145	0.00333	0.00479	-2.60245
D29	-0.55440	-0.00001	0.00179	0.00304	0.00483	-0.54956
D30	-1.47404	0.00006	0.00006	0.00827	0.00833	-1.46571
D31	0.59635	0.00012	-0.00020	0.00922	0.00902	0.60537
D32	2.64920	0.00008	0.00013	0.00893	0.00906	2.65826
D33	-1.32297	0.00000	-0.00383	-0.00092	-0.00475	-1.32772
D34	0.74016	0.00008	-0.00351	-0.00041	-0.00392	0.73625
D35	2.88576	-0.00008	-0.00312	-0.00162	-0.00474	2.88102
D36	2.91099	-0.00001	-0.00404	-0.00076	-0.00481	2.90619
D37	-1.30905	0.00008	-0.00372	-0.00025	-0.00397	-1.31303
D38	0.83654	-0.00008	-0.00334	-0.00146	-0.00480	0.83174
D39	0.79791	-0.00003	-0.00421	-0.00134	-0.00554	0.79236
D40	2.86104	0.00005	-0.00389	-0.00082	-0.00471	2.85633
D41	-1.27655	-0.00011	-0.00350	-0.00203	-0.00554	-1.28208
D42	2.88563	0.00003	0.00324	0.00032	0.00357	2.88919
D43	-1.33295	-0.00007	0.00263	0.00004	0.00267	-1.33028
D44	0.79985	0.00014	0.00357	0.00106	0.00463	0.80448
D45	2.86446	0.00003	0.00296	0.00078	0.00374	2.86820
D46	-1.31276	0.00003	0.00353	-0.00026	0.00327	-1.30949
D47	0.75184	-0.00008	0.00292	-0.00055	0.00238	0.75422
D48	-3.13643	0.00001	-0.00024	0.00010	-0.00013	-3.13657
D49	0.00581	0.00001	-0.00025	0.00017	-0.00008	0.00573
D50	0.00443	-0.00002	-0.00029	-0.00071	-0.00100	0.00343
D51	-3.13651	-0.00002	-0.00031	-0.00064	-0.00095	-3.13746

Item	Value	Threshold	Converged?
Maximum Force	0.000439	0.000450	YES
RMS Force	0.000108	0.000300	YES
Maximum Displacement	0.027741	0.001800	NO
RMS Displacement	0.006894	0.001200	NO

Predicted change in Energy=-6.014924D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.814105	-1.993202	0.277029
2	6	0	-2.821074	-1.110167	0.053373
3	7	0	-2.241847	0.154515	0.018081
4	6	0	-0.915056	0.027951	0.218793
5	7	0	-0.640355	-1.265985	0.380851
6	6	0	0.730836	-1.790319	0.561772
7	6	0	1.448329	-2.004486	-0.779391
8	1	0	-1.833515	-3.064953	0.375273
9	1	0	-3.875011	-1.272306	-0.079564
10	1	0	1.277207	-1.039209	1.132928
11	1	0	0.664940	-2.712204	1.139897
12	1	0	1.072950	-2.909039	-1.268696
13	1	0	1.227892	-1.144891	-1.426127
14	35	0	1.948159	1.598411	0.050775
15	1	0	-0.130881	0.814954	0.209816
16	6	0	-2.867809	1.414164	-0.186863
17	6	0	-4.173998	1.595696	-0.330982
18	1	0	-2.150939	2.225090	-0.214736
19	1	0	-4.552820	2.596127	-0.487400
20	1	0	-4.897793	0.791207	-0.300749
21	7	0	2.868257	-2.167953	-0.488719
22	1	0	3.362727	-2.543823	-1.289473
23	1	0	3.269429	-1.254661	-0.280605

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357852	0.000000			
3	N	2.205154	1.391464	0.000000		
4	C	2.212858	2.226114	1.347842	0.000000	
5	N	1.384670	2.210669	2.171221	1.332664	0.000000

6	C	2.568845	3.652005	3.593719	2.476428	1.479129
7	C	3.429231	4.440846	4.349097	3.273035	2.500829
8	H	1.076420	2.213613	3.264858	3.230187	2.158691
9	H	2.212281	1.074590	2.170847	3.246693	3.267265
10	H	3.346472	4.238678	3.879639	2.603937	2.072219
11	H	2.721611	3.987399	4.233905	3.294429	2.090811
12	H	3.400457	4.488567	4.693510	3.845867	2.890682
13	H	3.588052	4.310946	3.976591	2.945088	2.601957
14	Br	5.206294	5.484705	4.431935	3.269950	3.874806
15	H	3.274675	3.311753	2.220162	1.111029	2.149215
16	C	3.596614	2.536168	1.421460	2.428866	3.530872
17	C	4.338083	3.049561	2.435581	3.657975	4.602451
18	H	4.260197	3.412463	2.085605	2.557885	3.850220
19	H	5.398783	4.126499	3.399644	4.508610	5.565713
20	H	4.194746	2.837849	2.749742	4.088359	4.777279
21	N	4.747780	5.812165	5.635943	4.431255	3.725594
22	H	5.436608	6.488298	6.356255	5.214242	4.521894
23	H	5.167080	6.101365	5.696415	4.405043	3.965358

		6	7	8	9	10
6	C	0.000000				
7	C	1.536028	0.000000			
8	H	2.869733	3.637079	0.000000		
9	H	4.679046	5.418837	2.754663	0.000000	
10	H	1.090370	2.148954	3.788703	5.298096	0.000000
11	H	1.090158	2.190486	2.636542	4.916456	1.781526
12	H	2.172370	1.094781	3.342825	5.345582	3.050538
13	H	2.148344	1.098073	4.037808	5.279118	2.561711
14	Br	3.636823	3.730934	6.012763	6.493636	2.928868
15	H	2.766563	3.379597	4.240285	4.296383	2.504549
16	C	4.876414	5.537807	4.631226	2.871078	4.994201
17	C	6.026566	6.691259	5.262918	2.894484	6.229076
18	H	5.003109	5.582373	5.332301	3.901599	4.921792
19	H	6.946848	7.567344	6.339295	3.948484	7.059062
20	H	6.252174	6.951134	4.971597	2.313674	6.598218
21	N	2.411370	1.458563	4.863923	6.814782	2.536777
22	H	3.304804	2.053287	5.481231	7.447516	3.532886
23	H	2.727816	2.031607	5.454115	7.147290	2.452232

		11	12	13	14	15
11	H	0.000000				
12	H	2.450824	0.000000			
13	H	3.059063	1.777922	0.000000		
14	Br	4.627552	4.777457	3.197770	0.000000	
15	H	3.733526	4.183698	2.891983	2.227443	0.000000
16	C	5.591737	5.948952	4.985911	4.825346	2.829697

17	C	6.643553	6.978711	6.155532	6.134048	4.153170
18	H	5.843036	6.153338	4.923489	4.155217	2.499873
19	H	7.619153	7.909903	6.949321	6.599076	4.817908
20	H	6.730033	7.090734	6.522190	6.902333	4.794236
21	N	2.793422	2.093012	2.148531	3.914477	4.287249
22	H	3.634316	2.318813	2.556014	4.577704	5.072923
23	H	3.305393	2.921953	2.343532	3.161579	4.010725

		16	17	18	19	20
16	C	0.000000				
17	C	1.326594	0.000000			
18	H	1.082719	2.121890	0.000000		
19	H	2.080053	1.081127	2.445618	0.000000	
20	H	2.126471	1.082588	3.099778	1.847047	0.000000
21	N	6.769426	7.986444	6.675794	8.818664	8.312851
22	H	7.463310	8.651968	7.368725	9.471975	8.963046
23	H	6.693064	7.970675	6.441536	8.721176	8.419590

		21	22	23
21	N	0.000000		
22	H	1.013404	0.000000	
23	H	1.018996	1.639652	0.000000

Stoichiometry C7H12BrN3
Framework group C1[X(C7H12BrN3)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.730764	2.061413	-0.297313
2	6	0	-2.767678	1.221425	-0.046336
3	7	0	-2.237742	-0.064461	-0.003485
4	6	0	-0.910438	0.007441	-0.226579
5	7	0	-0.588113	1.287475	-0.409917
6	6	0	0.799392	1.755316	-0.619150
7	6	0	1.546261	1.957961	0.707690
8	1	0	-1.709925	3.131786	-0.409326
9	1	0	-3.812201	1.426429	0.100932
10	1	0	1.306745	0.976258	-1.188858
11	1	0	0.760188	2.671762	-1.208246
12	1	0	1.214412	2.882600	1.190872
13	1	0	1.302925	1.115843	1.369043

14	35	0	1.891659	-1.671885	-0.082747
15	1	0	-0.157525	-0.809539	-0.219526
16	6	0	-2.908986	-1.295923	0.227774
17	6	0	-4.218765	-1.424264	0.394689
18	1	0	-2.223947	-2.133930	0.255088
19	1	0	-4.633759	-2.407029	0.570157
20	1	0	-4.911013	-0.592446	0.365209
21	7	0	2.966606	2.061955	0.392712
22	1	0	3.488233	2.428143	1.180619
23	1	0	3.328424	1.131095	0.190374

Rotational constants (GHZ): 0.8897000 0.4599595 0.3138358

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 365 symmetry adapted cartesian basis functions of A symmetry.

There are 352 symmetry adapted basis functions of A symmetry.

352 basis functions, 562 primitive gaussians, 365 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 843.1065821910 Hartrees.

NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 352 RedAO= T EigKep= 4.31D-06 NBF= 352

NBsUse= 352 1.00D-06 EigRej= -1.00D+00 NBFU= 352

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999999 -0.000325 0.000112 -0.001272 Ang= -0.15 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3012.46805263 A.U. after 11 cycles

NFock= 11 Conv=0.36D-08 -V/T= 2.0017

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000029739	0.000019397	0.000038796
2	6	-0.000012355	0.000006387	-0.000056094
3	7	-0.000075731	0.000030927	0.000005009
4	6	0.000034846	-0.000023331	-0.000103504
5	7	-0.000002760	0.000051999	0.000110732
6	6	0.000107449	0.000217289	-0.000098323
7	6	0.000052576	0.000013236	-0.000164894
8	1	0.000024525	0.000005731	0.000013503
9	1	-0.000007054	-0.000001436	0.000026444
10	1	0.000002072	-0.000140815	0.000025523
11	1	-0.000028495	0.000009728	0.000010335
12	1	-0.000052630	-0.000140097	0.000084430
13	1	0.000161011	0.000053873	0.000122032
14	35	-0.000020849	-0.000025200	0.000028589
15	1	0.000030153	-0.000072299	0.000001315
16	6	0.000024117	-0.000081458	0.000015167
17	6	-0.000000382	0.000019369	-0.000020071
18	1	-0.000029715	0.000010927	0.000000644
19	1	-0.000002826	-0.000004029	0.000000456
20	1	-0.000000124	-0.000002754	0.000000444
21	7	-0.000095571	-0.000101067	0.000141304
22	1	-0.000013987	0.000030337	-0.000118336
23	1	-0.000064532	0.000123288	-0.000063497

Cartesian Forces: Max 0.000217289 RMS 0.000069183

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000195434 RMS 0.000054351

Search for a local minimum.

Step number 31 out of a maximum of 121

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 24 23 26 27 28
29 30 31
DE= -7.63D-06 DEPred=-6.01D-06 R= 1.27D+00
TightC=F SS= 1.41D+00 RLast= 3.65D-02 DXNew= 4.0000D-01 1.0964D-01
Trust test= 1.27D+00 RLast= 3.65D-02 DXMaxT set to 2.38D-01
ITU= 1 1 0 1 1 0 -1 -1 0 -1 -1 0 -1 0 0 0 1 1 -1 1
ITU= -1 1 1 1 1 1 1 0 1 0 0
Eigenvalues --- 0.00161 0.00221 0.00332 0.00695 0.00969
Eigenvalues --- 0.01366 0.01825 0.02014 0.02150 0.02311
Eigenvalues --- 0.02386 0.02770 0.03060 0.03069 0.03326
Eigenvalues --- 0.04047 0.04185 0.04485 0.05054 0.05289
Eigenvalues --- 0.05440 0.08903 0.09552 0.10091 0.12675
Eigenvalues --- 0.12917 0.15294 0.15846 0.15947 0.16000
Eigenvalues --- 0.16008 0.16030 0.16225 0.18975 0.21346
Eigenvalues --- 0.22046 0.23091 0.23739 0.24857 0.25089
Eigenvalues --- 0.27612 0.29889 0.34123 0.34628 0.34764
Eigenvalues --- 0.34889 0.35393 0.35690 0.35776 0.35859
Eigenvalues --- 0.36438 0.36660 0.38085 0.41441 0.42164
Eigenvalues --- 0.43079 0.46830 0.47696 0.48687 0.50027
Eigenvalues --- 0.54277 0.59957 0.60414
En-DIIS/RFO-DIIS IScMMF= 0 using points: 31 30 29 28 27
RFO step: Lambda=-1.02258603D-06.
DidBck=F Rises=F RFO-DIIS coefs: 1.51159 -0.21988 -0.36396 -0.04680
0.11905
Iteration 1 RMS(Cart)= 0.00622309 RMS(Int)= 0.00003138
Iteration 2 RMS(Cart)= 0.00004817 RMS(Int)= 0.00000135
Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00000135

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56597	0.00001	-0.00008	0.00009	0.00001	2.56598
R2	2.61665	0.00001	-0.00013	0.00000	-0.00012	2.61653
R3	2.03414	0.00000	0.00000	-0.00002	-0.00001	2.03412
R4	2.62949	-0.00001	-0.00001	-0.00004	-0.00005	2.62944
R5	2.03068	0.00000	0.00000	0.00000	0.00000	2.03068
R6	2.54705	0.00008	0.00010	0.00010	0.00020	2.54725
R7	2.68617	-0.00004	-0.00018	-0.00001	-0.00020	2.68597
R8	2.51837	-0.00011	0.00006	-0.00011	-0.00005	2.51832
R9	2.09954	-0.00006	-0.00066	0.00006	-0.00060	2.09894
R10	2.79515	0.00003	0.00015	0.00003	0.00018	2.79533
R11	2.90267	-0.00001	0.00044	-0.00007	0.00038	2.90305
R12	2.06050	-0.00009	-0.00048	0.00015	-0.00034	2.06016
R13	2.06010	0.00000	0.00005	-0.00004	0.00001	2.06011

R14	2.06884	0.00010	0.00007	0.00005	0.00013	2.06896
R15	2.07506	-0.00006	-0.00035	0.00009	-0.00025	2.07481
R16	2.75628	-0.00018	-0.00008	0.00011	0.00003	2.75632
R17	4.20926	-0.00003	0.00539	0.00016	0.00555	4.21481
R18	2.50690	0.00000	0.00000	0.00002	0.00002	2.50692
R19	2.04604	-0.00001	-0.00011	0.00004	-0.00007	2.04597
R20	2.04303	0.00000	-0.00002	0.00000	-0.00002	2.04302
R21	2.04579	0.00000	0.00000	0.00000	-0.00001	2.04579
R22	1.91506	0.00007	0.00013	0.00015	0.00028	1.91534
R23	1.92562	0.00007	0.00026	0.00025	0.00051	1.92613
A1	1.87490	0.00002	0.00016	0.00007	0.00023	1.87512
A2	2.27727	0.00001	-0.00003	0.00011	0.00007	2.27735
A3	2.13100	-0.00003	-0.00012	-0.00017	-0.00030	2.13070
A4	1.86141	-0.00002	-0.00013	0.00002	-0.00011	1.86130
A5	2.27784	0.00001	0.00000	0.00005	0.00006	2.27790
A6	2.14393	0.00001	0.00012	-0.00007	0.00005	2.14398
A7	1.89721	-0.00002	0.00009	-0.00014	-0.00004	1.89717
A8	2.24691	-0.00002	-0.00028	0.00000	-0.00028	2.24663
A9	2.13906	0.00004	0.00018	0.00014	0.00033	2.13939
A10	1.88829	0.00002	-0.00011	0.00019	0.00008	1.88837
A11	2.24858	0.00013	0.00038	0.00008	0.00046	2.24904
A12	2.14512	-0.00015	-0.00015	-0.00025	-0.00040	2.14472
A13	1.90295	0.00000	-0.00002	-0.00013	-0.00015	1.90280
A14	2.22536	0.00001	-0.00083	0.00003	-0.00080	2.22456
A15	2.15334	-0.00001	0.00071	0.00011	0.00082	2.15416
A16	1.95589	-0.00007	-0.00051	0.00016	-0.00035	1.95555
A17	1.85918	0.00007	0.00059	0.00050	0.00109	1.86027
A18	1.88452	-0.00002	-0.00056	-0.00042	-0.00098	1.88354
A19	1.89584	0.00003	0.00044	0.00019	0.00062	1.89646
A20	1.95343	0.00003	-0.00003	-0.00014	-0.00018	1.95325
A21	1.91243	-0.00004	0.00011	-0.00027	-0.00015	1.91228
A22	1.92334	-0.00010	-0.00069	-0.00008	-0.00076	1.92257
A23	1.88739	-0.00001	-0.00020	-0.00012	-0.00033	1.88706
A24	1.87167	0.00010	-0.00007	-0.00010	-0.00017	1.87150
A25	1.89097	0.00011	0.00194	0.00009	0.00204	1.89300
A26	1.90738	0.00003	0.00030	0.00022	0.00052	1.90791
A27	1.98290	-0.00014	-0.00134	-0.00002	-0.00137	1.98154
A28	2.71050	-0.00006	-0.00390	0.00112	-0.00279	2.70772
A29	2.17793	0.00002	0.00015	0.00004	0.00019	2.17812
A30	1.95612	0.00002	0.00020	0.00007	0.00027	1.95639
A31	2.14913	-0.00004	-0.00035	-0.00011	-0.00046	2.14867
A32	2.07985	0.00000	0.00007	-0.00003	0.00005	2.07990
A33	2.15744	0.00000	-0.00009	0.00004	-0.00005	2.15739
A34	2.04589	0.00000	0.00002	-0.00001	0.00000	2.04590

A35	1.93811	-0.00011	-0.00087	-0.00052	-0.00140	1.93671
A36	1.90024	-0.00020	-0.00201	-0.00027	-0.00228	1.89796
A37	1.87728	0.00006	-0.00047	-0.00021	-0.00068	1.87660
D1	0.00416	-0.00001	-0.00015	-0.00013	-0.00028	0.00388
D2	-3.13661	0.00000	0.00015	0.00090	0.00105	-3.13556
D3	3.13935	0.00000	0.00056	-0.00070	-0.00014	3.13921
D4	-0.00142	0.00002	0.00086	0.00033	0.00119	-0.00023
D5	-0.00548	0.00002	-0.00054	0.00072	0.00018	-0.00530
D6	-3.08857	0.00004	0.00187	0.00066	0.00253	-3.08604
D7	-3.14132	0.00000	-0.00118	0.00123	0.00005	-3.14127
D8	0.05877	0.00003	0.00123	0.00117	0.00241	0.06117
D9	-0.00148	0.00001	0.00078	-0.00050	0.00029	-0.00120
D10	3.14143	0.00001	0.00014	0.00047	0.00061	-3.14114
D11	3.13937	-0.00001	0.00051	-0.00143	-0.00091	3.13845
D12	-0.00090	-0.00001	-0.00013	-0.00046	-0.00059	-0.00149
D13	-0.00191	0.00000	-0.00113	0.00095	-0.00018	-0.00209
D14	3.08763	0.00002	0.00138	0.00142	0.00280	3.09043
D15	3.13846	0.00000	-0.00053	0.00005	-0.00048	3.13798
D16	-0.05519	0.00002	0.00198	0.00052	0.00250	-0.05269
D17	0.05166	-0.00002	-0.00340	-0.00112	-0.00452	0.04714
D18	-3.08849	-0.00001	-0.00294	-0.00160	-0.00454	-3.09303
D19	-3.08844	-0.00001	-0.00412	-0.00003	-0.00415	-3.09260
D20	0.05459	-0.00001	-0.00366	-0.00051	-0.00417	0.05042
D21	0.00454	-0.00001	0.00103	-0.00103	0.00000	0.00454
D22	3.09057	-0.00004	-0.00132	-0.00097	-0.00230	3.08827
D23	-3.08876	-0.00004	-0.00132	-0.00148	-0.00279	-3.09155
D24	-0.00273	-0.00006	-0.00367	-0.00142	-0.00509	-0.00783
D25	-2.78869	-0.00004	-0.01720	-0.00600	-0.02320	-2.81188
D26	0.29400	-0.00002	-0.01436	-0.00545	-0.01980	0.27419
D27	1.60965	-0.00003	0.00112	0.00263	0.00376	1.61341
D28	-2.60245	0.00001	0.00174	0.00326	0.00500	-2.59745
D29	-0.54956	-0.00001	0.00190	0.00300	0.00489	-0.54467
D30	-1.46571	0.00000	0.00389	0.00257	0.00646	-1.45925
D31	0.60537	0.00004	0.00450	0.00320	0.00771	0.61308
D32	2.65826	0.00002	0.00466	0.00294	0.00760	2.66586
D33	-1.32772	0.00003	-0.00487	0.00120	-0.00367	-1.33139
D34	0.73625	0.00010	-0.00303	0.00120	-0.00183	0.73441
D35	2.88102	-0.00002	-0.00481	0.00104	-0.00377	2.87725
D36	2.90619	-0.00004	-0.00557	0.00038	-0.00520	2.90099
D37	-1.31303	0.00003	-0.00374	0.00037	-0.00336	-1.31639
D38	0.83174	-0.00008	-0.00551	0.00022	-0.00530	0.82644
D39	0.79236	-0.00003	-0.00599	0.00068	-0.00531	0.78705
D40	2.85633	0.00004	-0.00415	0.00067	-0.00348	2.85285
D41	-1.28208	-0.00007	-0.00593	0.00051	-0.00541	-1.28750

D42	2.88919	0.00005	0.00294	0.00200	0.00495	2.89414
D43	-1.33028	-0.00006	0.00061	0.00127	0.00187	-1.32840
D44	0.80448	0.00009	0.00363	0.00203	0.00567	0.81015
D45	2.86820	-0.00002	0.00130	0.00130	0.00260	2.87079
D46	-1.30949	0.00003	0.00183	0.00177	0.00360	-1.30590
D47	0.75422	-0.00008	-0.00051	0.00103	0.00052	0.75475
D48	-3.13657	0.00000	-0.00019	-0.00023	-0.00041	-3.13698
D49	0.00573	0.00000	-0.00017	-0.00013	-0.00030	0.00542
D50	0.00343	0.00000	-0.00069	0.00030	-0.00039	0.00304
D51	-3.13746	0.00000	-0.00068	0.00039	-0.00028	-3.13775

Item	Value	Threshold	Converged?
Maximum Force	0.000195	0.000450	YES
RMS Force	0.000054	0.000300	YES
Maximum Displacement	0.031140	0.001800	NO
RMS Displacement	0.006221	0.001200	NO

Predicted change in Energy=-3.004798D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.814444	-1.992666	0.283447
2	6	0	-2.821202	-1.109838	0.058001
3	7	0	-2.241260	0.154354	0.018189
4	6	0	-0.914201	0.027515	0.217666
5	7	0	-0.640079	-1.266039	0.383509
6	6	0	0.730917	-1.792088	0.561669
7	6	0	1.446396	-2.003547	-0.781227
8	1	0	-1.834221	-3.064075	0.385205
9	1	0	-3.875504	-1.271707	-0.072328
10	1	0	1.279121	-1.044234	1.134995
11	1	0	0.663648	-2.715814	1.136705
12	1	0	1.071611	-2.908753	-1.269928
13	1	0	1.224094	-1.142992	-1.425818
14	35	0	1.956880	1.588957	0.067254
15	1	0	-0.129719	0.813757	0.207841
16	6	0	-2.867069	1.413524	-0.189437
17	6	0	-4.172933	1.594758	-0.336950
18	1	0	-2.150630	2.224814	-0.216327
19	1	0	-4.551578	2.595018	-0.494826
20	1	0	-4.896628	0.790134	-0.308040
21	7	0	2.867245	-2.163809	-0.493198

22	1	0	3.360854	-2.533633	-1.297480
23	1	0	3.264227	-1.248720	-0.283638

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357856	0.000000			
3	N	2.205046	1.391438	0.000000		
4	C	2.212667	2.226144	1.347949	0.000000	
5	N	1.384606	2.210803	2.171349	1.332640	0.000000
6	C	2.568366	3.651945	3.594141	2.477036	1.479223
7	C	3.430266	4.440204	4.346770	3.270385	2.500781
8	H	1.076412	2.213648	3.264762	3.229929	2.158452
9	H	2.212312	1.074588	2.170851	3.246750	3.267383
10	H	3.345864	4.239914	3.882906	2.607835	2.072983
11	H	2.718811	3.985842	4.234080	3.295465	2.090181
12	H	3.403161	4.489264	4.692227	3.844224	2.891755
13	H	3.588348	4.308971	3.972020	2.939971	2.600758
14	Br	5.205540	5.487590	4.436763	3.271670	3.872365
15	H	3.274145	3.311609	2.220222	1.110714	2.148692
16	C	3.596355	2.535880	1.421356	2.429084	3.530978
17	C	4.337854	3.049263	2.435621	3.658304	4.602638
18	H	4.260274	3.412452	2.085669	2.558365	3.850666
19	H	5.398560	4.126230	3.399646	4.508906	5.565883
20	H	4.194484	2.837477	2.749840	4.088726	4.777478
21	N	4.748755	5.811463	5.633136	4.427930	3.725041
22	H	5.438353	6.487090	6.351374	5.208766	4.521060
23	H	5.164101	6.096593	5.689473	4.397652	3.960933

		6	7	8	9	10
6	C	0.000000				
7	C	1.536227	0.000000			
8	H	2.868628	3.639744	0.000000		
9	H	4.678874	5.418555	2.754769	0.000000	
10	H	1.090191	2.149458	3.786139	5.299012	0.000000
11	H	1.090165	2.190543	2.631614	4.914377	1.781288
12	H	2.172041	1.094847	3.347754	5.346785	3.050106
13	H	2.148175	1.097940	4.040255	5.277726	2.563307
14	Br	3.630275	3.726472	6.010345	6.497659	2.921151
15	H	2.767005	3.376328	4.239619	4.296342	2.509298
16	C	4.877050	5.534670	4.630970	2.870735	4.998559
17	C	6.027105	6.687454	5.262681	2.893978	6.233442
18	H	5.004409	5.580031	5.332383	3.901485	4.927063
19	H	6.947492	7.563367	6.339071	3.948055	7.063818
20	H	6.252483	6.947123	4.971303	2.312887	6.602056

21	N	2.411393	1.458580	4.866812	6.814517	2.535073
22	H	3.304980	2.052477	5.486493	7.447035	3.531127
23	H	2.725335	2.030239	5.453168	7.142894	2.448464

		11	12	13	14	15
11	H	0.000000				
12	H	2.448579	0.000000			
13	H	3.058495	1.779176	0.000000		
14	Br	4.620305	4.775055	3.198403	0.000000	
15	H	3.734981	4.181396	2.886263	2.230379	0.000000
16	C	5.592499	5.946658	4.980163	4.833958	2.830307
17	C	6.644186	6.975479	6.148887	6.143128	4.153835
18	H	5.844713	6.151945	4.918714	4.166098	2.501017
19	H	7.620066	7.906487	6.942467	6.609699	4.818659
20	H	6.730203	7.087093	6.515339	6.910104	4.794801
21	N	2.795913	2.093454	2.147509	3.902066	4.282422
22	H	3.637769	2.319937	2.552665	4.563923	5.065087
23	H	3.306470	2.921651	2.340491	3.143992	4.001778

		16	17	18	19	20
16	C	0.000000				
17	C	1.326607	0.000000			
18	H	1.082682	2.121610	0.000000		
19	H	2.080087	1.081118	2.445233	0.000000	
20	H	2.126451	1.082585	3.099552	1.847039	0.000000
21	N	6.765496	7.982189	6.672012	8.813930	8.308898
22	H	7.456195	8.644315	7.361262	9.463292	8.956140
23	H	6.684999	7.962384	6.433557	8.712389	8.411723

		21	22	23
21	N	0.000000		
22	H	1.013553	0.000000	
23	H	1.019264	1.639578	0.000000

Stoichiometry C7H12BrN3
Framework group C1[X(C7H12BrN3)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.734682	2.056210	-0.307905
2	6	0	-2.771305	1.216493	-0.054805
3	7	0	-2.239837	-0.068393	-0.002766

4	6	0	-0.911846	0.004017	-0.222227
5	7	0	-0.590626	1.283317	-0.412327
6	6	0	0.796899	1.753223	-0.617421
7	6	0	1.538933	1.957505	0.712108
8	1	0	-1.714737	3.125893	-0.426413
9	1	0	-3.816659	1.420945	0.087230
10	1	0	1.307796	0.976030	-1.186167
11	1	0	0.757012	2.669909	-1.206109
12	1	0	1.206154	2.883915	1.191393
13	1	0	1.292904	1.116186	1.373262
14	35	0	1.898993	-1.664650	-0.085978
15	1	0	-0.158078	-0.811692	-0.210546
16	6	0	-2.910537	-1.299113	0.233334
17	6	0	-4.220176	-1.427488	0.401419
18	1	0	-2.225475	-2.136959	0.263398
19	1	0	-4.634680	-2.409833	0.580308
20	1	0	-4.912772	-0.596054	0.369540
21	7	0	2.960664	2.058325	0.402311
22	1	0	3.479462	2.421128	1.193836
23	1	0	3.319199	1.125474	0.201963

Rotational constants (GHZ): 0.8929855 0.4589105 0.3139285

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 365 symmetry adapted cartesian basis functions of A symmetry.

There are 352 symmetry adapted basis functions of A symmetry.

352 basis functions, 562 primitive gaussians, 365 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 843.2699748345 Hartrees.

NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 352 RedAO= T EigKep= 4.31D-06 NBF= 352

NBsUse= 352 1.00D-06 EigRej= -1.00D+00 NBFU= 352

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000054 0.000139 -0.000925 Ang= -0.11 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3012.46805644 A.U. after 11 cycles
NFock= 11 Conv=0.31D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000053991	-0.000025925	-0.000001241
2	6	0.000022449	0.000000974	0.000015853
3	7	-0.000027519	0.000002839	0.000039729
4	6	0.000031222	-0.000009828	-0.000100700
5	7	-0.000012748	0.000035450	0.000025675
6	6	-0.000006961	0.000009148	-0.000079319
7	6	0.000071187	0.000024017	0.000129862
8	1	0.000010212	-0.000000445	0.000008219
9	1	-0.000001706	-0.000001839	0.000014896
10	1	0.000002377	0.000020822	0.000025153
11	1	0.000003361	0.000000071	0.000018276
12	1	-0.000020929	-0.000004357	-0.000031408
13	1	-0.000004165	-0.000003783	-0.000039775
14	35	-0.000041941	0.000007236	0.000001654
15	1	0.000067519	-0.000041445	0.000002499
16	6	0.000003039	-0.000004298	0.000001537
17	6	-0.000000054	-0.000017294	-0.000002540
18	1	0.000005113	0.000006987	0.000003328
19	1	0.000000459	-0.000000666	-0.000005343
20	1	-0.000006259	0.000001767	-0.000001516
21	7	-0.000055442	-0.000000989	0.000009664
22	1	0.000014025	0.000008368	-0.000021732
23	1	0.000000753	-0.000006809	-0.000012772

Cartesian Forces: Max 0.000129862 RMS 0.000031044

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000084635 RMS 0.000017741
Search for a local minimum.
Step number 32 out of a maximum of 121
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 24 27 28 29 30
31 32
DE= -3.82D-06 DEPred=-3.00D-06 R= 1.27D+00
TightC=F SS= 1.41D+00 RLast= 4.01D-02 DXNew= 4.0000D-01 1.2018D-01
Trust test= 1.27D+00 RLast= 4.01D-02 DXMaxT set to 2.38D-01
ITU= 1 1 1 0 1 1 0 -1 -1 0 -1 -1 0 -1 0 0 0 1 1 -1
ITU= 1 -1 1 1 1 1 1 1 0 1 0 0
Eigenvalues --- 0.00146 0.00220 0.00329 0.00620 0.00965
Eigenvalues --- 0.01387 0.01822 0.02022 0.02159 0.02308
Eigenvalues --- 0.02388 0.02889 0.03061 0.03080 0.03345
Eigenvalues --- 0.04043 0.04168 0.04616 0.05007 0.05310
Eigenvalues --- 0.05508 0.08910 0.09543 0.10231 0.12603
Eigenvalues --- 0.12939 0.15470 0.15780 0.15932 0.16000
Eigenvalues --- 0.16010 0.16027 0.16253 0.18850 0.21804
Eigenvalues --- 0.22183 0.23081 0.23784 0.24921 0.25086
Eigenvalues --- 0.26862 0.29875 0.34173 0.34477 0.34782
Eigenvalues --- 0.35012 0.35424 0.35690 0.35810 0.35859
Eigenvalues --- 0.36438 0.36661 0.37915 0.41014 0.42166
Eigenvalues --- 0.43033 0.46769 0.47709 0.48659 0.49993
Eigenvalues --- 0.54224 0.59721 0.60401
En-DIIS/RFO-DIIS IScMMF= 0 using points: 32 31 30 29 28
RFO step: Lambda=-1.02199268D-07.
DidBck=F Rises=F RFO-DIIS coefs: 1.06287 -0.02858 -0.07779 0.03875
0.00474
Iteration 1 RMS(Cart)= 0.00148538 RMS(Int)= 0.00000191
Iteration 2 RMS(Cart)= 0.00000267 RMS(Int)= 0.00000013
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000013

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56598	-0.00001	0.00000	-0.00002	-0.00002	2.56595
R2	2.61653	0.00003	0.00001	0.00005	0.00005	2.61658
R3	2.03412	0.00000	0.00000	0.00000	0.00000	2.03413

R4	2.62944	0.00001	0.00001	0.00001	0.00003	2.62946
R5	2.03068	0.00000	0.00000	0.00000	0.00000	2.03068
R6	2.54725	0.00001	0.00000	-0.00002	-0.00001	2.54724
R7	2.68597	-0.00001	-0.00001	-0.00003	-0.00004	2.68593
R8	2.51832	-0.00006	0.00000	-0.00004	-0.00004	2.51829
R9	2.09894	-0.00001	0.00009	0.00000	0.00009	2.09904
R10	2.79533	-0.00001	-0.00002	-0.00001	-0.00003	2.79530
R11	2.90305	-0.00003	0.00006	-0.00011	-0.00006	2.90299
R12	2.06016	0.00003	-0.00001	0.00003	0.00001	2.06018
R13	2.06011	0.00001	0.00001	0.00001	0.00002	2.06013
R14	2.06896	0.00002	0.00001	0.00000	0.00001	2.06897
R15	2.07481	0.00002	-0.00003	0.00000	-0.00003	2.07477
R16	2.75632	-0.00004	0.00008	-0.00005	0.00003	2.75634
R17	4.21481	-0.00004	-0.00039	-0.00123	-0.00162	4.21319
R18	2.50692	0.00000	0.00000	0.00000	0.00001	2.50693
R19	2.04597	0.00001	0.00000	0.00000	0.00001	2.04598
R20	2.04302	0.00000	0.00000	0.00000	0.00000	2.04302
R21	2.04579	0.00000	0.00000	0.00000	0.00000	2.04579
R22	1.91534	0.00002	0.00004	0.00000	0.00004	1.91537
R23	1.92613	-0.00001	0.00004	-0.00005	-0.00001	1.92612
A1	1.87512	-0.00002	-0.00001	-0.00005	-0.00007	1.87506
A2	2.27735	0.00002	0.00002	0.00006	0.00008	2.27743
A3	2.13070	0.00000	0.00000	-0.00001	-0.00002	2.13068
A4	1.86130	0.00000	0.00000	0.00002	0.00002	1.86132
A5	2.27790	0.00000	0.00000	-0.00002	-0.00002	2.27788
A6	2.14398	0.00000	0.00000	-0.00001	0.00000	2.14398
A7	1.89717	0.00000	0.00001	0.00001	0.00002	1.89719
A8	2.24663	0.00001	-0.00001	0.00004	0.00002	2.24665
A9	2.13939	-0.00001	0.00000	-0.00005	-0.00004	2.13935
A10	1.88837	0.00000	-0.00002	-0.00003	-0.00004	1.88833
A11	2.24904	0.00001	0.00008	0.00011	0.00019	2.24922
A12	2.14472	-0.00001	-0.00007	-0.00003	-0.00010	2.14462
A13	1.90280	0.00002	0.00002	0.00005	0.00007	1.90287
A14	2.22456	0.00004	-0.00001	0.00006	0.00005	2.22461
A15	2.15416	-0.00006	-0.00003	-0.00011	-0.00014	2.15401
A16	1.95555	0.00003	-0.00005	0.00006	0.00001	1.95555
A17	1.86027	-0.00001	0.00001	0.00004	0.00005	1.86032
A18	1.88354	-0.00002	-0.00001	-0.00001	-0.00002	1.88352
A19	1.89646	-0.00001	0.00017	0.00004	0.00021	1.89667
A20	1.95325	0.00001	-0.00003	-0.00003	-0.00005	1.95320
A21	1.91228	0.00000	-0.00010	-0.00011	-0.00020	1.91208
A22	1.92257	0.00000	-0.00014	-0.00005	-0.00019	1.92239
A23	1.88706	0.00001	0.00001	0.00006	0.00007	1.88714
A24	1.87150	0.00001	0.00006	0.00010	0.00016	1.87167

A25	1.89300	-0.00002	0.00012	-0.00006	0.00005	1.89306
A26	1.90791	0.00000	0.00007	-0.00010	-0.00003	1.90787
A27	1.98154	-0.00001	-0.00013	0.00005	-0.00008	1.98146
A28	2.70772	0.00008	0.00061	0.00103	0.00165	2.70937
A29	2.17812	0.00000	0.00000	0.00004	0.00003	2.17816
A30	1.95639	0.00000	0.00001	-0.00002	0.00000	1.95639
A31	2.14867	0.00000	-0.00001	-0.00002	-0.00003	2.14864
A32	2.07990	-0.00001	0.00000	-0.00004	-0.00004	2.07986
A33	2.15739	0.00001	0.00000	0.00005	0.00005	2.15744
A34	2.04590	0.00000	0.00000	-0.00001	-0.00001	2.04589
A35	1.93671	0.00000	-0.00008	-0.00004	-0.00012	1.93659
A36	1.89796	0.00000	-0.00003	-0.00013	-0.00016	1.89780
A37	1.87660	-0.00001	-0.00011	-0.00019	-0.00031	1.87629
D1	0.00388	0.00001	0.00001	0.00001	0.00002	0.00390
D2	-3.13556	0.00001	0.00007	0.00046	0.00053	-3.13504
D3	3.13921	-0.00001	0.00002	-0.00034	-0.00032	3.13890
D4	-0.00023	0.00000	0.00009	0.00010	0.00019	-0.00004
D5	-0.00530	-0.00002	-0.00007	-0.00025	-0.00032	-0.00562
D6	-3.08604	-0.00002	0.00040	-0.00023	0.00017	-3.08587
D7	-3.14127	0.00000	-0.00008	0.00006	-0.00002	-3.14129
D8	0.06117	0.00000	0.00039	0.00008	0.00047	0.06164
D9	-0.00120	0.00000	0.00005	0.00023	0.00028	-0.00092
D10	-3.14114	0.00000	0.00000	0.00022	0.00021	-3.14093
D11	3.13845	0.00000	0.00000	-0.00017	-0.00018	3.13828
D12	-0.00149	0.00000	-0.00006	-0.00019	-0.00024	-0.00173
D13	-0.00209	-0.00001	-0.00010	-0.00039	-0.00048	-0.00257
D14	3.09043	0.00001	-0.00014	0.00079	0.00064	3.09108
D15	3.13798	-0.00001	-0.00005	-0.00038	-0.00042	3.13756
D16	-0.05269	0.00001	-0.00009	0.00080	0.00071	-0.05198
D17	0.04714	-0.00001	0.00016	-0.00075	-0.00059	0.04655
D18	-3.09303	-0.00001	0.00018	-0.00064	-0.00046	-3.09349
D19	-3.09260	-0.00001	0.00010	-0.00076	-0.00066	-3.09326
D20	0.05042	-0.00001	0.00012	-0.00065	-0.00053	0.04989
D21	0.00454	0.00002	0.00010	0.00039	0.00050	0.00504
D22	3.08827	0.00002	-0.00035	0.00039	0.00004	3.08831
D23	-3.09155	-0.00001	0.00014	-0.00070	-0.00056	-3.09211
D24	-0.00783	0.00000	-0.00031	-0.00071	-0.00101	-0.00884
D25	-2.81188	-0.00002	0.00096	-0.00461	-0.00366	-2.81554
D26	0.27419	0.00001	0.00090	-0.00328	-0.00238	0.27181
D27	1.61341	0.00002	0.00031	0.00213	0.00244	1.61585
D28	-2.59745	0.00002	0.00049	0.00224	0.00273	-2.59473
D29	-0.54467	0.00000	0.00038	0.00213	0.00251	-0.54216
D30	-1.45925	0.00002	0.00084	0.00214	0.00298	-1.45626
D31	0.61308	0.00002	0.00102	0.00225	0.00327	0.61635

D32	2.66586	0.00000	0.00091	0.00214	0.00306	2.66892
D33	-1.33139	0.00001	0.00017	0.00053	0.00070	-1.33069
D34	0.73441	-0.00001	0.00024	0.00047	0.00071	0.73512
D35	2.87725	0.00000	0.00012	0.00062	0.00075	2.87799
D36	2.90099	0.00001	0.00008	0.00043	0.00050	2.90149
D37	-1.31639	0.00000	0.00015	0.00036	0.00051	-1.31589
D38	0.82644	0.00000	0.00003	0.00051	0.00055	0.82699
D39	0.78705	0.00001	0.00010	0.00055	0.00065	0.78770
D40	2.85285	0.00000	0.00017	0.00048	0.00065	2.85350
D41	-1.28750	0.00001	0.00006	0.00064	0.00069	-1.28680
D42	2.89414	0.00001	0.00058	-0.00065	-0.00007	2.89407
D43	-1.32840	0.00000	0.00037	-0.00098	-0.00061	-1.32901
D44	0.81015	0.00000	0.00067	-0.00059	0.00007	0.81022
D45	2.87079	-0.00001	0.00046	-0.00093	-0.00046	2.87033
D46	-1.30590	0.00002	0.00055	-0.00047	0.00008	-1.30581
D47	0.75475	0.00001	0.00035	-0.00081	-0.00046	0.75429
D48	-3.13698	0.00000	0.00002	0.00013	0.00014	-3.13684
D49	0.00542	0.00000	0.00004	-0.00004	0.00000	0.00542
D50	0.00304	0.00000	-0.00001	0.00001	0.00000	0.00304
D51	-3.13775	0.00000	0.00001	-0.00015	-0.00014	-3.13789

Item	Value	Threshold	Converged?
Maximum Force	0.000085	0.000450	YES
RMS Force	0.000018	0.000300	YES
Maximum Displacement	0.005005	0.001800	NO
RMS Displacement	0.001487	0.001200	NO

Predicted change in Energy=-2.740036D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.814973	-1.992993	0.284871
2	6	0	-2.821511	-1.109996	0.059169
3	7	0	-2.241150	0.153975	0.017991
4	6	0	-0.913991	0.026842	0.216566
5	7	0	-0.640320	-1.266614	0.383754
6	6	0	0.730642	-1.792853	0.561500
7	6	0	1.446523	-2.002186	-0.781480
8	1	0	-1.835042	-3.064284	0.387819
9	1	0	-3.875989	-1.271572	-0.070094
10	1	0	1.278597	-1.046020	1.136406
11	1	0	0.663233	-2.717520	1.135024

12	1	0	1.071303	-2.906301	-1.271873
13	1	0	1.225004	-1.140343	-1.424591
14	35	0	1.955970	1.589935	0.067994
15	1	0	-0.129149	0.812787	0.206158
16	6	0	-2.866623	1.413198	-0.190163
17	6	0	-4.172456	1.594773	-0.337560
18	1	0	-2.149942	2.224256	-0.217707
19	1	0	-4.550758	2.595073	-0.496006
20	1	0	-4.896441	0.790429	-0.308138
21	7	0	2.867218	-2.163867	-0.493416
22	1	0	3.360693	-2.532521	-1.298342
23	1	0	3.264685	-1.249282	-0.282598

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357844	0.000000			
3	N	2.205067	1.391452	0.000000		
4	C	2.212728	2.226164	1.347941	0.000000	
5	N	1.384635	2.210764	2.171292	1.332620	0.000000
6	C	2.568411	3.651906	3.594035	2.476911	1.479209
7	C	3.431406	4.440586	4.345930	3.268803	2.500750
8	H	1.076413	2.213678	3.264795	3.229972	2.158470
9	H	2.212292	1.074589	2.170862	3.246766	3.267347
10	H	3.345451	4.239742	3.883228	2.608559	2.073015
11	H	2.718309	3.985603	4.234227	3.295864	2.090164
12	H	3.404141	4.489140	4.690562	3.841897	2.891250
13	H	3.590367	4.310076	3.971212	2.937860	2.601057
14	Br	5.206190	5.487625	4.436248	3.271393	3.873022
15	H	3.274232	3.311723	2.220357	1.110763	2.148661
16	C	3.596354	2.535885	1.421333	2.429029	3.530892
17	C	4.337881	3.049299	2.435623	3.658286	4.602587
18	H	4.260279	3.412463	2.085650	2.558280	3.850569
19	H	5.398577	4.126264	3.399624	4.508841	5.565799
20	H	4.194585	2.837581	2.749910	4.088800	4.777521
21	N	4.749510	5.811852	5.632881	4.427282	3.725227
22	H	5.439226	6.487377	6.350640	5.207515	4.521070
23	H	5.165080	6.097375	5.689789	4.397612	3.961489

		6	7	8	9	10
6	C	0.000000				
7	C	1.536197	0.000000			
8	H	2.868699	3.641975	0.000000		
9	H	4.678856	5.419317	2.754808	0.000000	
10	H	1.090198	2.149591	3.785303	5.298705	0.000000

11	H	1.090175	2.190487	2.630577	4.914022	1.781176
12	H	2.171882	1.094851	3.350578	5.347178	3.050151
13	H	2.148191	1.097923	4.043546	5.279396	2.563294
14	Br	3.631561	3.726187	6.011307	6.497618	2.923798
15	H	2.766743	3.373758	4.239663	4.296473	2.510433
16	C	4.876892	5.533329	4.630990	2.870754	4.999039
17	C	6.026997	6.686412	5.262746	2.894022	6.233806
18	H	5.004208	5.578101	5.332399	3.901518	4.927799
19	H	6.947330	7.561988	6.339131	3.948121	7.064255
20	H	6.252494	6.946649	4.971452	2.312971	6.602299
21	N	2.411526	1.458594	4.868118	6.815148	2.535669
22	H	3.305040	2.052425	5.488312	7.447695	3.531686
23	H	2.725683	2.030138	5.454439	7.143870	2.449374

		11	12	13	14	15
11	H	0.000000				
12	H	2.448532	0.000000			
13	H	3.058546	1.779200	0.000000		
14	Br	4.622109	4.774308	3.196332	0.000000	
15	H	3.735468	4.178190	2.882324	2.229523	0.000000
16	C	5.592748	5.944361	4.978534	4.832731	2.830429
17	C	6.644416	6.973494	6.147770	6.141833	4.153970
18	H	5.845082	6.149008	4.916031	4.164433	2.501102
19	H	7.620341	7.904091	6.940824	6.608019	4.818735
20	H	6.730408	7.085800	6.515093	6.909141	4.795005
21	N	2.795693	2.093446	2.147453	3.903406	4.281131
22	H	3.637552	2.319854	2.552501	4.564510	5.062963
23	H	3.306498	2.921524	2.340152	3.145918	4.001140

		16	17	18	19	20
16	C	0.000000				
17	C	1.326610	0.000000			
18	H	1.082684	2.121598	0.000000		
19	H	2.080067	1.081118	2.445173	0.000000	
20	H	2.126481	1.082584	3.099564	1.847033	0.000000
21	N	6.764931	7.981772	6.671097	8.813279	8.308826
22	H	7.454946	8.643263	7.359469	9.461872	8.955599
23	H	6.685079	7.962584	6.433340	8.712391	8.412197

		21	22	23
21	N	0.000000		
22	H	1.013572	0.000000	
23	H	1.019259	1.639407	0.000000

Stoichiometry C7H12BrN3

Framework group C1[X(C7H12BrN3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.735434	2.056315	-0.309057
2	6	0	-2.771638	1.216141	-0.055818
3	7	0	-2.239398	-0.068387	-0.002494
4	6	0	-0.911291	0.004682	-0.220987
5	7	0	-0.590862	1.283977	-0.412309
6	6	0	0.796532	1.754451	-0.616885
7	6	0	1.538769	1.956682	0.712811
8	1	0	-1.716069	3.125887	-0.428664
9	1	0	-3.817255	1.420012	0.085121
10	1	0	1.307425	0.978438	-1.187258
11	1	0	0.756358	2.672142	-1.204005
12	1	0	1.205277	2.881922	1.193864
13	1	0	1.293635	1.113910	1.372417
14	35	0	1.898759	-1.664913	-0.086522
15	1	0	-0.156936	-0.810544	-0.208757
16	6	0	-2.909454	-1.299355	0.234001
17	6	0	-4.219053	-1.428421	0.401899
18	1	0	-2.223920	-2.136796	0.264683
19	1	0	-4.632966	-2.410930	0.581258
20	1	0	-4.912167	-0.597438	0.369546
21	7	0	2.960389	2.059312	0.403037
22	1	0	3.478886	2.421031	1.195281
23	1	0	3.319659	1.127034	0.201363

Rotational constants (GHZ): 0.8926169 0.4590174 0.3139476
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 365 symmetry adapted cartesian basis functions of A symmetry.
There are 352 symmetry adapted basis functions of A symmetry.
352 basis functions, 562 primitive gaussians, 365 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 843.2611166219 Hartrees.
NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.

NBasis= 352 RedAO= T EigKep= 4.31D-06 NBF= 352
NBsUse= 352 1.00D-06 EigRej= -1.00D+00 NBFU= 352
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 -0.000073 -0.000015 -0.000055 Ang= -0.01 deg.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3012.46805686 A.U. after 9 cycles
NFock= 9 Conv=0.42D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000031692	-0.000005868	0.000024674
2	6	0.000005940	0.000010953	0.000040713
3	7	-0.000023669	-0.000007425	0.000010957
4	6	-0.000001782	-0.000024913	-0.000030042
5	7	0.000008466	-0.000005732	-0.000042819
6	6	0.000003092	0.000009575	-0.000039645
7	6	0.000061082	-0.000009045	0.000110396
8	1	0.000007922	0.000000641	0.000001913
9	1	-0.000000946	-0.000001305	0.000006608
10	1	0.000008644	0.000021572	0.000009087
11	1	-0.000000843	0.000003779	0.000009218
12	1	-0.000020139	-0.000001785	-0.000036721
13	1	-0.000007422	-0.000001325	-0.000033312
14	35	-0.000029187	0.000008861	0.000004640
15	1	0.000060517	-0.000014413	-0.000005650
16	6	-0.000005149	0.000007847	-0.000020439
17	6	0.000001278	-0.000015541	-0.000007208
18	1	0.000006154	0.000005769	0.000007643
19	1	-0.000001524	-0.000000238	0.000001052
20	1	-0.000004490	-0.000000154	0.000000359
21	7	-0.000045540	0.000026255	-0.000000197
22	1	0.000003996	-0.000002554	-0.000012673
23	1	0.000005292	-0.000004952	0.000001446

Cartesian Forces: Max 0.000110396 RMS 0.000023437

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000073583 RMS 0.000014520
Search for a local minimum.
Step number 33 out of a maximum of 121
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 24 27 28 29 30
31 32 33
DE= -4.22D-07 DEPred=-2.74D-07 R= 1.54D+00
Trust test= 1.54D+00 RLast= 9.12D-03 DXMaxT set to 2.38D-01
ITU= 0 1 1 1 0 1 1 0 -1 -1 0 -1 -1 0 -1 0 0 0 1 1
ITU= -1 1 -1 1 1 1 1 1 1 0 1 0 0
Eigenvalues --- 0.00081 0.00208 0.00336 0.00528 0.00988
Eigenvalues --- 0.01444 0.01811 0.01914 0.02147 0.02176
Eigenvalues --- 0.02348 0.02399 0.03059 0.03063 0.03892
Eigenvalues --- 0.04157 0.04205 0.04593 0.04998 0.05315
Eigenvalues --- 0.05551 0.08950 0.09280 0.09709 0.12651
Eigenvalues --- 0.12990 0.15436 0.15774 0.15957 0.15984
Eigenvalues --- 0.16000 0.16015 0.16307 0.18831 0.21487
Eigenvalues --- 0.22013 0.23240 0.23945 0.24824 0.25095
Eigenvalues --- 0.26997 0.30119 0.34062 0.34484 0.34818
Eigenvalues --- 0.35045 0.35309 0.35690 0.35807 0.35858
Eigenvalues --- 0.36441 0.36661 0.38030 0.40838 0.42279
Eigenvalues --- 0.43003 0.46850 0.47698 0.48660 0.50002
Eigenvalues --- 0.54208 0.59686 0.60391
En-DIIS/RFO-DIIS IScMMF= 0 using points: 33 32 31 30 29
RFO step: Lambda=-1.16293372D-07.
DidBck=F Rises=F RFO-DIIS coefs: 2.86393 -1.77644 -0.14392 0.07726 -0.02084
Iteration 1 RMS(Cart)= 0.00506534 RMS(Int)= 0.00002377
Iteration 2 RMS(Cart)= 0.00004299 RMS(Int)= 0.00000068
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000068

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56595	0.00000	-0.00004	0.00002	-0.00002	2.56593
R2	2.61658	0.00002	0.00009	0.00005	0.00014	2.61672
R3	2.03413	0.00000	0.00000	-0.00001	-0.00001	2.03412
R4	2.62946	0.00000	0.00003	0.00000	0.00003	2.62949
R5	2.03068	0.00000	0.00000	0.00001	0.00001	2.03069
R6	2.54724	0.00001	0.00000	0.00003	0.00003	2.54727

R7	2.68593	0.00001	-0.00009	0.00000	-0.00009	2.68584
R8	2.51829	-0.00003	-0.00008	-0.00006	-0.00014	2.51815
R9	2.09904	0.00002	0.00008	0.00025	0.00033	2.09937
R10	2.79530	-0.00001	-0.00002	-0.00002	-0.00004	2.79526
R11	2.90299	-0.00003	-0.00014	-0.00016	-0.00030	2.90270
R12	2.06018	0.00002	0.00001	0.00006	0.00007	2.06024
R13	2.06013	0.00000	0.00004	0.00000	0.00003	2.06016
R14	2.06897	0.00002	0.00003	0.00009	0.00013	2.06909
R15	2.07477	0.00002	-0.00006	0.00003	-0.00003	2.07474
R16	2.75634	-0.00004	-0.00001	-0.00005	-0.00006	2.75629
R17	4.21319	-0.00002	-0.00250	-0.00125	-0.00375	4.20944
R18	2.50693	0.00000	0.00001	0.00000	0.00001	2.50694
R19	2.04598	0.00001	0.00000	0.00002	0.00002	2.04600
R20	2.04302	0.00000	0.00000	0.00001	0.00001	2.04303
R21	2.04579	0.00000	0.00000	0.00000	-0.00001	2.04578
R22	1.91537	0.00001	0.00008	0.00005	0.00014	1.91551
R23	1.92612	0.00000	0.00001	0.00006	0.00007	1.92619
A1	1.87506	-0.00001	-0.00009	-0.00002	-0.00011	1.87494
A2	2.27743	0.00001	0.00015	0.00006	0.00022	2.27764
A3	2.13068	0.00000	-0.00006	-0.00005	-0.00011	2.13057
A4	1.86132	0.00000	0.00003	0.00001	0.00004	1.86136
A5	2.27788	0.00000	-0.00003	-0.00001	-0.00003	2.27785
A6	2.14398	0.00000	-0.00001	0.00000	-0.00001	2.14397
A7	1.89719	0.00000	0.00002	-0.00001	0.00001	1.89719
A8	2.24665	0.00001	0.00002	0.00007	0.00009	2.24674
A9	2.13935	-0.00001	-0.00005	-0.00005	-0.00010	2.13925
A10	1.88833	0.00001	-0.00006	0.00002	-0.00004	1.88829
A11	2.24922	0.00000	0.00035	0.00022	0.00057	2.24980
A12	2.14462	-0.00001	-0.00019	-0.00018	-0.00037	2.14425
A13	1.90287	0.00000	0.00009	0.00000	0.00010	1.90297
A14	2.22461	0.00004	0.00002	0.00028	0.00030	2.22492
A15	2.15401	-0.00004	-0.00016	-0.00021	-0.00037	2.15364
A16	1.95555	0.00003	0.00004	0.00018	0.00022	1.95577
A17	1.86032	-0.00001	0.00021	-0.00014	0.00008	1.86040
A18	1.88352	-0.00002	-0.00014	-0.00001	-0.00015	1.88337
A19	1.89667	-0.00001	0.00034	-0.00009	0.00025	1.89692
A20	1.95320	0.00000	-0.00010	0.00005	-0.00004	1.95316
A21	1.91208	0.00000	-0.00035	-0.00001	-0.00036	1.91172
A22	1.92239	0.00001	-0.00032	0.00021	-0.00010	1.92228
A23	1.88714	0.00001	0.00009	-0.00005	0.00004	1.88717
A24	1.87167	-0.00001	0.00024	-0.00008	0.00016	1.87183
A25	1.89306	-0.00002	0.00024	-0.00024	0.00000	1.89306
A26	1.90787	0.00001	-0.00005	0.00039	0.00035	1.90822
A27	1.98146	0.00000	-0.00022	-0.00022	-0.00044	1.98101

A28	2.70937	0.00007	0.00259	0.00155	0.00414	2.71351
A29	2.17816	0.00000	0.00008	0.00003	0.00011	2.17827
A30	1.95639	0.00000	0.00002	-0.00002	-0.00001	1.95638
A31	2.14864	0.00000	-0.00010	-0.00001	-0.00011	2.14854
A32	2.07986	-0.00001	-0.00007	-0.00004	-0.00011	2.07975
A33	2.15744	0.00001	0.00009	0.00005	0.00015	2.15759
A34	2.04589	0.00000	-0.00002	-0.00001	-0.00003	2.04585
A35	1.93659	-0.00001	-0.00035	0.00007	-0.00029	1.93631
A36	1.89780	0.00001	-0.00052	0.00030	-0.00022	1.89758
A37	1.87629	0.00000	-0.00059	0.00000	-0.00059	1.87570
D1	0.00390	0.00001	0.00001	0.00008	0.00008	0.00399
D2	-3.13504	0.00000	0.00106	0.00014	0.00120	-3.13383
D3	3.13890	0.00000	-0.00064	-0.00003	-0.00068	3.13822
D4	-0.00004	0.00000	0.00041	0.00003	0.00044	0.00040
D5	-0.00562	0.00000	-0.00052	0.00024	-0.00029	-0.00591
D6	-3.08587	-0.00001	0.00029	-0.00119	-0.00090	-3.08677
D7	-3.14129	0.00000	0.00006	0.00033	0.00039	-3.14089
D8	0.06164	-0.00001	0.00087	-0.00109	-0.00022	0.06142
D9	-0.00092	-0.00001	0.00050	-0.00036	0.00014	-0.00077
D10	-3.14093	0.00000	0.00050	-0.00003	0.00047	-3.14046
D11	3.13828	0.00000	-0.00045	-0.00042	-0.00087	3.13741
D12	-0.00173	0.00000	-0.00046	-0.00009	-0.00055	-0.00228
D13	-0.00257	0.00000	-0.00083	0.00051	-0.00032	-0.00289
D14	3.09108	0.00002	0.00158	0.00214	0.00372	3.09480
D15	3.13756	0.00000	-0.00083	0.00020	-0.00062	3.13693
D16	-0.05198	0.00002	0.00158	0.00184	0.00342	-0.04856
D17	0.04655	-0.00001	-0.00153	-0.00194	-0.00347	0.04308
D18	-3.09349	-0.00001	-0.00133	-0.00232	-0.00365	-3.09714
D19	-3.09326	-0.00001	-0.00154	-0.00157	-0.00311	-3.09637
D20	0.04989	-0.00001	-0.00134	-0.00195	-0.00329	0.04660
D21	0.00504	0.00000	0.00084	-0.00046	0.00038	0.00542
D22	3.08831	0.00001	0.00007	0.00092	0.00099	3.08929
D23	-3.09211	-0.00001	-0.00141	-0.00199	-0.00340	-3.09551
D24	-0.00884	0.00000	-0.00218	-0.00061	-0.00279	-0.01163
D25	-2.81554	-0.00002	-0.00971	-0.01123	-0.02094	-2.83648
D26	0.27181	0.00000	-0.00698	-0.00937	-0.01635	0.25546
D27	1.61585	0.00002	0.00456	0.00466	0.00922	1.62507
D28	-2.59473	0.00002	0.00512	0.00457	0.00969	-2.58503
D29	-0.54216	0.00001	0.00476	0.00448	0.00924	-0.53292
D30	-1.45626	0.00001	0.00548	0.00303	0.00851	-1.44776
D31	0.61635	0.00000	0.00604	0.00294	0.00898	0.62533
D32	2.66892	-0.00001	0.00567	0.00285	0.00852	2.67744
D33	-1.33069	0.00001	0.00094	0.00034	0.00129	-1.32940
D34	0.73512	0.00000	0.00110	0.00015	0.00125	0.73637

D35	2.87799	0.00000	0.00103	-0.00020	0.00083	2.87883
D36	2.90149	0.00001	0.00044	0.00046	0.00090	2.90240
D37	-1.31589	0.00000	0.00060	0.00027	0.00087	-1.31502
D38	0.82699	0.00000	0.00053	-0.00008	0.00045	0.82744
D39	0.78770	0.00001	0.00072	0.00050	0.00122	0.78891
D40	2.85350	0.00000	0.00088	0.00031	0.00118	2.85469
D41	-1.28680	0.00000	0.00081	-0.00004	0.00076	-1.28604
D42	2.89407	0.00000	0.00011	0.00087	0.00098	2.89505
D43	-1.32901	0.00001	-0.00114	0.00110	-0.00004	-1.32906
D44	0.81022	-0.00001	0.00037	0.00045	0.00082	0.81105
D45	2.87033	-0.00001	-0.00088	0.00067	-0.00020	2.87013
D46	-1.30581	0.00001	0.00025	0.00062	0.00087	-1.30495
D47	0.75429	0.00001	-0.00100	0.00084	-0.00016	0.75413
D48	-3.13684	-0.00001	0.00021	-0.00056	-0.00035	-3.13718
D49	0.00542	0.00000	-0.00004	-0.00032	-0.00036	0.00506
D50	0.00304	0.00000	0.00000	-0.00014	-0.00015	0.00289
D51	-3.13789	0.00000	-0.00026	0.00010	-0.00016	-3.13805

Item	Value	Threshold	Converged?
Maximum Force	0.000074	0.000450	YES
RMS Force	0.000015	0.000300	YES
Maximum Displacement	0.018885	0.001800	NO
RMS Displacement	0.005081	0.001200	NO

Predicted change in Energy=-7.845839D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.816919	-1.993769	0.290357
2	6	0	-2.822920	-1.110207	0.064538
3	7	0	-2.241015	0.152854	0.017147
4	6	0	-0.913397	0.024657	0.212026
5	7	0	-0.641022	-1.268469	0.383254
6	6	0	0.729837	-1.795308	0.559848
7	6	0	1.447007	-1.998930	-0.783143
8	1	0	-1.837975	-3.064604	0.397730
9	1	0	-3.878119	-1.270740	-0.060100
10	1	0	1.277198	-1.051118	1.138802
11	1	0	0.661909	-2.722424	1.129374
12	1	0	1.071346	-2.900376	-1.278235
13	1	0	1.227121	-1.133840	-1.422415
14	35	0	1.955143	1.590520	0.076540

15	1	0	-0.127414	0.809680	0.199709
16	6	0	-2.865389	1.412228	-0.193071
17	6	0	-4.171087	1.594878	-0.340381
18	1	0	-2.147981	2.222606	-0.222136
19	1	0	-4.548334	2.595366	-0.500176
20	1	0	-4.895970	0.791397	-0.309633
21	7	0	2.867294	-2.162844	-0.494479
22	1	0	3.361247	-2.527280	-1.301123
23	1	0	3.264965	-1.249359	-0.279148

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357834	0.000000			
3	N	2.205106	1.391468	0.000000		
4	C	2.212811	2.226196	1.347955	0.000000	
5	N	1.384711	2.210725	2.171214	1.332547	0.000000
6	C	2.568653	3.651955	3.593858	2.476584	1.479188
7	C	3.435934	4.443047	4.344208	3.264471	2.500784
8	H	1.076410	2.213775	3.264861	3.229994	2.158473
9	H	2.212269	1.074593	2.170874	3.246795	3.267318
10	H	3.343951	4.238927	3.884003	2.610538	2.073080
11	H	2.716519	3.984614	4.234529	3.296903	2.090050
12	H	3.409470	4.491442	4.687426	3.836131	2.890652
13	H	3.597116	4.314443	3.969368	2.931779	2.601639
14	Br	5.207811	5.488530	4.436007	3.270903	3.874012
15	H	3.274442	3.312098	2.220824	1.110938	2.148531
16	C	3.596361	2.535912	1.421288	2.428936	3.530736
17	C	4.338010	3.049426	2.435660	3.658319	4.602583
18	H	4.260290	3.412531	2.085614	2.558061	3.850329
19	H	5.398679	4.126407	3.399590	4.508719	5.565677
20	H	4.194960	2.837893	2.750147	4.089120	4.777837
21	N	4.752515	5.813697	5.631966	4.424696	3.725399
22	H	5.443422	6.489765	6.348724	5.203324	4.521049
23	H	5.167594	6.099166	5.689447	4.395802	3.961802

		6	7	8	9	10
6	C	0.000000				
7	C	1.536040	0.000000			
8	H	2.868981	3.649826	0.000000		
9	H	4.678970	5.423100	2.754949	0.000000	
10	H	1.090234	2.149663	3.782541	5.297442	0.000000
11	H	1.090192	2.190330	2.627129	4.912645	1.780992
12	H	2.171717	1.094918	3.361544	5.351333	3.050279
13	H	2.148069	1.097907	4.054083	5.285651	2.563042

14	Br	3.633014	3.725776	6.013409	6.498648	2.926818
15	H	2.765961	3.366465	4.239730	4.296910	2.513443
16	C	4.876558	5.530004	4.631053	2.870823	5.000299
17	C	6.026842	6.683897	5.262983	2.894159	6.234829
18	H	5.003695	5.573153	5.332441	3.901679	4.929632
19	H	6.946996	7.558554	6.339365	3.948371	7.065403
20	H	6.252738	6.945754	4.971965	2.313157	6.603092
21	N	2.411516	1.458564	4.873270	6.818000	2.536128
22	H	3.305044	2.052260	5.496065	7.451674	3.532074
23	H	2.725592	2.029985	5.458322	7.146473	2.449714

		11	12	13	14	15
11	H	0.000000				
12	H	2.448651	0.000000			
13	H	3.058544	1.779243	0.000000		
14	Br	4.624111	4.773328	3.193590	0.000000	
15	H	3.736718	4.169636	2.871118	2.227538	0.000000
16	C	5.593392	5.939193	4.974172	4.831357	2.830874
17	C	6.645083	6.969217	6.144701	6.140402	4.154459
18	H	5.845971	6.142016	4.908942	4.162255	2.501401
19	H	7.621086	7.898694	6.936381	6.605871	4.819030
20	H	6.731099	7.083518	6.514373	6.908363	4.795716
21	N	2.795309	2.093719	2.147111	3.904590	4.276221
22	H	3.637558	2.320210	2.551643	4.564138	5.055547
23	H	3.306019	2.921644	2.339490	3.147548	3.997146

		16	17	18	19	20
16	C	0.000000				
17	C	1.326616	0.000000			
18	H	1.082696	2.121552	0.000000		
19	H	2.080008	1.081123	2.444985	0.000000	
20	H	2.126565	1.082582	3.099590	1.847015	0.000000
21	N	6.762813	7.980165	6.667782	8.810910	8.308428
22	H	7.451074	8.640097	7.353722	9.457510	8.954234
23	H	6.683763	7.961677	6.431001	8.710821	8.412281

		21	22	23
21	N	0.000000		
22	H	1.013646	0.000000	
23	H	1.019297	1.639142	0.000000

Stoichiometry C7H12BrN3
Framework group C1[X(C7H12BrN3)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.738274	2.055452	-0.315962
2	6	0	-2.773589	1.214238	-0.062594
3	7	0	-2.238825	-0.068899	-0.001201
4	6	0	-0.910029	0.005980	-0.214923
5	7	0	-0.591699	1.284944	-0.411393
6	6	0	0.795476	1.756799	-0.614113
7	6	0	1.537461	1.955273	0.716107
8	1	0	-1.720625	3.124413	-0.441139
9	1	0	-3.820295	1.416430	0.072593
10	1	0	1.306879	0.983117	-1.187258
11	1	0	0.754798	2.676344	-1.198322
12	1	0	1.202405	2.878235	1.200589
13	1	0	1.293797	1.109688	1.372624
14	35	0	1.899389	-1.664395	-0.089135
15	1	0	-0.153906	-0.807786	-0.199243
16	6	0	-2.907097	-1.300240	0.238112
17	6	0	-4.216659	-1.431132	0.404919
18	1	0	-2.220223	-2.136481	0.271828
19	1	0	-4.628968	-2.413942	0.586335
20	1	0	-4.911281	-0.601528	0.369731
21	7	0	2.958951	2.060810	0.406851
22	1	0	3.476828	2.419569	1.200937
23	1	0	3.319247	1.129581	0.201994

Rotational constants (GHZ): 0.8922497 0.4590431 0.3139910

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 365 symmetry adapted cartesian basis functions of A symmetry.

There are 352 symmetry adapted basis functions of A symmetry.

352 basis functions, 562 primitive gaussians, 365 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 843.2536351564 Hartrees.

NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 352 RedAO= T EigKep= 4.31D-06 NBF= 352

NBsUse= 352 1.00D-06 EigRej= -1.00D+00 NBFU= 352

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000157 -0.000017 -0.000279 Ang= -0.04 deg.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3012.46805807 A.U. after 10 cycles

NFock= 10 Conv=0.92D-08 -V/T= 2.0017

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000032686	0.000031520	0.000059166
2	6	-0.000018952	0.000020315	0.000060111
3	7	0.000005226	-0.000024121	0.000007395
4	6	-0.000053196	-0.000012036	0.000033347
5	7	0.000006696	-0.000093882	-0.000122769
6	6	-0.000005385	-0.000013255	0.000091842
7	6	0.000030951	-0.000008508	0.000028282
8	1	-0.000002698	-0.000001198	-0.000014137
9	1	0.000003543	-0.000003293	-0.000014504
10	1	0.000016094	0.000024135	-0.000017991
11	1	-0.000007300	0.000008830	-0.000010979
12	1	0.000018947	0.000023271	-0.000015911
13	1	-0.000035730	-0.000002716	-0.000035835
14	35	0.000010014	0.000023629	0.000005417
15	1	0.000017061	0.000021524	-0.000028676
16	6	-0.000019949	0.000037379	-0.000026564
17	6	0.000001036	-0.000006805	-0.000007557
18	1	0.000006518	-0.000003183	0.000006586
19	1	-0.000004695	-0.000003225	0.000001250
20	1	0.000001037	-0.000006697	0.000001086
21	7	0.000030394	0.000025731	-0.000048402
22	1	-0.000021676	-0.000016921	0.000032450
23	1	-0.000010621	-0.000020496	0.000016393

Cartesian Forces: Max 0.000122769 RMS 0.000030990

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000072720 RMS 0.000017099
Search for a local minimum.
Step number 34 out of a maximum of 121
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 24 27 28 29 30
31 32 33 34
DE= -1.21D-06 DEPred=-7.85D-07 R= 1.54D+00
TightC=F SS= 1.41D+00 RLast= 3.66D-02 DXNew= 4.0000D-01 1.0974D-01
Trust test= 1.54D+00 RLast= 3.66D-02 DXMaxT set to 2.38D-01
ITU= 1 0 1 1 1 0 1 1 0 -1 -1 0 -1 -1 0 -1 0 0 0 1
ITU= 1 -1 1 -1 1 1 1 1 1 1 0 1 0 0
Eigenvalues --- 0.00044 0.00205 0.00350 0.00550 0.00986
Eigenvalues --- 0.01394 0.01822 0.01861 0.02126 0.02259
Eigenvalues --- 0.02365 0.02433 0.03059 0.03064 0.03827
Eigenvalues --- 0.04096 0.04328 0.04595 0.05089 0.05335
Eigenvalues --- 0.05524 0.08925 0.09218 0.09699 0.12742
Eigenvalues --- 0.13004 0.15400 0.15762 0.15964 0.16000
Eigenvalues --- 0.16010 0.16033 0.16355 0.18901 0.20998
Eigenvalues --- 0.22050 0.23256 0.23943 0.24879 0.25345
Eigenvalues --- 0.27295 0.29910 0.34010 0.34608 0.34839
Eigenvalues --- 0.35039 0.35339 0.35690 0.35811 0.35859
Eigenvalues --- 0.36441 0.36663 0.38358 0.41240 0.42319
Eigenvalues --- 0.42985 0.47047 0.47723 0.48829 0.50010
Eigenvalues --- 0.54224 0.60361 0.61077
En-DIIS/RFO-DIIS IScMMF= 0 using points: 34 33 32 31 30
RFO step: Lambda=-9.07463692D-08.
DidBck=F Rises=F RFO-DIIS coefs: 1.68674 -1.26517 0.56508 0.02036 -0.00700
Iteration 1 RMS(Cart)= 0.00452243 RMS(Int)= 0.00002209
Iteration 2 RMS(Cart)= 0.00004762 RMS(Int)= 0.00000063
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000063

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56593	0.00002	0.00000	0.00002	0.00002	2.56595
R2	2.61672	-0.00002	0.00007	-0.00004	0.00003	2.61675
R3	2.03412	0.00000	0.00000	0.00000	-0.00001	2.03411
R4	2.62949	-0.00002	0.00001	-0.00004	-0.00003	2.62946
R5	2.03069	0.00000	0.00000	0.00000	0.00000	2.03069
R6	2.54727	-0.00001	0.00002	0.00000	0.00002	2.54729
R7	2.68584	0.00003	-0.00003	0.00003	0.00000	2.68584
R8	2.51815	0.00005	-0.00007	0.00002	-0.00005	2.51810

R9	2.09937	0.00005	0.00018	0.00004	0.00022	2.09959
R10	2.79526	0.00001	-0.00001	0.00002	0.00001	2.79527
R11	2.90270	0.00002	-0.00017	0.00008	-0.00009	2.90261
R12	2.06024	0.00001	0.00004	0.00004	0.00008	2.06033
R13	2.06016	-0.00001	0.00001	-0.00004	-0.00003	2.06013
R14	2.06909	-0.00002	0.00008	-0.00011	-0.00004	2.06906
R15	2.07474	0.00003	0.00000	0.00007	0.00007	2.07481
R16	2.75629	0.00000	-0.00005	0.00005	0.00000	2.75629
R17	4.20944	0.00002	-0.00166	0.00019	-0.00146	4.20797
R18	2.50694	0.00000	0.00000	-0.00001	0.00000	2.50694
R19	2.04600	0.00000	0.00001	-0.00002	-0.00001	2.04599
R20	2.04303	0.00000	0.00001	0.00000	0.00000	2.04303
R21	2.04578	0.00000	0.00000	0.00000	-0.00001	2.04578
R22	1.91551	-0.00003	0.00007	-0.00010	-0.00003	1.91548
R23	1.92619	-0.00002	0.00005	-0.00007	-0.00002	1.92617
A1	1.87494	0.00002	-0.00004	0.00004	0.00000	1.87494
A2	2.27764	-0.00002	0.00010	-0.00002	0.00009	2.27773
A3	2.13057	0.00000	-0.00006	-0.00002	-0.00008	2.13049
A4	1.86136	0.00000	0.00002	-0.00001	0.00001	1.86137
A5	2.27785	0.00000	-0.00001	-0.00001	-0.00002	2.27782
A6	2.14397	0.00000	-0.00001	0.00002	0.00002	2.14398
A7	1.89719	0.00000	0.00000	-0.00002	-0.00002	1.89718
A8	2.24674	0.00001	0.00005	0.00003	0.00008	2.24682
A9	2.13925	0.00000	-0.00005	-0.00002	-0.00006	2.13918
A10	1.88829	0.00001	0.00000	0.00004	0.00003	1.88832
A11	2.24980	-0.00004	0.00028	-0.00011	0.00016	2.24996
A12	2.14425	0.00003	-0.00020	0.00015	-0.00005	2.14420
A13	1.90297	-0.00002	0.00003	-0.00005	-0.00002	1.90295
A14	2.22492	0.00002	0.00019	0.00007	0.00025	2.22517
A15	2.15364	0.00001	-0.00018	0.00006	-0.00012	2.15352
A16	1.95577	0.00002	0.00014	-0.00001	0.00013	1.95590
A17	1.86040	0.00000	0.00001	0.00013	0.00013	1.86053
A18	1.88337	-0.00001	-0.00008	-0.00011	-0.00019	1.88318
A19	1.89692	-0.00002	0.00005	-0.00007	-0.00002	1.89690
A20	1.95316	0.00000	0.00000	-0.00006	-0.00006	1.95310
A21	1.91172	0.00002	-0.00013	0.00014	0.00001	1.91173
A22	1.92228	0.00003	0.00004	0.00002	0.00006	1.92234
A23	1.88717	0.00001	-0.00001	0.00013	0.00012	1.88729
A24	1.87183	-0.00003	0.00002	0.00001	0.00003	1.87186
A25	1.89306	-0.00002	-0.00005	-0.00014	-0.00019	1.89288
A26	1.90822	-0.00001	0.00025	-0.00040	-0.00015	1.90808
A27	1.98101	0.00003	-0.00025	0.00037	0.00013	1.98114
A28	2.71351	0.00007	0.00190	0.00081	0.00270	2.71621
A29	2.17827	-0.00001	0.00006	0.00000	0.00006	2.17833

A30	1.95638	0.00000	-0.00001	-0.00002	-0.00003	1.95635
A31	2.14854	0.00002	-0.00005	0.00002	-0.00003	2.14851
A32	2.07975	0.00000	-0.00005	0.00002	-0.00003	2.07971
A33	2.15759	-0.00001	0.00007	-0.00002	0.00005	2.15763
A34	2.04585	0.00000	-0.00002	0.00000	-0.00001	2.04584
A35	1.93631	0.00000	-0.00011	0.00006	-0.00005	1.93625
A36	1.89758	0.00001	-0.00004	0.00003	-0.00001	1.89757
A37	1.87570	0.00001	-0.00022	0.00021	-0.00001	1.87570
D1	0.00399	0.00000	0.00005	-0.00022	-0.00017	0.00382
D2	-3.13383	-0.00001	0.00051	-0.00026	0.00025	-3.13359
D3	3.13822	0.00001	-0.00028	0.00007	-0.00021	3.13801
D4	0.00040	0.00000	0.00019	0.00003	0.00021	0.00061
D5	-0.00591	0.00001	-0.00002	0.00003	0.00001	-0.00589
D6	-3.08677	-0.00002	-0.00073	-0.00134	-0.00207	-3.08884
D7	-3.14089	0.00000	0.00027	-0.00023	0.00004	-3.14085
D8	0.06142	-0.00002	-0.00044	-0.00160	-0.00204	0.05939
D9	-0.00077	-0.00001	-0.00006	0.00033	0.00027	-0.00050
D10	-3.14046	-0.00001	0.00019	0.00008	0.00026	-3.14020
D11	3.13741	0.00001	-0.00048	0.00037	-0.00011	3.13730
D12	-0.00228	0.00001	-0.00023	0.00012	-0.00012	-0.00240
D13	-0.00289	0.00001	0.00005	-0.00031	-0.00026	-0.00316
D14	3.09480	0.00002	0.00215	0.00166	0.00382	3.09861
D15	3.13693	0.00001	-0.00018	-0.00008	-0.00026	3.13668
D16	-0.04856	0.00001	0.00192	0.00190	0.00382	-0.04474
D17	0.04308	-0.00001	-0.00201	-0.00197	-0.00399	0.03910
D18	-3.09714	-0.00001	-0.00221	-0.00186	-0.00406	-3.10121
D19	-3.09637	-0.00001	-0.00174	-0.00226	-0.00399	-3.10036
D20	0.04660	-0.00001	-0.00193	-0.00214	-0.00407	0.04252
D21	0.00542	-0.00001	-0.00002	0.00017	0.00015	0.00557
D22	3.08929	0.00001	0.00067	0.00148	0.00215	3.09144
D23	-3.09551	-0.00001	-0.00198	-0.00165	-0.00363	-3.09914
D24	-0.01163	0.00001	-0.00129	-0.00034	-0.00164	-0.01327
D25	-2.83648	-0.00001	-0.01207	-0.01398	-0.02606	-2.86253
D26	0.25546	-0.00001	-0.00969	-0.01175	-0.02144	0.23402
D27	1.62507	0.00001	0.00490	0.00365	0.00855	1.63362
D28	-2.58503	0.00000	0.00505	0.00364	0.00869	-2.57634
D29	-0.53292	0.00001	0.00486	0.00381	0.00867	-0.52425
D30	-1.44776	-0.00001	0.00409	0.00210	0.00619	-1.44157
D31	0.62533	-0.00002	0.00423	0.00209	0.00632	0.63165
D32	2.67744	-0.00001	0.00405	0.00226	0.00631	2.68375
D33	-1.32940	0.00000	0.00049	0.00059	0.00108	-1.32832
D34	0.73637	-0.00001	0.00045	0.00052	0.00096	0.73733
D35	2.87883	0.00001	0.00016	0.00105	0.00120	2.88003
D36	2.90240	0.00000	0.00037	0.00048	0.00085	2.90325

D37	-1.31502	-0.00001	0.00032	0.00041	0.00073	-1.31429
D38	0.82744	0.00001	0.00003	0.00094	0.00097	0.82841
D39	0.78891	0.00000	0.00049	0.00039	0.00089	0.78980
D40	2.85469	-0.00001	0.00045	0.00032	0.00077	2.85545
D41	-1.28604	0.00001	0.00016	0.00085	0.00101	-1.28503
D42	2.89505	-0.00001	0.00067	-0.00100	-0.00033	2.89472
D43	-1.32906	0.00001	0.00032	-0.00069	-0.00037	-1.32943
D44	0.81105	-0.00002	0.00048	-0.00082	-0.00034	0.81071
D45	2.87013	0.00000	0.00012	-0.00050	-0.00038	2.86974
D46	-1.30495	-0.00001	0.00052	-0.00060	-0.00008	-1.30503
D47	0.75413	0.00002	0.00017	-0.00029	-0.00012	0.75401
D48	-3.13718	-0.00001	-0.00032	0.00003	-0.00028	-3.13747
D49	0.00506	0.00000	-0.00025	-0.00016	-0.00041	0.00465
D50	0.00289	0.00000	-0.00010	-0.00010	-0.00020	0.00270
D51	-3.13805	0.00000	-0.00003	-0.00029	-0.00032	-3.13837

Item	Value	Threshold	Converged?
Maximum Force	0.000073	0.000450	YES
RMS Force	0.000017	0.000300	YES
Maximum Displacement	0.022437	0.001800	NO
RMS Displacement	0.004531	0.001200	NO

Predicted change in Energy=-4.541730D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.818345	-1.993975	0.295190
2	6	0	-2.824206	-1.110117	0.069855
3	7	0	-2.241223	0.152195	0.016585
4	6	0	-0.913051	0.023233	0.207213
5	7	0	-0.641393	-1.269575	0.381750
6	6	0	0.729398	-1.796761	0.557866
7	6	0	1.447742	-1.996526	-0.785023
8	1	0	-1.840044	-3.064424	0.406188
9	1	0	-3.880006	-1.269974	-0.050505
10	1	0	1.276340	-1.054287	1.139495
11	1	0	0.660932	-2.725538	1.124583
12	1	0	1.071877	-2.895983	-1.283526
13	1	0	1.229194	-1.129218	-1.421807
14	35	0	1.955209	1.591361	0.088413
15	1	0	-0.126531	0.807850	0.193032
16	6	0	-2.864971	1.411603	-0.195280

17	6	0	-4.170560	1.594774	-0.342895
18	1	0	-2.147154	2.221580	-0.225269
19	1	0	-4.547245	2.595310	-0.503725
20	1	0	-4.895883	0.791718	-0.311529
21	7	0	2.867584	-2.162762	-0.495497
22	1	0	3.361892	-2.525224	-1.302791
23	1	0	3.265966	-1.250343	-0.277036

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357843	0.000000			
3	N	2.205105	1.391452	0.000000		
4	C	2.212787	2.226177	1.347965	0.000000	
5	N	1.384726	2.210742	2.171228	1.332522	0.000000
6	C	2.568830	3.652087	3.593884	2.476485	1.479192
7	C	3.440086	4.445906	4.343735	3.261487	2.500860
8	H	1.076407	2.213823	3.264869	3.229943	2.158435
9	H	2.212267	1.074594	2.170870	3.246787	3.267332
10	H	3.342595	4.238128	3.884555	2.612208	2.073216
11	H	2.714755	3.983495	4.234561	3.297686	2.089899
12	H	3.414579	4.494489	4.685969	3.831979	2.890267
13	H	3.603246	4.319198	3.969229	2.927637	2.602232
14	Br	5.209328	5.490094	4.436935	3.271094	3.874705
15	H	3.274584	3.312284	2.221022	1.111054	2.148580
16	C	3.596379	2.535947	1.421287	2.428902	3.530719
17	C	4.338108	3.049502	2.435693	3.658377	4.602676
18	H	4.260269	3.412579	2.085593	2.557886	3.850189
19	H	5.398769	4.126506	3.399600	4.508701	5.565707
20	H	4.195167	2.838004	2.750249	4.089329	4.778101
21	N	4.755166	5.815854	5.632154	4.423299	3.725622
22	H	5.447075	6.492650	6.348560	5.200950	4.521130
23	H	5.170169	6.101655	5.690558	4.395529	3.962552

		6	7	8	9	10
6	C	0.000000				
7	C	1.535993	0.000000			
8	H	2.869147	3.656354	0.000000		
9	H	4.679127	5.426996	2.755007	0.000000	
10	H	1.090278	2.149642	3.780243	5.296274	0.000000
11	H	1.090175	2.190233	2.624084	4.911173	1.781019
12	H	2.171705	1.094899	3.370874	5.355875	3.050357
13	H	2.148142	1.097943	4.062857	5.291900	2.562831
14	Br	3.633507	3.727378	6.015086	6.500482	2.926617
15	H	2.765813	3.361465	4.239820	4.297120	2.516226

16	C	4.876507	5.528347	4.631096	2.870907	5.001269
17	C	6.026896	6.682680	5.263132	2.894252	6.235681
18	H	5.003491	5.570369	5.332437	3.901828	4.930943
19	H	6.946959	7.556716	6.339517	3.948549	7.066391
20	H	6.252988	6.945507	4.972232	2.313160	6.603751
21	N	2.411507	1.458565	4.877273	6.820928	2.536528
22	H	3.304955	2.052213	5.501952	7.455800	3.532413
23	H	2.725767	2.029970	5.461595	7.149588	2.450226

		11	12	13	14	15
11	H	0.000000				
12	H	2.448860	0.000000			
13	H	3.058637	1.779137	0.000000		
14	Br	4.624329	4.774804	3.195217	0.000000	
15	H	3.738010	4.163506	2.863202	2.226763	0.000000
16	C	5.593743	5.936190	4.972155	4.831866	2.830964
17	C	6.645442	6.966694	6.143413	6.140935	4.154592
18	H	5.846488	6.137713	4.905026	4.162326	2.501305
19	H	7.621544	7.895374	6.934136	6.606092	4.819046
20	H	6.731396	7.082237	6.514543	6.909185	4.795994
21	N	2.794761	2.093601	2.147227	3.907277	4.273561
22	H	3.636956	2.319914	2.551744	4.567327	5.051333
23	H	3.305591	2.921503	2.339575	3.150701	3.995767

		16	17	18	19	20
16	C	0.000000				
17	C	1.326614	0.000000			
18	H	1.082692	2.121530	0.000000		
19	H	2.079988	1.081125	2.444923	0.000000	
20	H	2.126587	1.082579	3.099589	1.847007	0.000000
21	N	6.762277	7.979839	6.666564	8.810165	8.308682
22	H	7.449765	8.639075	7.351380	9.455836	8.954080
23	H	6.684386	7.962471	6.431081	8.711298	8.413499

		21	22	23
21	N	0.000000		
22	H	1.013629	0.000000	
23	H	1.019285	1.639115	0.000000

Stoichiometry C7H12BrN3
Framework group C1[X(C7H12BrN3)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-1.740466	2.054095	-0.323938
2	6	0	-2.775485	1.212486	-0.070623
3	7	0	-2.238866	-0.069385	-0.000021
4	6	0	-0.909210	0.006660	-0.207968
5	7	0	-0.592151	1.285047	-0.409989
6	6	0	0.794954	1.757661	-0.611445
7	6	0	1.536146	1.955447	0.719266
8	1	0	-1.723988	3.122375	-0.454929
9	1	0	-3.823159	1.413606	0.058544
10	1	0	1.307159	0.984771	-1.185023
11	1	0	0.754038	2.677694	-1.194837
12	1	0	1.199688	2.877300	1.204844
13	1	0	1.293367	1.108775	1.374769
14	35	0	1.900468	-1.664344	-0.091740
15	1	0	-0.152054	-0.806203	-0.187774
16	6	0	-2.906073	-1.300647	0.242643
17	6	0	-4.215676	-1.432488	0.408360
18	1	0	-2.218316	-2.136006	0.279892
19	1	0	-4.627066	-2.415213	0.592324
20	1	0	-4.911206	-0.603791	0.369949
21	7	0	2.957599	2.063502	0.410709
22	1	0	3.474535	2.422249	1.205391
23	1	0	3.319419	1.133045	0.205097

Rotational constants (GHZ): 0.8917064 0.4588819 0.3139300
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 365 symmetry adapted cartesian basis functions of A symmetry.
There are 352 symmetry adapted basis functions of A symmetry.
352 basis functions, 562 primitive gaussians, 365 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 843.1635340307 Hartrees.
NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 352 RedAO= T EigKep= 4.32D-06 NBF= 352
NBsUse= 352 1.00D-06 EigRej= -1.00D+00 NBFU= 352
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 0.000001 0.000009 -0.000241 Ang= 0.03 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3012.46805909 A.U. after 10 cycles

NFock= 10 Conv=0.90D-08 -V/T= 2.0017

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000056422	0.000029067	0.000042924
2	6	-0.000029698	0.000012968	0.000068961
3	7	0.000029948	-0.000033138	-0.000016733
4	6	-0.000065493	0.000033665	0.000057581
5	7	-0.000010221	-0.000092241	-0.000118859
6	6	-0.000004009	-0.000013461	0.000098653
7	6	0.000028899	-0.000035167	0.000007248
8	1	-0.000010011	-0.000003244	-0.000013733
9	1	0.000004004	-0.000005012	-0.000011827
10	1	0.000007611	0.000030188	-0.000022266
11	1	-0.000004896	0.000002659	-0.000016480
12	1	-0.000001696	0.000013919	-0.000012455
13	1	-0.000016286	-0.000005227	-0.000015558
14	35	0.000021128	0.000017172	-0.000003312
15	1	0.000001947	0.000008529	-0.000017184
16	6	-0.000019828	0.000034871	-0.000033327
17	6	-0.000001410	-0.000004098	-0.000010571
18	1	0.000008626	-0.000001573	0.000007936
19	1	-0.000005226	-0.000004705	0.000004593

```
      20        1             0.000001702     -0.000009102      0.000004054
      21        7             0.000015983      0.000070842     -0.000051553
      22        1            -0.000010576     -0.000022149      0.000023167
      23        1             0.000003081     -0.000024762      0.000028741
 ---------------------------------------------------------------------
 Cartesian Forces:  Max        0.000118859 RMS        0.000033062

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 Internal  Forces:  Max        0.000054740 RMS        0.000014609
 Search for a local minimum.
 Step number  35 out of a maximum of  121
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swapping is turned off.
 Update second derivatives using D2CorX and points     24     27     28     29     30
                                                      31     32     33     34     35
 DE= -1.02D-06 DEPred=-4.54D-07 R= 2.24D+00
 TightC=F SS=  1.41D+00  RLast= 4.03D-02 DXNew= 4.0000D-01 1.2085D-01
 Trust test= 2.24D+00 RLast= 4.03D-02 DXMaxT set to 2.38D-01
 ITU=  1  1  0  1  1  1  0  1  1  0 -1 -1  0 -1 -1  0 -1  0  0  0
 ITU=  1  1 -1  1 -1  1  1  1  1  1  1  0  1  0  0
      Eigenvalues ---    0.00032    0.00204    0.00343    0.00541    0.00970
      Eigenvalues ---    0.01268    0.01830    0.01850    0.02114    0.02273
      Eigenvalues ---    0.02376    0.02494    0.03059    0.03065    0.03919
      Eigenvalues ---    0.04073    0.04373    0.04628    0.05057    0.05440
      Eigenvalues ---    0.05479    0.08767    0.09180    0.09718    0.12661
      Eigenvalues ---    0.12968    0.15299    0.15743    0.15966    0.16000
      Eigenvalues ---    0.16008    0.16060    0.16338    0.19047    0.20768
      Eigenvalues ---    0.22089    0.23228    0.23937    0.24903    0.25153
      Eigenvalues ---    0.26869    0.29924    0.33978    0.34581    0.34867
      Eigenvalues ---    0.34991    0.35376    0.35690    0.35817    0.35859
      Eigenvalues ---    0.36441    0.36663    0.38087    0.41387    0.42229
      Eigenvalues ---    0.43027    0.46945    0.47714    0.48759    0.50043
      Eigenvalues ---    0.54308    0.60341    0.60617
 En-DIIS/RFO-DIIS IScMMF=        0 using points:    35     34     33     32     31
 RFO step:  Lambda=-7.24394411D-08.
 DidBck=F Rises=F RFO-DIIS coefs:          1.65362       -0.30704       -1.88769          1.42896
0.11214
 Iteration  1 RMS(Cart)=  0.00290910 RMS(Int)=  0.00000869
 Iteration  2 RMS(Cart)=  0.00001961 RMS(Int)=  0.00000065
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000065
```

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56595	0.00002	0.00004	0.00001	0.00005	2.56600
R2	2.61675	-0.00003	0.00000	-0.00008	-0.00008	2.61667
R3	2.03411	0.00000	-0.00001	0.00001	0.00000	2.03412
R4	2.62946	0.00000	-0.00004	0.00003	-0.00002	2.62944
R5	2.03069	0.00000	0.00000	-0.00001	0.00000	2.03068
R6	2.54729	-0.00002	0.00002	-0.00005	-0.00003	2.54725
R7	2.68584	0.00003	0.00006	0.00002	0.00008	2.68593
R8	2.51810	0.00005	-0.00002	0.00006	0.00004	2.51814
R9	2.09959	0.00003	0.00018	-0.00009	0.00009	2.09968
R10	2.79527	0.00001	0.00001	0.00006	0.00007	2.79534
R11	2.90261	0.00003	-0.00012	0.00014	0.00002	2.90263
R12	2.06033	0.00001	0.00009	0.00000	0.00010	2.06042
R13	2.06013	-0.00001	-0.00004	0.00000	-0.00005	2.06009
R14	2.06906	0.00000	-0.00001	0.00000	-0.00001	2.06905
R15	2.07481	0.00001	0.00011	-0.00002	0.00009	2.07491
R16	2.75629	0.00001	-0.00006	-0.00008	-0.00015	2.75614
R17	4.20797	0.00003	-0.00038	0.00107	0.00068	4.20865
R18	2.50694	0.00000	-0.00001	0.00000	-0.00001	2.50693
R19	2.04599	0.00001	0.00000	0.00001	0.00002	2.04601
R20	2.04303	0.00000	0.00001	-0.00001	0.00000	2.04303
R21	2.04578	0.00000	0.00000	0.00001	0.00000	2.04578
R22	1.91548	-0.00002	-0.00006	-0.00001	-0.00007	1.91541
R23	1.92617	-0.00002	-0.00004	-0.00003	-0.00007	1.92610
A1	1.87494	0.00001	0.00004	-0.00002	0.00001	1.87496
A2	2.27773	-0.00002	0.00000	-0.00008	-0.00008	2.27765
A3	2.13049	0.00001	-0.00004	0.00010	0.00007	2.13056
A4	1.86137	0.00000	0.00000	0.00000	0.00000	1.86137
A5	2.27782	0.00000	0.00000	-0.00003	-0.00003	2.27779
A6	2.14398	0.00000	0.00001	0.00003	0.00003	2.14402
A7	1.89718	0.00000	-0.00003	0.00001	-0.00002	1.89715
A8	2.24682	0.00000	0.00008	-0.00002	0.00006	2.24689
A9	2.13918	0.00000	-0.00005	0.00001	-0.00004	2.13914
A10	1.88832	0.00000	0.00007	-0.00004	0.00003	1.88835
A11	2.24996	-0.00001	-0.00003	0.00017	0.00014	2.25010
A12	2.14420	0.00001	0.00003	-0.00011	-0.00008	2.14412
A13	1.90295	-0.00001	-0.00007	0.00005	-0.00002	1.90293
A14	2.22517	0.00002	0.00028	0.00006	0.00034	2.22551
A15	2.15352	-0.00001	-0.00008	-0.00007	-0.00015	2.15337
A16	1.95590	0.00003	0.00019	0.00005	0.00024	1.95614
A17	1.86053	-0.00001	-0.00009	-0.00004	-0.00013	1.86041
A18	1.88318	-0.00001	-0.00004	-0.00006	-0.00011	1.88308
A19	1.89690	-0.00002	-0.00032	-0.00001	-0.00033	1.89657

A20	1.95310	-0.00001	0.00005	-0.00008	-0.00003	1.95307
A21	1.91173	0.00002	0.00021	0.00015	0.00036	1.91208
A22	1.92234	0.00001	0.00038	-0.00015	0.00023	1.92257
A23	1.88729	0.00000	0.00001	0.00005	0.00007	1.88736
A24	1.87186	-0.00002	-0.00016	0.00008	-0.00008	1.87178
A25	1.89288	-0.00002	-0.00043	0.00003	-0.00040	1.89248
A26	1.90808	0.00001	0.00002	0.00001	0.00003	1.90811
A27	1.98114	0.00001	0.00021	-0.00003	0.00017	1.98131
A28	2.71621	0.00003	0.00098	-0.00020	0.00078	2.71699
A29	2.17833	-0.00002	0.00001	-0.00005	-0.00005	2.17828
A30	1.95635	0.00000	-0.00005	0.00000	-0.00005	1.95631
A31	2.14851	0.00002	0.00004	0.00005	0.00010	2.14860
A32	2.07971	0.00001	-0.00001	0.00004	0.00003	2.07974
A33	2.15763	-0.00001	0.00001	-0.00005	-0.00004	2.15759
A34	2.04584	0.00000	0.00000	0.00001	0.00001	2.04585
A35	1.93625	0.00001	0.00020	0.00007	0.00028	1.93653
A36	1.89757	0.00004	0.00042	-0.00004	0.00037	1.89794
A37	1.87570	0.00001	0.00034	0.00015	0.00049	1.87619
D1	0.00382	0.00001	-0.00008	0.00017	0.00009	0.00391
D2	-3.13359	-0.00001	-0.00035	-0.00001	-0.00036	-3.13395
D3	3.13801	0.00001	0.00013	0.00012	0.00025	3.13827
D4	0.00061	-0.00001	-0.00014	-0.00006	-0.00020	0.00041
D5	-0.00589	0.00000	0.00038	-0.00019	0.00019	-0.00570
D6	-3.08884	-0.00002	-0.00221	-0.00086	-0.00306	-3.09190
D7	-3.14085	0.00000	0.00019	-0.00014	0.00005	-3.14080
D8	0.05939	-0.00002	-0.00240	-0.00081	-0.00321	0.05618
D9	-0.00050	-0.00002	-0.00024	-0.00010	-0.00034	-0.00084
D10	-3.14020	-0.00001	-0.00007	-0.00008	-0.00015	-3.14034
D11	3.13730	0.00000	0.00001	0.00006	0.00007	3.13737
D12	-0.00240	0.00001	0.00018	0.00009	0.00026	-0.00213
D13	-0.00316	0.00002	0.00048	-0.00002	0.00046	-0.00269
D14	3.09861	0.00001	0.00248	0.00056	0.00304	3.10165
D15	3.13668	0.00001	0.00032	-0.00004	0.00028	3.13696
D16	-0.04474	0.00000	0.00232	0.00054	0.00286	-0.04188
D17	0.03910	0.00000	-0.00239	-0.00098	-0.00337	0.03572
D18	-3.10121	-0.00001	-0.00271	-0.00098	-0.00368	-3.10489
D19	-3.10036	0.00000	-0.00220	-0.00095	-0.00315	-3.10351
D20	0.04252	-0.00001	-0.00251	-0.00095	-0.00347	0.03906
D21	0.00557	-0.00001	-0.00053	0.00013	-0.00041	0.00517
D22	3.09144	0.00001	0.00194	0.00077	0.00271	3.09415
D23	-3.09914	0.00000	-0.00238	-0.00042	-0.00280	-3.10193
D24	-0.01327	0.00002	0.00010	0.00022	0.00032	-0.01295
D25	-2.86253	0.00000	-0.01605	-0.00237	-0.01842	-2.88095
D26	0.23402	-0.00001	-0.01379	-0.00171	-0.01550	0.21852

D27	1.63362	0.00001	0.00460	0.00142	0.00602	1.63964
D28	-2.57634	0.00000	0.00427	0.00140	0.00568	-2.57067
D29	-0.52425	0.00002	0.00445	0.00153	0.00598	-0.51827
D30	-1.44157	-0.00001	0.00167	0.00066	0.00233	-1.43924
D31	0.63165	-0.00002	0.00134	0.00064	0.00198	0.63364
D32	2.68375	-0.00001	0.00151	0.00077	0.00228	2.68603
D33	-1.32832	0.00000	0.00048	-0.00013	0.00036	-1.32796
D34	0.73733	-0.00001	0.00018	-0.00014	0.00004	0.73738
D35	2.88003	0.00000	0.00035	-0.00010	0.00024	2.88027
D36	2.90325	0.00001	0.00068	-0.00010	0.00058	2.90383
D37	-1.31429	0.00000	0.00038	-0.00011	0.00027	-1.31402
D38	0.82841	0.00001	0.00054	-0.00008	0.00046	0.82888
D39	0.78980	0.00000	0.00060	-0.00023	0.00037	0.79017
D40	2.85545	-0.00001	0.00030	-0.00024	0.00006	2.85551
D41	-1.28503	0.00000	0.00046	-0.00021	0.00026	-1.28478
D42	2.89472	-0.00001	-0.00032	0.00018	-0.00014	2.89458
D43	-1.32943	0.00002	0.00047	0.00037	0.00085	-1.32858
D44	0.81071	-0.00002	-0.00069	0.00030	-0.00039	0.81032
D45	2.86974	0.00001	0.00010	0.00050	0.00061	2.87035
D46	-1.30503	-0.00002	-0.00028	0.00027	-0.00001	-1.30504
D47	0.75401	0.00002	0.00051	0.00047	0.00098	0.75499
D48	-3.13747	-0.00001	-0.00048	-0.00003	-0.00051	-3.13797
D49	0.00465	0.00000	-0.00036	-0.00002	-0.00039	0.00427
D50	0.00270	0.00000	-0.00013	-0.00003	-0.00016	0.00254
D51	-3.13837	0.00001	-0.00001	-0.00003	-0.00004	-3.13841

Item	Value	Threshold	Converged?
Maximum Force	0.000055	0.000450	YES
RMS Force	0.000015	0.000300	YES
Maximum Displacement	0.014632	0.001800	NO
RMS Displacement	0.002909	0.001200	NO

Predicted change in Energy=-2.381059D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.819413	-1.993954	0.297724
2	6	0	-2.825356	-1.109809	0.073739
3	7	0	-2.241659	0.151977	0.016244
4	6	0	-0.913078	0.022466	0.203501
5	7	0	-0.641738	-1.270246	0.379410
6	6	0	0.729046	-1.797402	0.555980

7	6	0	1.448722	-1.995731	-0.786421
8	1	0	-1.841580	-3.064194	0.410650
9	1	0	-3.881576	-1.269227	-0.043450
10	1	0	1.275446	-1.055181	1.138535
11	1	0	0.660209	-2.726739	1.121685
12	1	0	1.073380	-2.894511	-1.286528
13	1	0	1.230720	-1.127799	-1.422626
14	35	0	1.956418	1.590502	0.096156
15	1	0	-0.126231	0.806800	0.188142
16	6	0	-2.865090	1.411473	-0.196320
17	6	0	-4.170626	1.594836	-0.344122
18	1	0	-2.147052	2.221264	-0.226351
19	1	0	-4.547169	2.595414	-0.505026
20	1	0	-4.896054	0.791874	-0.312729
21	7	0	2.868168	-2.162343	-0.495562
22	1	0	3.363526	-2.524061	-1.302501
23	1	0	3.266509	-1.250489	-0.274845

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357867	0.000000			
3	N	2.205117	1.391442	0.000000		
4	C	2.212751	2.226138	1.347949	0.000000	
5	N	1.384682	2.210738	2.171256	1.332544	0.000000
6	C	2.569041	3.652276	3.593951	2.476435	1.479229
7	C	3.443266	4.448874	4.344633	3.260546	2.501102
8	H	1.076410	2.213808	3.264870	3.229937	2.158436
9	H	2.212272	1.074592	2.170878	3.246758	3.267317
10	H	3.341618	4.237140	3.884173	2.612518	2.073191
11	H	2.713745	3.982690	4.234364	3.297942	2.089835
12	H	3.418934	4.498404	4.686981	3.830790	2.890539
13	H	3.607373	4.323330	3.970590	2.926306	2.602638
14	Br	5.210168	5.491588	4.438422	3.271738	3.874858
15	H	3.274614	3.312363	2.221121	1.111100	2.148593
16	C	3.596450	2.536015	1.421331	2.428899	3.530776
17	C	4.338154	3.049502	2.435697	3.658396	4.602743
18	H	4.260289	3.412652	2.085606	2.557768	3.850138
19	H	5.398829	4.126534	3.399630	4.508735	5.565783
20	H	4.195141	2.837877	2.750183	4.089325	4.778138
21	N	4.757213	5.817916	5.632793	4.422657	3.725702
22	H	5.450192	6.495876	6.349674	5.200210	4.521395
23	H	5.171767	6.103451	5.691358	4.395244	3.962680

	6	7	8	9	10

6	C	0.000000				
7	C	1.536004	0.000000			
8	H	2.869495	3.660694	0.000000		
9	H	4.679330	5.430644	2.754941	0.000000	
10	H	1.090328	2.149446	3.779128	5.295072	0.000000
11	H	1.090151	2.190204	2.622669	4.910162	1.781266
12	H	2.171878	1.094895	3.377306	5.360819	3.050393
13	H	2.148238	1.097993	4.068114	5.296952	2.562581
14	Br	3.632598	3.727971	6.015803	6.502285	2.924023
15	H	2.765623	3.359231	4.239873	4.297224	2.516926
16	C	4.876541	5.528674	4.631154	2.871021	5.001026
17	C	6.026961	6.683179	5.263145	2.894271	6.235429
18	H	5.003365	5.570127	5.332462	3.901993	4.930669
19	H	6.947014	7.557017	6.339545	3.948609	7.066186
20	H	6.253060	6.946316	4.972157	2.312966	6.603423
21	N	2.411383	1.458488	4.880193	6.823570	2.536305
22	H	3.304916	2.052302	5.506338	7.459981	3.532187
23	H	2.725454	2.030134	5.463698	7.151854	2.449514

		11	12	13	14	15
11	H	0.000000				
12	H	2.449153	0.000000			
13	H	3.058694	1.778918	0.000000		
14	Br	4.622817	4.775658	3.197264	0.000000	
15	H	3.738434	4.160940	2.859819	2.227123	0.000000
16	C	5.593717	5.936464	4.972664	4.833687	2.831040
17	C	6.645417	6.967207	6.144140	6.142844	4.154689
18	H	5.846422	6.137289	4.904757	4.164173	2.501246
19	H	7.621567	7.895606	6.934573	6.608170	4.819161
20	H	6.731288	7.083210	6.515702	6.910960	4.796072
21	N	2.794480	2.093553	2.147316	3.907078	4.271965
22	H	3.636713	2.319969	2.552027	4.567912	5.049263
23	H	3.304907	2.921665	2.340276	3.150430	3.994681

		16	17	18	19	20
16	C	0.000000				
17	C	1.326609	0.000000			
18	H	1.082701	2.121588	0.000000		
19	H	2.080001	1.081125	2.445037	0.000000	
20	H	2.126562	1.082579	3.099617	1.847012	0.000000
21	N	6.762541	7.980223	6.666402	8.810424	8.309270
22	H	7.450351	8.639864	7.351373	9.456431	8.955207
23	H	6.684962	7.963143	6.431334	8.711918	8.414280

		21	22	23
21	N	0.000000		
22	H	1.013592	0.000000	

23 H 1.019249 1.639352 0.000000

Stoichiometry C7H12BrN3

Framework group C1[X(C7H12BrN3)]

Deg. of freedom 63

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.741941	2.053002	-0.328825
2	6	0	-2.777122	1.211267	-0.076462
3	7	0	-2.239546	-0.069815	0.000692
4	6	0	-0.909265	0.006770	-0.202911
5	7	0	-0.592612	1.284803	-0.407932
6	6	0	0.794560	1.757336	-0.609394
7	6	0	1.535886	1.955741	0.721163
8	1	0	-1.726048	3.120860	-0.463305
9	1	0	-3.825410	1.411897	0.048384
10	1	0	1.306840	0.983946	-1.182326
11	1	0	0.753618	2.677089	-1.193180
12	1	0	1.199371	2.877586	1.206706
13	1	0	1.293236	1.109342	1.377148
14	35	0	1.901736	-1.663720	-0.093346
15	1	0	-0.151626	-0.805627	-0.179718
16	6	0	-2.906404	-1.300926	0.245327
17	6	0	-4.216073	-1.432954	0.410345
18	1	0	-2.218295	-2.135922	0.284420
19	1	0	-4.627291	-2.415526	0.595499
20	1	0	-4.911832	-0.604535	0.370106
21	7	0	2.957177	2.063966	0.412286
22	1	0	3.474407	2.423198	1.206513
23	1	0	3.319294	1.133793	0.206088

Rotational constants (GHZ): 0.8918921 0.4585798 0.3138477

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 365 symmetry adapted cartesian basis functions of A symmetry.

There are 352 symmetry adapted basis functions of A symmetry.

352 basis functions, 562 primitive gaussians, 365 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 843.1050180292 Hartrees.

NAtoms= 23 NActive= 23 NUniq= 23 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F

Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 352 RedAO= T EigKep= 4.32D-06 NBF= 352
NBsUse= 352 1.00D-06 EigRej= -1.00D+00 NBFU= 352
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/nh2/nh2.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 0.000025 0.000002 -0.000149 Ang= 0.02 deg.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3012.46805973 A.U. after 10 cycles
NFock= 10 Conv=0.50D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000037854	0.000020603	0.000021685
2	6	-0.000018410	0.000000759	0.000008840
3	7	0.000019873	-0.000014842	0.000004459
4	6	-0.000025370	0.000037292	0.000011073
5	7	-0.000003780	-0.000035352	-0.000032257
6	6	0.000002606	-0.000002061	0.000041883
7	6	-0.000001081	-0.000014374	-0.000026959
8	1	-0.000004959	-0.000000500	-0.000002258
9	1	0.000001911	-0.000004124	-0.000002996
10	1	-0.000001313	0.000006721	-0.000006085
11	1	0.000001549	0.000001433	-0.000006580
12	1	-0.000004385	-0.000003184	0.000008841
13	1	0.000002500	-0.000000608	0.000008007
14	35	0.000010459	0.000013314	-0.000005100
15	1	-0.000013693	-0.000016181	-0.000010857
16	6	-0.000010229	0.000010345	-0.000005312
17	6	-0.000001454	0.000000241	-0.000004450
18	1	-0.000001287	-0.000004337	-0.000001845
19	1	-0.000004122	-0.000005089	-0.000001084
20	1	0.000001421	-0.000006494	0.000001228
21	7	0.000006996	0.000024050	-0.000011450

```
      22        1             -0.000001531   -0.000003244    0.000007058
      23        1              0.000006444   -0.000004369    0.000004158
 ---------------------------------------------------------------------
 Cartesian Forces:  Max        0.000041883 RMS        0.000013761

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 Internal  Forces:  Max        0.000032712 RMS        0.000007024
 Search for a local minimum.
 Step number   36 out of a maximum of   121
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swapping is turned off.
 Update second derivatives using D2CorX and points     24     27     28     29     30
                                                       31     32     33     34     35
                                                       36
 DE= -6.42D-07 DEPred=-2.38D-07 R= 2.70D+00
 Trust test= 2.70D+00 RLast= 2.84D-02 DXMaxT set to 2.38D-01
 ITU=   0   1   1   0   1   1   1   0   1   1   0 -1 -1   0 -1 -1   0 -1   0   0
 ITU=   0   1   1 -1   1 -1   1   1   1   1   1   1   0   1   0   0
      Eigenvalues ---      0.00034     0.00205     0.00339     0.00537     0.00873
      Eigenvalues ---      0.01160     0.01824     0.01839     0.02110     0.02249
      Eigenvalues ---      0.02374     0.02412     0.03059     0.03065     0.03909
      Eigenvalues ---      0.04011     0.04165     0.04622     0.05023     0.05326
      Eigenvalues ---      0.05628     0.08597     0.09138     0.09736     0.12822
      Eigenvalues ---      0.13056     0.15363     0.15747     0.15917     0.16000
      Eigenvalues ---      0.16003     0.16029     0.16214     0.19202     0.20942
      Eigenvalues ---      0.22062     0.23150     0.23926     0.24848     0.25073
      Eigenvalues ---      0.27562     0.30003     0.34035     0.34557     0.34880
      Eigenvalues ---      0.35093     0.35380     0.35691     0.35839     0.35859
      Eigenvalues ---      0.36441     0.36661     0.37869     0.41126     0.42158
      Eigenvalues ---      0.43057     0.46902     0.47711     0.48653     0.50025
      Eigenvalues ---      0.54259     0.59646     0.60391
 En-DIIS/RFO-DIIS IScMMF=        0 using points:     36     35     34     33     32
 RFO step:  Lambda=-1.11931660D-08.
 DidBck=F Rises=F RFO-DIIS coefs:      1.15009     -0.07642     -0.23061      0.22485     -
0.06792
 Iteration  1 RMS(Cart)=  0.00034162 RMS(Int)=  0.00000019
 Iteration  2 RMS(Cart)=  0.00000020 RMS(Int)=  0.00000017
 Variable          Old X       -DE/DX      Delta X      Delta X      Delta X          New X
                                           (Linear)       (Quad)     (Total)
     R1            2.56600     0.00001     0.00001      0.00001      0.00002      2.56601
```

R2	2.61667	-0.00002	-0.00003	-0.00003	-0.00006	2.61661
R3	2.03412	0.00000	0.00000	0.00000	0.00000	2.03412
R4	2.62944	0.00000	-0.00001	0.00000	0.00000	2.62944
R5	2.03068	0.00000	0.00000	0.00000	0.00000	2.03068
R6	2.54725	-0.00001	-0.00001	-0.00002	-0.00003	2.54723
R7	2.68593	0.00001	0.00002	0.00001	0.00004	2.68596
R8	2.51814	0.00003	0.00002	0.00003	0.00005	2.51819
R9	2.09968	0.00000	-0.00002	-0.00002	-0.00004	2.09964
R10	2.79534	0.00001	0.00002	0.00001	0.00002	2.79536
R11	2.90263	0.00001	0.00004	0.00001	0.00005	2.90268
R12	2.06042	0.00000	0.00001	-0.00001	0.00000	2.06042
R13	2.06009	0.00000	-0.00001	0.00000	-0.00001	2.06007
R14	2.06905	0.00000	-0.00002	0.00002	-0.00001	2.06904
R15	2.07491	-0.00001	0.00002	-0.00003	-0.00001	2.07489
R16	2.75614	0.00001	-0.00001	0.00002	0.00001	2.75616
R17	4.20865	0.00002	0.00047	-0.00008	0.00040	4.20905
R18	2.50693	0.00000	0.00000	0.00000	0.00000	2.50692
R19	2.04601	0.00000	0.00000	0.00000	0.00000	2.04600
R20	2.04303	0.00000	0.00000	0.00000	0.00000	2.04303
R21	2.04578	0.00000	0.00000	0.00000	0.00000	2.04578
R22	1.91541	0.00000	-0.00003	0.00000	-0.00003	1.91538
R23	1.92610	0.00000	-0.00002	-0.00001	-0.00003	1.92607
A1	1.87496	0.00001	0.00002	0.00002	0.00004	1.87499
A2	2.27765	-0.00001	-0.00003	-0.00005	-0.00008	2.27757
A3	2.13056	0.00000	0.00002	0.00003	0.00005	2.13060
A4	1.86137	0.00000	0.00000	-0.00002	-0.00003	1.86134
A5	2.27779	0.00000	0.00000	0.00000	0.00000	2.27779
A6	2.14402	0.00000	0.00001	0.00002	0.00003	2.14404
A7	1.89715	0.00000	0.00000	0.00002	0.00001	1.89717
A8	2.24689	-0.00001	0.00000	-0.00002	-0.00001	2.24687
A9	2.13914	0.00000	0.00000	0.00000	0.00000	2.13914
A10	1.88835	0.00000	0.00001	-0.00001	0.00000	1.88836
A11	2.25010	-0.00001	-0.00004	0.00004	-0.00001	2.25009
A12	2.14412	0.00001	0.00004	-0.00003	0.00000	2.14413
A13	1.90293	-0.00001	-0.00002	-0.00001	-0.00003	1.90290
A14	2.22551	-0.00001	0.00003	-0.00003	0.00000	2.22551
A15	2.15337	0.00002	0.00002	0.00004	0.00006	2.15343
A16	1.95614	0.00000	0.00001	-0.00003	-0.00002	1.95612
A17	1.86041	0.00000	-0.00002	0.00000	-0.00002	1.86039
A18	1.88308	0.00000	-0.00001	0.00001	0.00000	1.88308
A19	1.89657	0.00000	-0.00008	0.00006	-0.00001	1.89656
A20	1.95307	-0.00001	-0.00001	-0.00006	-0.00006	1.95300
A21	1.91208	0.00000	0.00010	0.00002	0.00012	1.91220
A22	1.92257	-0.00001	0.00004	-0.00007	-0.00003	1.92254

A23	1.88736	0.00000	0.00002	-0.00005	-0.00004	1.88732
A24	1.87178	0.00000	-0.00002	0.00002	0.00000	1.87177
A25	1.89248	0.00000	-0.00007	0.00011	0.00004	1.89251
A26	1.90811	0.00000	-0.00006	0.00008	0.00002	1.90813
A27	1.98131	0.00000	0.00010	-0.00009	0.00001	1.98132
A28	2.71699	0.00002	-0.00022	0.00034	0.00012	2.71711
A29	2.17828	-0.00001	-0.00002	-0.00001	-0.00003	2.17824
A30	1.95631	0.00000	-0.00001	-0.00001	-0.00001	1.95629
A31	2.14860	0.00001	0.00003	0.00002	0.00005	2.14865
A32	2.07974	0.00000	0.00002	0.00002	0.00004	2.07978
A33	2.15759	-0.00001	-0.00002	-0.00003	-0.00005	2.15755
A34	2.04585	0.00000	0.00000	0.00001	0.00001	2.04586
A35	1.93653	0.00000	0.00007	0.00001	0.00009	1.93662
A36	1.89794	0.00002	0.00008	0.00013	0.00021	1.89816
A37	1.87619	0.00000	0.00014	-0.00002	0.00013	1.87631
D1	0.00391	0.00000	-0.00001	-0.00007	-0.00008	0.00382
D2	-3.13395	0.00000	-0.00019	-0.00008	-0.00027	-3.13422
D3	3.13827	0.00000	0.00011	0.00003	0.00014	3.13840
D4	0.00041	0.00000	-0.00007	0.00002	-0.00005	0.00036
D5	-0.00570	0.00000	0.00005	0.00008	0.00013	-0.00556
D6	-3.09190	0.00000	-0.00046	-0.00004	-0.00050	-3.09240
D7	-3.14080	0.00000	-0.00005	-0.00001	-0.00006	-3.14086
D8	0.05618	-0.00001	-0.00057	-0.00013	-0.00070	0.05548
D9	-0.00084	0.00000	-0.00003	0.00004	0.00001	-0.00084
D10	-3.14034	0.00000	-0.00006	0.00004	-0.00002	-3.14036
D11	3.13737	0.00000	0.00013	0.00005	0.00017	3.13754
D12	-0.00213	0.00000	0.00010	0.00005	0.00015	-0.00199
D13	-0.00269	0.00000	0.00007	0.00001	0.00008	-0.00262
D14	3.10165	0.00000	0.00020	-0.00010	0.00010	3.10175
D15	3.13696	0.00000	0.00009	0.00001	0.00010	3.13706
D16	-0.04188	0.00000	0.00022	-0.00010	0.00012	-0.04175
D17	0.03572	0.00000	-0.00030	0.00001	-0.00028	0.03544
D18	-3.10489	0.00000	-0.00031	-0.00002	-0.00033	-3.10522
D19	-3.10351	0.00000	-0.00032	0.00001	-0.00032	-3.10383
D20	0.03906	0.00000	-0.00034	-0.00002	-0.00036	0.03870
D21	0.00517	0.00000	-0.00008	-0.00006	-0.00013	0.00504
D22	3.09415	0.00000	0.00041	0.00006	0.00047	3.09462
D23	-3.10193	0.00000	-0.00019	0.00004	-0.00015	-3.10209
D24	-0.01295	0.00000	0.00030	0.00015	0.00045	-0.01250
D25	-2.88095	0.00000	-0.00165	-0.00005	-0.00169	-2.88264
D26	0.21852	0.00000	-0.00150	-0.00017	-0.00167	0.21685
D27	1.63964	0.00000	0.00025	0.00019	0.00044	1.64008
D28	-2.57067	0.00000	0.00016	0.00024	0.00040	-2.57027
D29	-0.51827	0.00001	0.00026	0.00027	0.00053	-0.51774

D30	-1.43924	-0.00001	-0.00033	0.00005	-0.00028	-1.43952
D31	0.63364	-0.00001	-0.00042	0.00011	-0.00032	0.63332
D32	2.68603	0.00000	-0.00032	0.00014	-0.00019	2.68584
D33	-1.32796	0.00000	-0.00002	0.00027	0.00025	-1.32771
D34	0.73738	0.00000	-0.00007	0.00033	0.00025	0.73763
D35	2.88027	0.00000	0.00005	0.00020	0.00024	2.88052
D36	2.90383	0.00000	0.00004	0.00025	0.00029	2.90412
D37	-1.31402	0.00000	-0.00001	0.00031	0.00030	-1.31372
D38	0.82888	0.00000	0.00011	0.00018	0.00029	0.82916
D39	0.79017	0.00000	-0.00003	0.00022	0.00020	0.79037
D40	2.85551	0.00000	-0.00008	0.00028	0.00020	2.85571
D41	-1.28478	0.00000	0.00004	0.00015	0.00019	-1.28459
D42	2.89458	-0.00001	-0.00020	-0.00022	-0.00042	2.89416
D43	-1.32858	0.00000	0.00007	-0.00015	-0.00008	-1.32866
D44	0.81032	0.00000	-0.00021	-0.00019	-0.00040	0.80993
D45	2.87035	0.00001	0.00006	-0.00012	-0.00006	2.87029
D46	-1.30504	-0.00001	-0.00014	-0.00032	-0.00046	-1.30550
D47	0.75499	0.00000	0.00013	-0.00025	-0.00012	0.75486
D48	-3.13797	0.00000	-0.00003	-0.00005	-0.00008	-3.13805
D49	0.00427	0.00000	-0.00003	0.00000	-0.00004	0.00423
D50	0.00254	0.00000	-0.00002	-0.00002	-0.00003	0.00251
D51	-3.13841	0.00000	-0.00001	0.00003	0.00001	-3.13840

Item	Value	Threshold	Converged?
Maximum Force	0.000033	0.000450	YES
RMS Force	0.000007	0.000300	YES
Maximum Displacement	0.001522	0.001800	YES
RMS Displacement	0.000342	0.001200	YES

Predicted change in Energy=-2.420970D-08

Optimization completed.

-- Stationary point found.

! Optimized Parameters !

! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.	
! R1	R(1,2)	1.3579	-DE/DX =	0.0 !
! R2	R(1,5)	1.3847	-DE/DX =	0.0 !
! R3	R(1,8)	1.0764	-DE/DX =	0.0 !
! R4	R(2,3)	1.3914	-DE/DX =	0.0 !
! R5	R(2,9)	1.0746	-DE/DX =	0.0 !
! R6	R(3,4)	1.3479	-DE/DX =	0.0 !
! R7	R(3,16)	1.4213	-DE/DX =	0.0 !
! R8	R(4,5)	1.3325	-DE/DX =	0.0 !

! R9	R(4,15)	1.1111	-DE/DX =	0.0	!
! R10	R(5,6)	1.4792	-DE/DX =	0.0	!
! R11	R(6,7)	1.536	-DE/DX =	0.0	!
! R12	R(6,10)	1.0903	-DE/DX =	0.0	!
! R13	R(6,11)	1.0902	-DE/DX =	0.0	!
! R14	R(7,12)	1.0949	-DE/DX =	0.0	!
! R15	R(7,13)	1.098	-DE/DX =	0.0	!
! R16	R(7,21)	1.4585	-DE/DX =	0.0	!
! R17	R(14,15)	2.2271	-DE/DX =	0.0	!
! R18	R(16,17)	1.3266	-DE/DX =	0.0	!
! R19	R(16,18)	1.0827	-DE/DX =	0.0	!
! R20	R(17,19)	1.0811	-DE/DX =	0.0	!
! R21	R(17,20)	1.0826	-DE/DX =	0.0	!
! R22	R(21,22)	1.0136	-DE/DX =	0.0	!
! R23	R(21,23)	1.0192	-DE/DX =	0.0	!
! A1	A(2,1,5)	107.427	-DE/DX =	0.0	!
! A2	A(2,1,8)	130.4998	-DE/DX =	0.0	!
! A3	A(5,1,8)	122.0719	-DE/DX =	0.0	!
! A4	A(1,2,3)	106.6486	-DE/DX =	0.0	!
! A5	A(1,2,9)	130.5079	-DE/DX =	0.0	!
! A6	A(3,2,9)	122.8431	-DE/DX =	0.0	!
! A7	A(2,3,4)	108.699	-DE/DX =	0.0	!
! A8	A(2,3,16)	128.7371	-DE/DX =	0.0	!
! A9	A(4,3,16)	122.5638	-DE/DX =	0.0	!
! A10	A(3,4,5)	108.1947	-DE/DX =	0.0	!
! A11	A(3,4,15)	128.9211	-DE/DX =	0.0	!
! A12	A(5,4,15)	122.8492	-DE/DX =	0.0	!
! A13	A(1,5,4)	109.0297	-DE/DX =	0.0	!
! A14	A(1,5,6)	127.5124	-DE/DX =	0.0	!
! A15	A(4,5,6)	123.379	-DE/DX =	0.0	!
! A16	A(5,6,7)	112.0788	-DE/DX =	0.0	!
! A17	A(5,6,10)	106.5934	-DE/DX =	0.0	!
! A18	A(5,6,11)	107.8923	-DE/DX =	0.0	!
! A19	A(7,6,10)	108.6657	-DE/DX =	0.0	!
! A20	A(7,6,11)	111.9026	-DE/DX =	0.0	!
! A21	A(10,6,11)	109.5543	-DE/DX =	0.0	!
! A22	A(6,7,12)	110.1552	-DE/DX =	0.0	!
! A23	A(6,7,13)	108.1376	-DE/DX =	0.0	!
! A24	A(6,7,21)	107.2449	-DE/DX =	0.0	!
! A25	A(12,7,13)	108.4309	-DE/DX =	0.0	!
! A26	A(12,7,21)	109.3265	-DE/DX =	0.0	!
! A27	A(13,7,21)	113.5209	-DE/DX =	0.0	!
! A28	A(4,15,14)	155.6721	-DE/DX =	0.0	!
! A29	A(3,16,17)	124.8061	-DE/DX =	0.0	!

! A30	A(3,16,18)	112.088	-DE/DX =	0.0	!
! A31	A(17,16,18)	123.1058	-DE/DX =	0.0	!
! A32	A(16,17,19)	119.1605	-DE/DX =	0.0	!
! A33	A(16,17,20)	123.6211	-DE/DX =	0.0	!
! A34	A(19,17,20)	117.2184	-DE/DX =	0.0	!
! A35	A(7,21,22)	110.955	-DE/DX =	0.0	!
! A36	A(7,21,23)	108.7441	-DE/DX =	0.0	!
! A37	A(22,21,23)	107.4976	-DE/DX =	0.0	!
! D1	D(5,1,2,3)	0.2238	-DE/DX =	0.0	!
! D2	D(5,1,2,9)	-179.5619	-DE/DX =	0.0	!
! D3	D(8,1,2,3)	179.8094	-DE/DX =	0.0	!
! D4	D(8,1,2,9)	0.0237	-DE/DX =	0.0	!
! D5	D(2,1,5,4)	-0.3264	-DE/DX =	0.0	!
! D6	D(2,1,5,6)	-177.1531	-DE/DX =	0.0	!
! D7	D(8,1,5,4)	-179.9546	-DE/DX =	0.0	!
! D8	D(8,1,5,6)	3.2188	-DE/DX =	0.0	!
! D9	D(1,2,3,4)	-0.0483	-DE/DX =	0.0	!
! D10	D(1,2,3,16)	-179.9283	-DE/DX =	0.0	!
! D11	D(9,2,3,4)	179.7578	-DE/DX =	0.0	!
! D12	D(9,2,3,16)	-0.1222	-DE/DX =	0.0	!
! D13	D(2,3,4,5)	-0.1543	-DE/DX =	0.0	!
! D14	D(2,3,4,15)	177.7116	-DE/DX =	0.0	!
! D15	D(16,3,4,5)	179.7346	-DE/DX =	0.0	!
! D16	D(16,3,4,15)	-2.3994	-DE/DX =	0.0	!
! D17	D(2,3,16,17)	2.0469	-DE/DX =	0.0	!
! D18	D(2,3,16,18)	-177.8971	-DE/DX =	0.0	!
! D19	D(4,3,16,17)	-177.8183	-DE/DX =	0.0	!
! D20	D(4,3,16,18)	2.2378	-DE/DX =	0.0	!
! D21	D(3,4,5,1)	0.296	-DE/DX =	0.0	!
! D22	D(3,4,5,6)	177.2818	-DE/DX =	0.0	!
! D23	D(15,4,5,1)	-177.7277	-DE/DX =	0.0	!
! D24	D(15,4,5,6)	-0.742	-DE/DX =	0.0	!
! D25	D(3,4,15,14)	-165.0663	-DE/DX =	0.0	!
! D26	D(5,4,15,14)	12.5204	-DE/DX =	0.0	!
! D27	D(1,5,6,7)	93.9444	-DE/DX =	0.0	!
! D28	D(1,5,6,10)	-147.2883	-DE/DX =	0.0	!
! D29	D(1,5,6,11)	-29.6948	-DE/DX =	0.0	!
! D30	D(4,5,6,7)	-82.4626	-DE/DX =	0.0	!
! D31	D(4,5,6,10)	36.3047	-DE/DX =	0.0	!
! D32	D(4,5,6,11)	153.8983	-DE/DX =	0.0	!
! D33	D(5,6,7,12)	-76.0866	-DE/DX =	0.0	!
! D34	D(5,6,7,13)	42.2485	-DE/DX =	0.0	!
! D35	D(5,6,7,21)	165.0276	-DE/DX =	0.0	!
! D36	D(10,6,7,12)	166.3769	-DE/DX =	0.0	!

! D37	D(10,6,7,13)	-75.2879	-DE/DX =	0.0 !
! D38	D(10,6,7,21)	47.4911	-DE/DX =	0.0 !
! D39	D(11,6,7,12)	45.2735	-DE/DX =	0.0 !
! D40	D(11,6,7,13)	163.6087	-DE/DX =	0.0 !
! D41	D(11,6,7,21)	-73.6123	-DE/DX =	0.0 !
! D42	D(6,7,21,22)	165.847	-DE/DX =	0.0 !
! D43	D(6,7,21,23)	-76.1221	-DE/DX =	0.0 !
! D44	D(12,7,21,22)	46.4281	-DE/DX =	0.0 !
! D45	D(12,7,21,23)	164.4589	-DE/DX =	0.0 !
! D46	D(13,7,21,22)	-74.7733	-DE/DX =	0.0 !
! D47	D(13,7,21,23)	43.2575	-DE/DX =	0.0 !
! D48	D(3,16,17,19)	-179.7926	-DE/DX =	0.0 !
! D49	D(3,16,17,20)	0.2445	-DE/DX =	0.0 !
! D50	D(18,16,17,19)	0.1454	-DE/DX =	0.0 !
! D51	D(18,16,17,20)	-179.8175	-DE/DX =	0.0 !

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.819413	-1.993954	0.297724
2	6	0	-2.825356	-1.109809	0.073739
3	7	0	-2.241659	0.151977	0.016244
4	6	0	-0.913078	0.022466	0.203501
5	7	0	-0.641738	-1.270246	0.379410
6	6	0	0.729046	-1.797402	0.555980
7	6	0	1.448722	-1.995731	-0.786421
8	1	0	-1.841580	-3.064194	0.410650
9	1	0	-3.881576	-1.269227	-0.043450
10	1	0	1.275446	-1.055181	1.138535
11	1	0	0.660209	-2.726739	1.121685
12	1	0	1.073380	-2.894511	-1.286528
13	1	0	1.230720	-1.127799	-1.422626
14	35	0	1.956418	1.590502	0.096156
15	1	0	-0.126231	0.806800	0.188142
16	6	0	-2.865090	1.411473	-0.196320
17	6	0	-4.170626	1.594836	-0.344122
18	1	0	-2.147052	2.221264	-0.226351
19	1	0	-4.547169	2.595414	-0.505026
20	1	0	-4.896054	0.791874	-0.312729
21	7	0	2.868168	-2.162343	-0.495562

22	1	0	3.363526	-2.524061	-1.302501
23	1	0	3.266509	-1.250489	-0.274845

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357867	0.000000			
3	N	2.205117	1.391442	0.000000		
4	C	2.212751	2.226138	1.347949	0.000000	
5	N	1.384682	2.210738	2.171256	1.332544	0.000000
6	C	2.569041	3.652276	3.593951	2.476435	1.479229
7	C	3.443266	4.448874	4.344633	3.260546	2.501102
8	H	1.076410	2.213808	3.264870	3.229937	2.158436
9	H	2.212272	1.074592	2.170878	3.246758	3.267317
10	H	3.341618	4.237140	3.884173	2.612518	2.073191
11	H	2.713745	3.982690	4.234364	3.297942	2.089835
12	H	3.418934	4.498404	4.686981	3.830790	2.890539
13	H	3.607373	4.323330	3.970590	2.926306	2.602638
14	Br	5.210168	5.491588	4.438422	3.271738	3.874858
15	H	3.274614	3.312363	2.221121	1.111100	2.148593
16	C	3.596450	2.536015	1.421331	2.428899	3.530776
17	C	4.338154	3.049502	2.435697	3.658396	4.602743
18	H	4.260289	3.412652	2.085606	2.557768	3.850138
19	H	5.398829	4.126534	3.399630	4.508735	5.565783
20	H	4.195141	2.837877	2.750183	4.089325	4.778138
21	N	4.757213	5.817916	5.632793	4.422657	3.725702
22	H	5.450192	6.495876	6.349674	5.200210	4.521395
23	H	5.171767	6.103451	5.691358	4.395244	3.962680

		6	7	8	9	10
6	C	0.000000				
7	C	1.536004	0.000000			
8	H	2.869495	3.660694	0.000000		
9	H	4.679330	5.430644	2.754941	0.000000	
10	H	1.090328	2.149446	3.779128	5.295072	0.000000
11	H	1.090151	2.190204	2.622669	4.910162	1.781266
12	H	2.171878	1.094895	3.377306	5.360819	3.050393
13	H	2.148238	1.097993	4.068114	5.296952	2.562581
14	Br	3.632598	3.727971	6.015803	6.502285	2.924023
15	H	2.765623	3.359231	4.239873	4.297224	2.516926
16	C	4.876541	5.528674	4.631154	2.871021	5.001026
17	C	6.026961	6.683179	5.263145	2.894271	6.235429
18	H	5.003365	5.570127	5.332462	3.901993	4.930669
19	H	6.947014	7.557017	6.339545	3.948609	7.066186
20	H	6.253060	6.946316	4.972157	2.312966	6.603423

21	N	2.411383	1.458488	4.880193	6.823570	2.536305
22	H	3.304916	2.052302	5.506338	7.459981	3.532187
23	H	2.725454	2.030134	5.463698	7.151854	2.449514

		11	12	13	14	15
11	H	0.000000				
12	H	2.449153	0.000000			
13	H	3.058694	1.778918	0.000000		
14	Br	4.622817	4.775658	3.197264	0.000000	
15	H	3.738434	4.160940	2.859819	2.227123	0.000000
16	C	5.593717	5.936464	4.972664	4.833687	2.831040
17	C	6.645417	6.967207	6.144140	6.142844	4.154689
18	H	5.846422	6.137289	4.904757	4.164173	2.501246
19	H	7.621567	7.895606	6.934573	6.608170	4.819161
20	H	6.731288	7.083210	6.515702	6.910960	4.796072
21	N	2.794480	2.093553	2.147316	3.907078	4.271965
22	H	3.636713	2.319969	2.552027	4.567912	5.049263
23	H	3.304907	2.921665	2.340276	3.150430	3.994681

		16	17	18	19	20
16	C	0.000000				
17	C	1.326609	0.000000			
18	H	1.082701	2.121588	0.000000		
19	H	2.080001	1.081125	2.445037	0.000000	
20	H	2.126562	1.082579	3.099617	1.847012	0.000000
21	N	6.762541	7.980223	6.666402	8.810424	8.309270
22	H	7.450351	8.639864	7.351373	9.456431	8.955207
23	H	6.684962	7.963143	6.431334	8.711918	8.414280

		21	22	23
21	N	0.000000		
22	H	1.013592	0.000000	
23	H	1.019249	1.639352	0.000000

Stoichiometry C7H12BrN3
Framework group C1[X(C7H12BrN3)]
Deg. of freedom 63
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.741941	2.053002	-0.328825
2	6	0	-2.777122	1.211267	-0.076462
3	7	0	-2.239546	-0.069815	0.000692

4	6	0	-0.909265	0.006770	-0.202911
5	7	0	-0.592612	1.284803	-0.407932
6	6	0	0.794560	1.757336	-0.609394
7	6	0	1.535886	1.955741	0.721163
8	1	0	-1.726048	3.120860	-0.463305
9	1	0	-3.825410	1.411897	0.048384
10	1	0	1.306840	0.983946	-1.182326
11	1	0	0.753618	2.677089	-1.193180
12	1	0	1.199371	2.877586	1.206706
13	1	0	1.293236	1.109342	1.377148
14	35	0	1.901736	-1.663720	-0.093346
15	1	0	-0.151626	-0.805627	-0.179718
16	6	0	-2.906404	-1.300926	0.245327
17	6	0	-4.216073	-1.432954	0.410345
18	1	0	-2.218295	-2.135922	0.284420
19	1	0	-4.627291	-2.415526	0.595499
20	1	0	-4.911832	-0.604535	0.370106
21	7	0	2.957177	2.063966	0.412286
22	1	0	3.474407	2.423198	1.206513
23	1	0	3.319294	1.133793	0.206088

Rotational constants (GHZ): 0.8918921 0.4585798 0.3138477

****

Population analysis using the SCF density.

****

Orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A)

The electronic state is 1-A.

Alpha occ. eigenvalues -- -482.69288 -62.34625 -56.16406 -56.16393 -56.16389
Alpha occ. eigenvalues -- -14.45414 -14.44036 -14.29508 -10.29534 -10.27329
Alpha occ. eigenvalues -- -10.27258 -10.27137 -10.23824 -10.22253 -10.21047
Alpha occ. eigenvalues -- -8.55532 -6.37859 -6.37799 -6.37789 -2.49098
Alpha occ. eigenvalues -- -2.49081 -2.49072 -2.49025 -2.49023 -1.11660
Alpha occ. eigenvalues -- -1.00233 -0.89365 -0.85310 -0.82543 -0.77403
Alpha occ. eigenvalues -- -0.71439 -0.67954 -0.65113 -0.63181 -0.62846
Alpha occ. eigenvalues -- -0.58582 -0.54324 -0.53272 -0.52228 -0.50751
Alpha occ. eigenvalues -- -0.50149 -0.49286 -0.48463 -0.45096 -0.43935
Alpha occ. eigenvalues -- -0.43518 -0.42839 -0.38634 -0.37114 -0.31616
Alpha occ. eigenvalues -- -0.30436 -0.24984 -0.19661 -0.19278 -0.18985
Alpha virt. eigenvalues -- -0.08470 -0.04620 -0.03229 -0.01762 -0.00870
Alpha virt. eigenvalues -- -0.00663 0.00260 0.00805 0.01235 0.01606
Alpha virt. eigenvalues -- 0.03444 0.03790 0.04625 0.04949 0.05387
Alpha virt. eigenvalues -- 0.05880 0.06472 0.07204 0.07620 0.07783
Alpha virt. eigenvalues -- 0.08384 0.08679 0.08758 0.09399 0.09626
Alpha virt. eigenvalues -- 0.10341 0.10762 0.11004 0.11310 0.11926
Alpha virt. eigenvalues -- 0.12268 0.12565 0.12938 0.13412 0.13627
Alpha virt. eigenvalues -- 0.13920 0.14308 0.14615 0.15585 0.15674
Alpha virt. eigenvalues -- 0.16098 0.16205 0.16374 0.17289 0.18021
Alpha virt. eigenvalues -- 0.18340 0.18788 0.18980 0.19736 0.20480
Alpha virt. eigenvalues -- 0.20838 0.21005 0.21548 0.21893 0.22514
Alpha virt. eigenvalues -- 0.22812 0.23576 0.24257 0.24529 0.25029
Alpha virt. eigenvalues -- 0.25662 0.26071 0.26736 0.27573 0.27813
Alpha virt. eigenvalues -- 0.28306 0.29488 0.30283 0.30671 0.30906
Alpha virt. eigenvalues -- 0.32447 0.33733 0.33798 0.34349 0.35173
Alpha virt. eigenvalues -- 0.36326 0.36704 0.39020 0.39780 0.41248

Alpha virt. eigenvalues --	0.43005	0.46329	0.46845	0.49029	0.49826
Alpha virt. eigenvalues --	0.50947	0.51569	0.52710	0.53156	0.53869
Alpha virt. eigenvalues --	0.54456	0.54904	0.55875	0.57590	0.57819
Alpha virt. eigenvalues --	0.59707	0.60622	0.61303	0.61973	0.63209
Alpha virt. eigenvalues --	0.64160	0.64640	0.65911	0.66414	0.68261
Alpha virt. eigenvalues --	0.68608	0.68899	0.70027	0.70592	0.71976
Alpha virt. eigenvalues --	0.72502	0.73918	0.74949	0.75291	0.75611
Alpha virt. eigenvalues --	0.76634	0.78247	0.79092	0.79468	0.80579
Alpha virt. eigenvalues --	0.80815	0.82630	0.84428	0.84923	0.86422
Alpha virt. eigenvalues --	0.87646	0.88622	0.90199	0.90607	0.92188
Alpha virt. eigenvalues --	0.94367	0.95911	0.96969	0.99456	1.00477
Alpha virt. eigenvalues --	1.01071	1.02826	1.03731	1.05306	1.07329
Alpha virt. eigenvalues --	1.09501	1.10546	1.11774	1.13186	1.15108
Alpha virt. eigenvalues --	1.20180	1.23965	1.27183	1.28425	1.31137
Alpha virt. eigenvalues --	1.32678	1.38448	1.40859	1.42933	1.44626
Alpha virt. eigenvalues --	1.46824	1.48737	1.49016	1.50424	1.52782
Alpha virt. eigenvalues --	1.54564	1.56131	1.57908	1.58658	1.59422
Alpha virt. eigenvalues --	1.59874	1.61904	1.64813	1.66646	1.67674
Alpha virt. eigenvalues --	1.68678	1.69708	1.70376	1.71779	1.72436
Alpha virt. eigenvalues --	1.73148	1.73470	1.76715	1.77396	1.79417
Alpha virt. eigenvalues --	1.81293	1.83583	1.84225	1.87608	1.89652
Alpha virt. eigenvalues --	1.90331	1.94352	1.97916	1.98903	2.01535
Alpha virt. eigenvalues --	2.03651	2.05291	2.07911	2.08433	2.08835
Alpha virt. eigenvalues --	2.10434	2.12066	2.13140	2.15341	2.15669
Alpha virt. eigenvalues --	2.18037	2.20546	2.22828	2.26130	2.28556
Alpha virt. eigenvalues --	2.31368	2.36301	2.39346	2.42286	2.42457
Alpha virt. eigenvalues --	2.44547	2.46423	2.46831	2.50937	2.51700
Alpha virt. eigenvalues --	2.53564	2.55550	2.56751	2.57966	2.60381
Alpha virt. eigenvalues --	2.61282	2.62648	2.64293	2.65636	2.68798
Alpha virt. eigenvalues --	2.69548	2.70936	2.71960	2.72491	2.75138
Alpha virt. eigenvalues --	2.75620	2.77595	2.79506	2.80891	2.82384
Alpha virt. eigenvalues --	2.82703	2.85931	2.87380	2.87937	2.90668
Alpha virt. eigenvalues --	2.92374	2.94053	2.96249	3.01518	3.08920
Alpha virt. eigenvalues --	3.14994	3.16374	3.21470	3.25952	3.37272
Alpha virt. eigenvalues --	3.49135	3.52285	3.54410	3.59108	3.63508
Alpha virt. eigenvalues --	3.64611	3.71719	3.75793	3.78765	3.81677
Alpha virt. eigenvalues --	3.82979	3.85876	3.87535	4.05180	4.07465
Alpha virt. eigenvalues --	4.08526	4.25910	4.26929	4.28708	4.30029
Alpha virt. eigenvalues --	4.34578	4.43196	4.68870	4.74227	4.83903
Alpha virt. eigenvalues --	4.92507	5.02254	5.22445	6.77222	7.68510
Alpha virt. eigenvalues --	7.72883	7.75506	23.69349	23.74236	23.84020
Alpha virt. eigenvalues --	23.87340	23.88657	24.13334	24.22097	35.43781
Alpha virt. eigenvalues --	35.56715	35.60716	48.05845	289.89287	289.93540
Alpha virt. eigenvalues --	289.957571	020.84698			

Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	8.104870	-2.390873	0.626770	-0.547320	-0.573751	0.644942
2	C	-2.390873	8.067432	-0.453285	0.533346	0.862983	-0.763244
3	N	0.626770	-0.453285	6.897964	-0.086320	-0.487830	0.114147
4	C	-0.547320	0.533346	-0.086320	7.076055	0.742281	-0.509416
5	N	-0.573751	0.862983	-0.487830	0.742281	7.035008	-0.200550
6	C	0.644942	-0.763244	0.114147	-0.509416	-0.200550	7.117414
7	C	-0.343551	0.421625	-0.115016	0.100909	0.215042	-0.688437
8	H	0.490608	-0.111734	0.033909	0.024595	-0.071962	-0.011741
9	H	-0.146137	0.547835	-0.085204	0.004741	0.034335	-0.004343
10	H	0.014485	-0.027083	0.015996	0.034342	-0.050964	0.401470
11	H	-0.048083	0.060814	0.008220	-0.020909	-0.063423	0.341878
12	H	0.097773	-0.111973	0.020650	-0.039656	-0.050610	0.189137
13	H	-0.125084	0.116232	-0.037284	0.021951	0.054053	-0.214791
14	Br	-0.017388	0.005264	0.006579	-0.168115	-0.032290	0.050127
15	H	0.151561	-0.307370	0.127767	-0.669558	-0.222901	0.174182
16	C	0.448250	-0.491381	0.311041	-0.357501	-0.188061	-0.035052
17	C	-0.187143	0.094943	-0.018890	-0.232259	-0.064414	-0.060426
18	H	-0.032742	0.052156	-0.093120	0.143143	0.029090	-0.010357
19	H	-0.000705	0.001849	0.022780	-0.009705	-0.000838	0.000662
20	H	-0.007909	0.012709	-0.035286	0.011767	0.002323	-0.002460
21	N	-0.002897	-0.002573	0.003463	0.048785	-0.002384	-0.216930
22	H	0.002262	0.000191	0.000246	0.001317	0.001612	0.012528
23	H	-0.001771	0.001502	0.000790	0.008484	-0.001686	-0.009935

		7	8	9	10	11	12
1	C	-0.343551	0.490608	-0.146137	0.014485	-0.048083	0.097773
2	C	0.421625	-0.111734	0.547835	-0.027083	0.060814	-0.111973
3	N	-0.115016	0.033909	-0.085204	0.015996	0.008220	0.020650
4	C	0.100909	0.024595	0.004741	0.034342	-0.020909	-0.039656
5	N	0.215042	-0.071962	0.034335	-0.050964	-0.063423	-0.050610
6	C	-0.688437	-0.011741	-0.004343	0.401470	0.341878	0.189137
7	C	6.274456	-0.000610	0.005108	-0.079314	-0.089879	0.243004
8	H	-0.000610	0.488154	-0.011776	0.002407	-0.019539	0.000100
9	H	0.005108	-0.011776	0.502221	-0.000446	0.003794	-0.000672
10	H	-0.079314	0.002407	-0.000446	0.469681	-0.047881	0.006995
11	H	-0.089879	-0.019539	0.003794	-0.047881	0.686594	-0.012938
12	H	0.243004	0.000100	-0.000672	0.006995	-0.012938	0.688329
13	H	0.520820	-0.002869	0.000935	-0.024493	0.028684	-0.112173
14	Br	-0.011431	-0.001157	-0.000697	-0.010014	0.018757	0.008195
15	H	-0.197733	-0.002281	-0.007962	-0.003213	0.013304	0.030695
16	C	-0.043267	0.003999	0.000130	0.012805	0.002712	0.003306
17	C	-0.009645	0.000775	-0.011275	-0.000608	-0.001476	-0.001585
18	H	0.008140	0.000253	0.002202	0.000550	-0.002072	-0.001334

19	H	-0.000283	-0.000185	-0.000636	-0.000068	0.000173	0.000049
20	H	0.000137	0.000631	0.004980	0.000130	-0.000419	-0.000185
21	N	0.232747	0.000518	-0.000282	0.007173	0.014791	-0.077911
22	H	-0.048356	0.000106	0.000030	-0.001950	-0.002688	-0.013505
23	H	-0.048600	-0.000095	0.000047	0.009217	0.007439	0.006433
		13	14	15	16	17	18
1	C	-0.125084	-0.017388	0.151561	0.448250	-0.187143	-0.032742
2	C	0.116232	0.005264	-0.307370	-0.491381	0.094943	0.052156
3	N	-0.037284	0.006579	0.127767	0.311041	-0.018890	-0.093120
4	C	0.021951	-0.168115	-0.669558	-0.357501	-0.232259	0.143143
5	N	0.054053	-0.032290	-0.222901	-0.188061	-0.064414	0.029090
6	C	-0.214791	0.050127	0.174182	-0.035052	-0.060426	-0.010357
7	C	0.520820	-0.011431	-0.197733	-0.043267	-0.009645	0.008140
8	H	-0.002869	-0.001157	-0.002281	0.003999	0.000775	0.000253
9	H	0.000935	-0.000697	-0.007962	0.000130	-0.011275	0.002202
10	H	-0.024493	-0.010014	-0.003213	0.012805	-0.000608	0.000550
11	H	0.028684	0.018757	0.013304	0.002712	-0.001476	-0.002072
12	H	-0.112173	0.008195	0.030695	0.003306	-0.001585	-0.001334
13	H	0.694204	-0.024830	-0.044409	-0.015444	0.005318	0.001450
14	Br	-0.024830	35.558632	0.269243	0.025255	0.031133	-0.004791
15	H	-0.044409	0.269243	1.542182	0.046049	0.138408	-0.081965
16	C	-0.015444	0.025255	0.046049	6.095783	-0.250365	0.409504
17	C	0.005318	0.031133	0.138408	-0.250365	6.332283	-0.100461
18	H	0.001450	-0.004791	-0.081965	0.409504	-0.100461	0.468427
19	H	0.000010	-0.000369	0.005859	-0.091182	0.449236	-0.010238
20	H	0.000141	0.000425	0.001560	0.070715	0.299947	0.004254
21	N	-0.060162	-0.045244	-0.015999	0.006180	0.000557	0.000668
22	H	-0.000573	-0.000482	-0.002183	0.000107	-0.000086	0.000086
23	H	-0.000013	0.020404	-0.012514	0.000258	-0.000139	0.000058
		19	20	21	22	23	
1	C	-0.000705	-0.007909	-0.002897	0.002262	-0.001771	
2	C	0.001849	0.012709	-0.002573	0.000191	0.001502	
3	N	0.022780	-0.035286	0.003463	0.000246	0.000790	
4	C	-0.009705	0.011767	0.048785	0.001317	0.008484	
5	N	-0.000838	0.002323	-0.002384	0.001612	-0.001686	
6	C	0.000662	-0.002460	-0.216930	0.012528	-0.009935	
7	C	-0.000283	0.000137	0.232747	-0.048356	-0.048600	
8	H	-0.000185	0.000631	0.000518	0.000106	-0.000095	
9	H	-0.000636	0.004980	-0.000282	0.000030	0.000047	
10	H	-0.000068	0.000130	0.007173	-0.001950	0.009217	
11	H	0.000173	-0.000419	0.014791	-0.002688	0.007439	
12	H	0.000049	-0.000185	-0.077911	-0.013505	0.006433	
13	H	0.000010	0.000141	-0.060162	-0.000573	-0.000013	
14	Br	-0.000369	0.000425	-0.045244	-0.000482	0.020404	

15	H	0.005859	0.001560	-0.015999	-0.002183	-0.012514
16	C	-0.091182	0.070715	0.006180	0.000107	0.000258
17	C	0.449236	0.299947	0.000557	-0.000086	-0.000139
18	H	-0.010238	0.004254	0.000668	0.000086	0.000058
19	H	0.464642	-0.021790	-0.000021	-0.000002	0.000003
20	H	-0.021790	0.533022	0.000048	0.000000	-0.000004
21	N	-0.000021	0.000048	6.645828	0.386886	0.396937
22	H	-0.000002	0.000000	0.386886	0.474870	-0.047249
23	H	0.000003	-0.000004	0.396937	-0.047249	0.428406

Mulliken charges:

		1
1	C	-0.156167
2	C	-0.119363
3	N	0.221912
4	C	-0.110958
5	N	0.034934
6	C	-0.318805
7	C	-0.345869
8	H	0.187893
9	H	0.163072
10	H	0.270784
11	H	0.122150
12	H	0.127877
13	H	0.218326
14	Br	-0.677207
15	H	0.067279
16	C	0.036160
17	C	-0.413828
18	H	0.217099
19	H	0.190761
20	H	0.125265
21	N	-0.320177
22	H	0.236833
23	H	0.242028

Sum of Mulliken charges = 0.00000

Mulliken charges with hydrogens summed into heavy atoms:

		1
1	C	0.031726
2	C	0.043709
3	N	0.221912
4	C	-0.043679
5	N	0.034934
6	C	0.074129
7	C	0.000334

14 Br -0.677207
16 C 0.253260
17 C -0.097802
21 N 0.158684
Electronic spatial extent (au): <R**2>= 3282.9008
Charge= 0.0000 electrons
Dipole moment (field-independent basis, Debye):
X= -10.8568 Y= 6.8535 Z= 0.9335
Tot= 12.8730
Quadrupole moment (field-independent basis, Debye-Ang):
XX= -72.4820 YY= -81.9221 ZZ= -83.6860
XY= 10.1606 XZ= 3.0924 YZ= -0.0670
Traceless Quadrupole moment (field-independent basis, Debye-Ang):
XX= 6.8814 YY= -2.5588 ZZ= -4.3226
XY= 10.1606 XZ= 3.0924 YZ= -0.0670
Octapole moment (field-independent basis, Debye-Ang**2):
XXX= -47.9482 YYY= -7.8376 ZZZ= -1.5191
XYY= -36.5917
XXY= 1.1842 XXZ= 23.0414 XZZ= 26.8731
YZZ= -4.6168
YYZ= 6.4699 XYZ= 14.3554
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX= -2304.2815 YYYY= -1301.1644 ZZZZ= -194.9067
XXXY= -11.2140
XXXZ= 16.9993 YYYX= -56.1907 YYYZ= 2.1255
ZZZX= 10.6970
ZZZY= 10.8328 XXYY= -661.0236 XXZZ= -498.6175
YYZZ= -253.5802
XXYZ= 22.2977 YYXZ= 25.3496 ZZXY= -7.8833
N-N= 8.431050180292D+02 E-N=-8.859190974210D+03 KE= 3.007463276976D+03
1\1\GINC-NODE12\FOpt\RB3LYP\6-311++G(d,p)\C7H12Br1N3\SUQIAN\20-Jul-202
4\0\\# opt b3lyp/6-311++g(d,p)\\oh\\0,1\C,-1.8194127754,-1.9939540463,
0.2977240836\C,-2.8253560048,-1.1098088699,0.0737390223\N,-2.241658869
5,0.1519766127,0.0162441466\C,-0.9130778391,0.0224655164,0.2035005146\
N,-0.64173791,-1.2702462573,0.379409687\C,0.7290464499,-1.79740169,0.5
559803443\C,1.4487220977,-1.9957313229,-0.7864211071\H,-1.8415798554,-
3.0641943909,0.4106497129\H,-3.8815759697,-1.2692267394,-0.04345049\H,
1.2754464604,-1.0551806835,1.138535278\H,0.6602090227,-2.7267390285,1.
121685224\H,1.0733803148,-2.8945114095,-1.2865280125\H,1.2307199425,-1
.1277992297,-1.4226259507\Br,1.9564180091,1.5905016501,0.0961560181\H,
-0.1262311996,0.8067997092,0.1881421968\C,-2.8650900021,1.4114729542,-
0.1963203874\C,-4.1706264741,1.5948357098,-0.3441222162\H,-2.147052310
2,2.2212637198,-0.226351132\H,-4.5471691084,2.5954135631,-0.5050257152
\H,-4.8960537266,0.7918738252,-0.3127294357\N,2.8681684367,-2.16234265

56,-0.4955619347\H,3.3635261162,-2.5240612417,-1.3025006948\H,3.266508
685,-1.2504892053,-0.2748446619\\Version=EM64L-G09RevD.01\State=1-A\HF
=-3012.4680597\RMSD=5.014e-09\RMSF=1.376e-05\Dipole=-4.3716519,-2.5296
895,-0.3736571\Quadrupole=4.5004534,-1.3406218,-3.1598316,-7.741675,-2
.5375706,0.1530448\PG=C01 [X(C7H12Br1N3)]\\@

THE RED LIGHT IS ALWAYS LONGER THAN THE GREEN LIGHT.

-- PETER'S THEORY OF RELATIVITY

Job cpu time: 0 days 10 hours 59 minutes 32.8 seconds.
File lengths (MBytes): RWF= 75 Int= 0 D2E= 0 Chk= 10 Scr= 1
Normal termination of Gaussian 09 at Sat Jul 20 21:30:23 2024.

Entering Gaussian System, Link 0=/opt/gaussian/g09/g09
Initial command:
/opt/gaussian/g09/l1.exe "/tmp/Gau-6630.inp" -scrdir="/tmp/"
Entering Link 1 = /opt/gaussian/g09/l1.exe PID= 6631.

Cite this work as:
Gaussian 09, Revision D.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci,
G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian,
A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada,
M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima,
Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr.,
J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers,
K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand,
K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi,
M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross,
V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,
O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,
R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth,
P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels,
O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski,
and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

```
*****************************************
Gaussian 09:    EM64L-G09RevD.01 24-Apr-2013
                22-Jul-2024
*****************************************
%chk=/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk
%mem=40000MB
%nprocl=1
Will use up to        1 processors via Linda.
%nprocs=8
Will use up to        8 processors via shared memory.
-------------------------
# opt b3lyp/6-311++g(d,p)
-------------------------
1/14=-1,18=20,19=15,26=3,38=1/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=4,6=6,7=1111,11=2,16=1,25=1,30=1,71=1,74=-5/1,2,3;
4//1;
5/5=2,38=5/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(2);
2/9=110/2;
99//99;
2/9=110/2;
3/5=4,6=6,7=1111,11=2,16=1,25=1,30=1,71=1,74=-5/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;
--
oh
--
Symbolic Z-matrix:
Charge =    0 Multiplicity = 1
C                            -1.85298    -2.00477     0.26195
C                            -2.84494    -1.10868     0.02227
N                             -2.2526      0.1497      0.01266
C                            -0.93264     0.00637     0.24353
N                            -0.67446    -1.292       0.4013
C                             0.68899    -1.82956     0.59657
C                             1.47835    -1.92564    -0.73551
```

H	-1.88574	-3.07712	0.34901
H	-3.89688	-1.25872	-0.13791
H	1.21191	-1.1335	1.25067
H	0.59178	-2.79327	1.09741
H	1.34487	-2.9108	-1.19079
H	1.08962	-1.16668	-1.42475
Br	2.0255	1.47738	0.09935
H	-0.1445	0.78154	0.25732
C	-2.86233	1.41676	-0.19872
C	-4.16281	1.61048	-0.37392
H	-2.13902	2.2222	-0.2043
H	-4.52894	2.61515	-0.53341
H	-4.89412	0.81234	-0.36723
O	2.85001	-1.74993	-0.50409
H	2.97789	-0.79367	-0.33511
C	5.02891	2.32267	-0.02622
C	5.70243	1.28787	-0.80621
O	4.27439	1.23764	-0.6477
H	5.0356	2.30003	1.07929
H	4.82935	3.32222	-0.45494
H	6.02983	1.47781	-1.84517
C	6.44565	0.12879	-0.11645
H	6.37202	-0.75156	-0.72016
H	7.47564	0.39006	0.00909
H	6.00568	-0.05746	0.84096

Add virtual bond connecting atoms H15 and Br14 Dist= 4.32D+00.
Add virtual bond connecting atoms O25 and Br14 Dist= 4.50D+00.
Add virtual bond connecting atoms O25 and H22 Dist= 4.59D+00.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.

! Initial Parameters !
! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.	!
! R1	R(1,2)	1.3581	estimate D2E/DX2	!
! R2	R(1,5)	1.3843	estimate D2E/DX2	!
! R3	R(1,8)	1.0764	estimate D2E/DX2	!
! R4	R(2,3)	1.3909	estimate D2E/DX2	!
! R5	R(2,9)	1.0746	estimate D2E/DX2	!

! R6	R(3,4)	1.3476	estimate D2E/DX2	!
! R7	R(3,16)	1.4219	estimate D2E/DX2	!
! R8	R(4,5)	1.3332	estimate D2E/DX2	!
! R9	R(4,15)	1.1056	estimate D2E/DX2	!
! R10	R(5,6)	1.4785	estimate D2E/DX2	!
! R11	R(6,7)	1.5514	estimate D2E/DX2	!
! R12	R(6,10)	1.0889	estimate D2E/DX2	!
! R13	R(6,11)	1.0904	estimate D2E/DX2	!
! R14	R(7,12)	1.0935	estimate D2E/DX2	!
! R15	R(7,13)	1.0964	estimate D2E/DX2	!
! R16	R(7,21)	1.4021	estimate D2E/DX2	!
! R17	R(14,15)	2.2843	estimate D2E/DX2	!
! R18	R(14,25)	2.3818	estimate D2E/DX2	!
! R19	R(16,17)	1.3265	estimate D2E/DX2	!
! R20	R(16,18)	1.0826	estimate D2E/DX2	!
! R21	R(17,19)	1.0811	estimate D2E/DX2	!
! R22	R(17,20)	1.0825	estimate D2E/DX2	!
! R23	R(21,22)	0.9795	estimate D2E/DX2	!
! R24	R(22,25)	2.43	estimate D2E/DX2	!
! R25	R(23,24)	1.4604	estimate D2E/DX2	!
! R26	R(23,25)	1.4604	estimate D2E/DX2	!
! R27	R(23,26)	1.1058	estimate D2E/DX2	!
! R28	R(23,27)	1.1058	estimate D2E/DX2	!
! R29	R(24,25)	1.4377	estimate D2E/DX2	!
! R30	R(24,28)	1.1058	estimate D2E/DX2	!
! R31	R(24,29)	1.54	estimate D2E/DX2	!
! R32	R(29,30)	1.07	estimate D2E/DX2	!
! R33	R(29,31)	1.07	estimate D2E/DX2	!
! R34	R(29,32)	1.07	estimate D2E/DX2	!
! A1	A(2,1,5)	107.4487	estimate D2E/DX2	!
! A2	A(2,1,8)	130.4957	estimate D2E/DX2	!
! A3	A(5,1,8)	122.0547	estimate D2E/DX2	!
! A4	A(1,2,3)	106.6857	estimate D2E/DX2	!
! A5	A(1,2,9)	130.4812	estimate D2E/DX2	!
! A6	A(3,2,9)	122.8331	estimate D2E/DX2	!
! A7	A(2,3,4)	108.6462	estimate D2E/DX2	!
! A8	A(2,3,16)	128.6538	estimate D2E/DX2	!
! A9	A(4,3,16)	122.6999	estimate D2E/DX2	!
! A10	A(3,4,5)	108.2726	estimate D2E/DX2	!
! A11	A(3,4,15)	128.7417	estimate D2E/DX2	!
! A12	A(5,4,15)	122.9107	estimate D2E/DX2	!
! A13	A(1,5,4)	108.9455	estimate D2E/DX2	!
! A14	A(1,5,6)	127.6728	estimate D2E/DX2	!
! A15	A(4,5,6)	123.2506	estimate D2E/DX2	!

! A16	A(5,6,7)	112.2301	estimate D2E/DX2	!
! A17	A(5,6,10)	106.8437	estimate D2E/DX2	!
! A18	A(5,6,11)	107.4442	estimate D2E/DX2	!
! A19	A(7,6,10)	108.1204	estimate D2E/DX2	!
! A20	A(7,6,11)	112.6443	estimate D2E/DX2	!
! A21	A(10,6,11)	109.3802	estimate D2E/DX2	!
! A22	A(6,7,12)	110.5609	estimate D2E/DX2	!
! A23	A(6,7,13)	108.4511	estimate D2E/DX2	!
! A24	A(6,7,21)	110.3829	estimate D2E/DX2	!
! A25	A(12,7,13)	108.5799	estimate D2E/DX2	!
! A26	A(12,7,21)	107.5209	estimate D2E/DX2	!
! A27	A(13,7,21)	111.3365	estimate D2E/DX2	!
! A28	A(15,14,25)	152.6194	estimate D2E/DX2	!
! A29	A(4,15,14)	152.8661	estimate D2E/DX2	!
! A30	A(3,16,17)	124.7632	estimate D2E/DX2	!
! A31	A(3,16,18)	112.1624	estimate D2E/DX2	!
! A32	A(17,16,18)	123.0742	estimate D2E/DX2	!
! A33	A(16,17,19)	119.1583	estimate D2E/DX2	!
! A34	A(16,17,20)	123.6301	estimate D2E/DX2	!
! A35	A(19,17,20)	117.2116	estimate D2E/DX2	!
! A36	A(7,21,22)	106.174	estimate D2E/DX2	!
! A37	A(21,22,25)	149.7232	estimate D2E/DX2	!
! A38	A(24,23,26)	121.1085	estimate D2E/DX2	!
! A39	A(24,23,27)	121.1085	estimate D2E/DX2	!
! A40	A(25,23,26)	114.4165	estimate D2E/DX2	!
! A41	A(25,23,27)	114.4165	estimate D2E/DX2	!
! A42	A(26,23,27)	114.0306	estimate D2E/DX2	!
! A43	A(23,24,28)	121.1085	estimate D2E/DX2	!
! A44	A(23,24,29)	121.1085	estimate D2E/DX2	!
! A45	A(25,24,28)	113.8091	estimate D2E/DX2	!
! A46	A(25,24,29)	113.8091	estimate D2E/DX2	!
! A47	A(28,24,29)	114.0306	estimate D2E/DX2	!
! A48	A(14,25,22)	62.6147	estimate D2E/DX2	!
! A49	A(14,25,23)	106.2333	estimate D2E/DX2	!
! A50	A(22,25,23)	147.349	estimate D2E/DX2	!
! A51	A(22,25,24)	124.9845	estimate D2E/DX2	!
! A52	A(24,29,30)	109.4712	estimate D2E/DX2	!
! A53	A(24,29,31)	109.4712	estimate D2E/DX2	!
! A54	A(24,29,32)	109.4712	estimate D2E/DX2	!
! A55	A(30,29,31)	109.4713	estimate D2E/DX2	!
! A56	A(30,29,32)	109.4712	estimate D2E/DX2	!
! A57	A(31,29,32)	109.4712	estimate D2E/DX2	!
! A58	L(14,25,24,22,-1)	187.5992	estimate D2E/DX2	!
! A59	L(14,25,24,22,-2)	194.2234	estimate D2E/DX2	!

! D1	D(5,1,2,3)	0.2541	estimate D2E/DX2	!
! D2	D(5,1,2,9)	-179.7257	estimate D2E/DX2	!
! D3	D(8,1,2,3)	179.9213	estimate D2E/DX2	!
! D4	D(8,1,2,9)	-0.0585	estimate D2E/DX2	!
! D5	D(2,1,5,4)	-0.3687	estimate D2E/DX2	!
! D6	D(2,1,5,6)	-176.2729	estimate D2E/DX2	!
! D7	D(8,1,5,4)	179.9299	estimate D2E/DX2	!
! D8	D(8,1,5,6)	4.0256	estimate D2E/DX2	!
! D9	D(1,2,3,4)	-0.0562	estimate D2E/DX2	!
! D10	D(1,2,3,16)	179.8446	estimate D2E/DX2	!
! D11	D(9,2,3,4)	179.9255	estimate D2E/DX2	!
! D12	D(9,2,3,16)	-0.1737	estimate D2E/DX2	!
! D13	D(2,3,4,5)	-0.1729	estimate D2E/DX2	!
! D14	D(2,3,4,15)	176.707	estimate D2E/DX2	!
! D15	D(16,3,4,5)	179.9192	estimate D2E/DX2	!
! D16	D(16,3,4,15)	-3.2009	estimate D2E/DX2	!
! D17	D(2,3,16,17)	3.0504	estimate D2E/DX2	!
! D18	D(2,3,16,18)	-176.7973	estimate D2E/DX2	!
! D19	D(4,3,16,17)	-177.0614	estimate D2E/DX2	!
! D20	D(4,3,16,18)	3.0909	estimate D2E/DX2	!
! D21	D(3,4,5,1)	0.3336	estimate D2E/DX2	!
! D22	D(3,4,5,6)	176.4574	estimate D2E/DX2	!
! D23	D(15,4,5,1)	-176.7678	estimate D2E/DX2	!
! D24	D(15,4,5,6)	-0.644	estimate D2E/DX2	!
! D25	D(3,4,15,14)	-157.7623	estimate D2E/DX2	!
! D26	D(5,4,15,14)	18.7081	estimate D2E/DX2	!
! D27	D(1,5,6,7)	96.5542	estimate D2E/DX2	!
! D28	D(1,5,6,10)	-145.1004	estimate D2E/DX2	!
! D29	D(1,5,6,11)	-27.8065	estimate D2E/DX2	!
! D30	D(4,5,6,7)	-78.8125	estimate D2E/DX2	!
! D31	D(4,5,6,10)	39.5329	estimate D2E/DX2	!
! D32	D(4,5,6,11)	156.8268	estimate D2E/DX2	!
! D33	D(5,6,7,12)	-91.7943	estimate D2E/DX2	!
! D34	D(5,6,7,13)	27.1459	estimate D2E/DX2	!
! D35	D(5,6,7,21)	149.3646	estimate D2E/DX2	!
! D36	D(10,6,7,12)	150.6177	estimate D2E/DX2	!
! D37	D(10,6,7,13)	-90.4421	estimate D2E/DX2	!
! D38	D(10,6,7,21)	31.7765	estimate D2E/DX2	!
! D39	D(11,6,7,12)	29.6316	estimate D2E/DX2	!
! D40	D(11,6,7,13)	148.5719	estimate D2E/DX2	!
! D41	D(11,6,7,21)	-89.2095	estimate D2E/DX2	!
! D42	D(6,7,21,22)	-74.5924	estimate D2E/DX2	!
! D43	D(12,7,21,22)	164.7311	estimate D2E/DX2	!
! D44	D(13,7,21,22)	45.9129	estimate D2E/DX2	!

! D45	D(25,14,15,4)	23.9892	estimate D2E/DX2	!
! D46	D(15,14,25,22)	-27.5846	estimate D2E/DX2	!
! D47	D(15,14,25,23)	-174.3868	estimate D2E/DX2	!
! D48	D(3,16,17,19)	-179.6544	estimate D2E/DX2	!
! D49	D(3,16,17,20)	0.3485	estimate D2E/DX2	!
! D50	D(18,16,17,19)	0.1773	estimate D2E/DX2	!
! D51	D(18,16,17,20)	-179.8198	estimate D2E/DX2	!
! D52	D(7,21,22,25)	-138.9065	estimate D2E/DX2	!
! D53	D(21,22,25,14)	162.2392	estimate D2E/DX2	!
! D54	D(21,22,25,23)	-120.7569	estimate D2E/DX2	!
! D55	D(21,22,25,24)	-31.9842	estimate D2E/DX2	!
! D56	D(26,23,24,28)	-156.8753	estimate D2E/DX2	!
! D57	D(26,23,24,29)	0.0	estimate D2E/DX2	!
! D58	D(27,23,24,28)	0.0	estimate D2E/DX2	!
! D59	D(27,23,24,29)	156.8753	estimate D2E/DX2	!
! D60	D(26,23,25,14)	61.1869	estimate D2E/DX2	!
! D61	D(26,23,25,22)	-3.1182	estimate D2E/DX2	!
! D62	D(27,23,25,14)	-73.0187	estimate D2E/DX2	!
! D63	D(27,23,25,22)	-137.3239	estimate D2E/DX2	!
! D64	D(28,24,25,22)	104.7601	estimate D2E/DX2	!
! D65	D(29,24,25,22)	-28.1776	estimate D2E/DX2	!
! D66	D(23,24,29,30)	147.4407	estimate D2E/DX2	!
! D67	D(23,24,29,31)	-92.5593	estimate D2E/DX2	!
! D68	D(23,24,29,32)	27.4407	estimate D2E/DX2	!
! D69	D(25,24,29,30)	78.6702	estimate D2E/DX2	!
! D70	D(25,24,29,31)	-161.3298	estimate D2E/DX2	!
! D71	D(25,24,29,32)	-41.3298	estimate D2E/DX2	!
! D72	D(28,24,29,30)	-54.1618	estimate D2E/DX2	!
! D73	D(28,24,29,31)	65.8383	estimate D2E/DX2	!
! D74	D(28,24,29,32)	-174.1618	estimate D2E/DX2	!

Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-06

Number of steps in this run= 177 maximum allowed number of steps= 192.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.852977	-2.004770	0.261946
2	6	0	-2.844936	-1.108684	0.022270
3	7	0	-2.252596	0.149697	0.012664
4	6	0	-0.932640	0.006366	0.243529

5	7	0	-0.674460	-1.291997	0.401298
6	6	0	0.688990	-1.829559	0.596565
7	6	0	1.478350	-1.925642	-0.735506
8	1	0	-1.885737	-3.077123	0.349012
9	1	0	-3.896876	-1.258715	-0.137907
10	1	0	1.211914	-1.133502	1.250666
11	1	0	0.591782	-2.793267	1.097412
12	1	0	1.344868	-2.910804	-1.190791
13	1	0	1.089622	-1.166684	-1.424751
14	35	0	2.025502	1.477383	0.099347
15	1	0	-0.144502	0.781540	0.257320
16	6	0	-2.862333	1.416758	-0.198718
17	6	0	-4.162812	1.610481	-0.373924
18	1	0	-2.139017	2.222199	-0.204304
19	1	0	-4.528939	2.615146	-0.533412
20	1	0	-4.894120	0.812340	-0.367232
21	8	0	2.850009	-1.749930	-0.504093
22	1	0	2.977890	-0.793667	-0.335111
23	6	0	5.028905	2.322671	-0.026222
24	6	0	5.702430	1.287870	-0.806209
25	8	0	4.274393	1.237636	-0.647703
26	1	0	5.035601	2.300029	1.079288
27	1	0	4.829352	3.322217	-0.454937
28	1	0	6.029830	1.477806	-1.845171
29	6	0	6.445646	0.128789	-0.116454
30	1	0	6.372016	-0.751562	-0.720160
31	1	0	7.475636	0.390056	0.009086
32	1	0	6.005675	-0.057463	0.840957

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.358086	0.000000			
3	N	2.205349	1.390856	0.000000		
4	C	2.211793	2.224673	1.347637	0.000000	
5	N	1.384329	2.210935	2.172563	1.333152	0.000000
6	C	2.569876	3.652138	3.593233	2.474861	1.478546
7	C	3.478349	4.464577	4.334368	3.240993	2.515635
8	H	1.076380	2.213950	3.264978	3.229152	2.157916
9	H	2.212240	1.074590	2.170243	3.245400	3.267387
10	H	3.336200	4.238821	3.896419	2.629208	2.074838
11	H	2.701218	3.975523	4.234171	3.300140	2.083688
12	H	3.627334	4.719493	4.874086	3.969156	3.038580
13	H	3.493741	4.192610	3.869036	2.872063	2.542075

14	Br	5.214828	5.514966	4.480222	3.306854	3.879489
15	H	3.268399	3.304624	2.214304	1.105553	2.145027
16	C	3.596924	2.535152	1.421937	2.430741	3.533293
17	C	4.337016	3.047561	2.435624	3.659022	4.603688
18	H	4.262215	3.412395	2.086921	2.562385	3.855030
19	H	5.397869	4.124507	3.399761	4.510292	5.567446
20	H	4.192914	2.835701	2.749739	4.088514	4.777489
21	O	4.771775	5.755055	5.469205	4.236974	3.667604
22	H	5.016027	5.842282	5.326243	4.033252	3.759028
23	C	8.134500	8.589175	7.598920	6.401411	6.765869
24	C	8.310632	8.915566	8.077650	6.838740	6.984162
25	O	6.991804	7.525884	6.649909	5.424345	5.656023
26	H	8.164058	8.650981	7.673293	6.448200	6.779905
27	H	8.575793	8.874419	7.774157	6.684555	7.232984
28	H	8.871692	9.430734	8.591508	7.416454	7.593809
29	C	8.576852	9.373659	8.699225	7.388077	7.278915
30	H	8.377683	9.253699	8.702484	7.406831	7.155597
31	H	9.634425	10.428835	9.731201	8.420290	8.331098
32	H	8.116999	8.950343	8.302291	6.964281	6.807465

		6	7	8	9	10
6	C	0.000000				
7	C	1.551365	0.000000			
8	H	2.871745	3.717414	0.000000		
9	H	4.679261	5.449309	2.754701	0.000000	
10	H	1.088941	2.154844	3.766442	5.295616	0.000000
11	H	1.090427	2.213225	2.603608	4.901930	1.778446
12	H	2.189500	1.093456	3.582662	5.595877	3.022779
13	H	2.164631	1.096442	3.955853	5.150689	2.678416
14	Br	3.601299	3.546397	6.008631	6.528176	2.967184
15	H	2.761817	3.308804	4.234334	4.289424	2.548330
16	C	4.876776	5.504662	4.631276	2.869169	5.020361
17	C	6.026251	6.667654	5.261306	2.891144	6.249513
18	H	5.005573	5.529205	5.334147	3.900159	4.960484
19	H	6.946872	7.533068	6.337753	3.944962	7.084680
20	H	6.251372	6.945541	4.969034	2.310055	6.609656
21	O	2.426477	1.402097	4.991645	6.774647	2.478410
22	H	2.679581	1.921016	5.416370	6.893299	2.397675
23	C	6.038522	5.581908	8.781279	9.618127	5.305186
24	C	6.068008	5.307967	8.829948	9.953814	5.500774
25	O	4.879652	4.222783	7.586685	8.559282	4.313338
26	H	6.014943	5.814104	8.794998	9.692026	5.141895
27	H	6.692462	6.232813	9.310763	9.860654	5.987351
28	H	6.739830	5.790578	9.392445	10.437566	6.294081
29	C	6.122304	5.410909	8.939042	10.435199	5.554669

30	H	5.932337	5.032561	8.645337	10.297882	5.536848
31	H	7.164522	6.471809	9.988602	11.492348	6.564827
32	H	5.609563	5.145095	8.463731	10.023059	4.930098

		11	12	13	14	15
11	H	0.000000				
12	H	2.411810	0.000000			
13	H	3.042191	1.778157	0.000000		
14	Br	4.614124	4.624273	3.192152	0.000000	
15	H	3.745279	4.236585	2.854470	2.284310	0.000000
16	C	5.597783	6.116579	4.878040	4.897290	2.828087
17	C	6.645599	7.172435	6.033651	6.207812	4.151196
18	H	5.857186	6.281587	4.837161	4.241482	2.503335
19	H	7.624454	8.091346	6.831175	6.682483	4.817744
20	H	6.726121	7.311978	6.390622	6.967148	4.790604
21	O	2.958540	2.021047	2.070447	3.385188	3.994394
22	H	3.426957	2.807351	2.211790	2.500693	3.547053
23	C	6.864652	6.505199	5.445130	3.122613	5.405518
24	C	6.811621	6.063424	5.261695	3.791536	5.964401
25	O	5.731948	5.107506	4.065381	2.381822	4.533622
26	H	6.759402	6.776987	5.818854	3.270738	5.460303
27	H	7.600390	7.178695	5.922529	3.401796	5.630415
28	H	7.514867	6.452673	5.619229	4.451493	6.559545
29	C	6.654292	6.034174	5.663646	4.626332	6.632936
30	H	6.394000	5.491451	5.345321	4.952976	6.765418
31	H	7.661947	7.065528	6.727592	5.558272	7.634224
32	H	6.071296	5.830324	5.525521	4.329840	6.234520

		16	17	18	19	20
16	C	0.000000				
17	C	1.326451	0.000000			
18	H	1.082568	2.121018	0.000000		
19	H	2.079839	1.081128	2.444268	0.000000	
20	H	2.126470	1.082536	3.099168	1.846912	0.000000
21	O	6.538503	7.777465	6.384204	8.573425	8.158155
22	H	6.246022	7.534657	5.940984	8.246927	8.034229
23	C	7.944940	9.225821	7.170838	9.575760	10.043098
24	C	8.587248	9.879977	7.919820	10.320707	10.616294
25	O	7.153079	8.449876	6.503676	8.911187	9.182656
26	H	8.049275	9.337993	7.288951	9.704665	10.144210
27	H	7.928331	9.153994	7.059109	9.385293	10.042563
28	H	9.043511	10.299132	8.365203	10.700554	11.043543
29	C	9.397026	10.714526	8.836658	11.260432	11.363117
30	H	9.499827	10.801932	9.030340	11.410540	11.379638
31	H	10.390904	11.708527	9.789986	12.221094	12.382681
32	H	9.049631	10.375746	8.522056	10.954900	11.000992

		21	22	23	24	25
21	O	0.000000				
22	H	0.979463	0.000000			
23	C	4.643494	3.743480	0.000000		
24	C	4.178015	3.460903	1.460421	0.000000	
25	O	3.312861	2.429985	1.460421	1.437685	0.000000
26	H	4.866834	3.975632	1.105762	2.241478	2.165783
27	H	5.444896	4.514728	1.105762	2.241478	2.165783
28	H	4.725255	4.093191	2.241478	1.105762	2.138497
29	C	4.075347	3.595006	2.613124	1.540000	2.495216
30	H	3.667146	3.416157	3.425844	2.148263	2.891743
31	H	5.122432	4.663624	3.118130	2.148263	3.376050
32	H	3.825158	3.330558	2.714980	2.148263	2.625020

		26	27	28	29	30
26	H	0.000000				
27	H	1.855062	0.000000			
28	H	3.196405	2.603027	0.000000		
29	C	2.851720	3.595130	2.231863	0.000000	
30	H	3.786321	4.364153	2.520481	1.070000	0.000000
31	H	3.278276	3.976896	2.590719	1.070000	1.747303
32	H	2.560393	3.805958	3.094014	1.070000	1.747303

		31	32
31	H	0.000000	
32	H	1.747303	0.000000

Stoichiometry C10H17BrN2O2
Framework group C1[X(C10H17BrN2O2)]
Deg. of freedom 90
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.377565	1.817649	-0.193450
2	6	0	-4.220960	0.784347	0.062229
3	7	0	-3.454108	-0.375436	0.025840
4	6	0	-2.177919	-0.039753	-0.247632
5	7	0	-2.114910	1.284499	-0.387922
6	6	0	-0.850999	2.015982	-0.619348
7	6	0	-0.034651	2.204855	0.686270
8	1	0	-3.567193	2.875250	-0.257598
9	1	0	-5.276852	0.778648	0.261732

10	1	0	-0.258219	1.412557	-1.305120
11	1	0	-1.104141	2.963020	-1.096913
12	1	0	-0.291205	3.153495	1.165758
13	1	0	-0.284468	1.387475	1.373050
14	35	0	0.964099	-1.070704	-0.235760
15	1	0	-1.287696	-0.692843	-0.304393
16	6	0	-3.867287	-1.720232	0.232504
17	6	0	-5.119046	-2.102127	0.448668
18	1	0	-3.036101	-2.412911	0.196736
19	1	0	-5.330920	-3.151382	0.600359
20	1	0	-5.957128	-1.417807	0.483460
21	8	0	1.338463	2.232333	0.404000
22	1	0	1.595971	1.307169	0.211364
23	6	0	4.060330	-1.475734	-0.231383
24	6	0	4.606797	-0.366464	0.545613
25	8	0	3.181453	-0.520356	0.437690
26	1	0	4.022604	-1.435723	-1.335777
27	1	0	4.022459	-2.499950	0.183656
28	1	0	4.996473	-0.522808	1.568560
29	6	0	5.149702	0.897949	-0.145846
30	1	0	4.972907	1.749284	0.477750
31	1	0	6.201149	0.789900	-0.312232
32	1	0	4.652262	1.033182	-1.083484

Rotational constants (GHZ): 0.8595191 0.2035802 0.1694573

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.

475 basis functions, 751 primitive gaussians, 492 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1350.4616834160 Hartrees.

NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 475 RedAO= T EigKep= 4.43D-06 NBF= 475

NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid=
0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0
NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
EnCoef did 7 forward-backward iterations
SCF Done: E(RB3LYP) = -3225.46834355 A.U. after 17 cycles
NFock= 17 Conv=0.54D-08 -V/T= 2.0017

****

Population analysis using the SCF density.

****

Orbital symmetries:
Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A)

The electronic state is 1-A.

Alpha occ. eigenvalues -- -482.68264 -62.33656 -56.15425 -56.15422 -56.15410
Alpha occ. eigenvalues -- -19.10183 -19.09272 -14.45177 -14.43827 -10.29176
Alpha occ. eigenvalues -- -10.27091 -10.27018 -10.26969 -10.23541 -10.22253
Alpha occ. eigenvalues -- -10.22087 -10.19521 -10.19217 -10.13568 -8.54629
Alpha occ. eigenvalues -- -6.36935 -6.36916 -6.36884 -2.48191 -2.48187
Alpha occ. eigenvalues -- -2.48159 -2.48143 -2.48138 -1.11421 -1.03187
Alpha occ. eigenvalues -- -1.01195 -0.99805 -0.85368 -0.82336 -0.77654
Alpha occ. eigenvalues -- -0.71788 -0.71253 -0.68050 -0.65029 -0.63900
Alpha occ. eigenvalues -- -0.63338 -0.62218 -0.58419 -0.56352 -0.54072
Alpha occ. eigenvalues -- -0.53198 -0.51913 -0.50868 -0.49221 -0.49119
Alpha occ. eigenvalues -- -0.47886 -0.47328 -0.46208 -0.44232 -0.43786
Alpha occ. eigenvalues -- -0.43619 -0.40365 -0.39711 -0.38712 -0.38055
Alpha occ. eigenvalues -- -0.34380 -0.33763 -0.33384 -0.31172 -0.30274
Alpha occ. eigenvalues -- -0.28798 -0.26740 -0.24286 -0.18856 -0.18170
Alpha occ. eigenvalues -- -0.16247
Alpha virt. eigenvalues -- -0.08290 -0.04386 -0.03080 -0.01604 -0.00692
Alpha virt. eigenvalues -- -0.00479 0.00890 0.01248 0.01278 0.01540
Alpha virt. eigenvalues -- 0.02846 0.03431 0.03461 0.03966 0.04212
Alpha virt. eigenvalues -- 0.04937 0.05330 0.05859 0.06132 0.06376
Alpha virt. eigenvalues -- 0.06841 0.07226 0.07527 0.07917 0.08262
Alpha virt. eigenvalues -- 0.08785 0.08857 0.09214 0.09316 0.09863
Alpha virt. eigenvalues -- 0.10091 0.10406 0.10849 0.11459 0.11496
Alpha virt. eigenvalues -- 0.12268 0.12644 0.12842 0.13004 0.13180
Alpha virt. eigenvalues -- 0.13633 0.13657 0.13931 0.14020 0.14441
Alpha virt. eigenvalues -- 0.14799 0.14950 0.14969 0.15413 0.15580

Alpha virt. eigenvalues --	0.15948	0.16084	0.16992	0.17098	0.17473
Alpha virt. eigenvalues --	0.17882	0.18136	0.18332	0.18538	0.18726
Alpha virt. eigenvalues --	0.19559	0.19691	0.19929	0.20340	0.20885
Alpha virt. eigenvalues --	0.21336	0.21615	0.21796	0.22391	0.22605
Alpha virt. eigenvalues --	0.23234	0.23307	0.23781	0.24271	0.24512
Alpha virt. eigenvalues --	0.25055	0.25222	0.25510	0.25726	0.26026
Alpha virt. eigenvalues --	0.26913	0.27647	0.27874	0.28680	0.29459
Alpha virt. eigenvalues --	0.29749	0.30389	0.30614	0.30960	0.31685
Alpha virt. eigenvalues --	0.32005	0.32746	0.33358	0.33743	0.34336
Alpha virt. eigenvalues --	0.34699	0.35106	0.35757	0.36784	0.36904
Alpha virt. eigenvalues --	0.36972	0.38081	0.38768	0.39283	0.40454
Alpha virt. eigenvalues --	0.41103	0.41841	0.43366	0.43926	0.44856
Alpha virt. eigenvalues --	0.45422	0.47655	0.48168	0.48550	0.50162
Alpha virt. eigenvalues --	0.51495	0.52090	0.52501	0.53576	0.54198
Alpha virt. eigenvalues --	0.54307	0.55219	0.55545	0.56366	0.57129
Alpha virt. eigenvalues --	0.57395	0.58371	0.59649	0.60056	0.60471
Alpha virt. eigenvalues --	0.61303	0.61750	0.63049	0.63597	0.64157
Alpha virt. eigenvalues --	0.64880	0.65242	0.66202	0.66524	0.67547
Alpha virt. eigenvalues --	0.68129	0.68800	0.69318	0.70040	0.70307
Alpha virt. eigenvalues --	0.70425	0.71163	0.72343	0.72857	0.73198
Alpha virt. eigenvalues --	0.74555	0.75047	0.75238	0.76209	0.76495
Alpha virt. eigenvalues --	0.77215	0.77664	0.77987	0.79432	0.79948
Alpha virt. eigenvalues --	0.81550	0.81922	0.83081	0.83339	0.84310
Alpha virt. eigenvalues --	0.86324	0.87190	0.88025	0.89352	0.90039
Alpha virt. eigenvalues --	0.91576	0.92549	0.93608	0.94405	0.97719
Alpha virt. eigenvalues --	0.98656	0.99355	1.00179	1.01426	1.03678
Alpha virt. eigenvalues --	1.04324	1.05026	1.05493	1.06418	1.09106
Alpha virt. eigenvalues --	1.10314	1.11008	1.12113	1.13086	1.14625
Alpha virt. eigenvalues --	1.15874	1.18223	1.19668	1.20799	1.22359
Alpha virt. eigenvalues --	1.24860	1.27221	1.29026	1.30015	1.31705
Alpha virt. eigenvalues --	1.33921	1.35385	1.37544	1.38585	1.39461
Alpha virt. eigenvalues --	1.43726	1.44623	1.46148	1.47223	1.48104
Alpha virt. eigenvalues --	1.48886	1.49141	1.50063	1.50810	1.51139
Alpha virt. eigenvalues --	1.53548	1.54261	1.54953	1.56244	1.58041
Alpha virt. eigenvalues --	1.58798	1.59904	1.60125	1.60546	1.61750
Alpha virt. eigenvalues --	1.62169	1.63034	1.63779	1.66020	1.66882
Alpha virt. eigenvalues --	1.67190	1.69233	1.69915	1.70479	1.71193
Alpha virt. eigenvalues --	1.72263	1.72889	1.73600	1.73936	1.75071
Alpha virt. eigenvalues --	1.76028	1.77265	1.78311	1.81749	1.82065
Alpha virt. eigenvalues --	1.83593	1.85975	1.86436	1.86673	1.88177
Alpha virt. eigenvalues --	1.89431	1.90061	1.90293	1.94648	1.95272
Alpha virt. eigenvalues --	1.97450	1.98412	2.01044	2.04017	2.05568
Alpha virt. eigenvalues --	2.05908	2.06626	2.08851	2.10105	2.11971
Alpha virt. eigenvalues --	2.12380	2.13097	2.13922	2.15256	2.17386

Alpha virt. eigenvalues --	2.19281	2.20218	2.21391	2.22394	2.22822	
Alpha virt. eigenvalues --	2.26662	2.27743	2.29264	2.30596	2.35630	
Alpha virt. eigenvalues --	2.37581	2.39069	2.42633	2.43003	2.44588	
Alpha virt. eigenvalues --	2.45492	2.46897	2.49757	2.50619	2.51333	
Alpha virt. eigenvalues --	2.53124	2.54371	2.55776	2.56105	2.56939	
Alpha virt. eigenvalues --	2.57201	2.58654	2.59290	2.60426	2.61189	
Alpha virt. eigenvalues --	2.62126	2.64117	2.64538	2.70603	2.70908	
Alpha virt. eigenvalues --	2.71690	2.71861	2.72626	2.73335	2.74335	
Alpha virt. eigenvalues --	2.75537	2.76566	2.78327	2.79621	2.80089	
Alpha virt. eigenvalues --	2.81152	2.82699	2.83189	2.84536	2.85090	
Alpha virt. eigenvalues --	2.85660	2.87333	2.89764	2.91204	2.93860	
Alpha virt. eigenvalues --	2.95190	2.96078	2.97631	3.02192	3.09520	
Alpha virt. eigenvalues --	3.11158	3.11405	3.14822	3.15631	3.16571	
Alpha virt. eigenvalues --	3.23001	3.25874	3.26384	3.27718	3.35547	
Alpha virt. eigenvalues --	3.36151	3.37631	3.49319	3.54862	3.59808	
Alpha virt. eigenvalues --	3.63792	3.64910	3.71868	3.72044	3.75774	
Alpha virt. eigenvalues --	3.76310	3.76906	3.82593	3.84478	3.85392	
Alpha virt. eigenvalues --	3.88218	3.88414	3.89911	3.90589	3.96818	
Alpha virt. eigenvalues --	4.05763	4.08497	4.09609	4.12114	4.20229	
Alpha virt. eigenvalues --	4.31065	4.32784	4.36724	4.42318	4.46691	
Alpha virt. eigenvalues --	4.58743	4.69157	4.91286	5.02376	5.10665	
Alpha virt. eigenvalues --	5.11878	5.22775	5.44171	5.52283	5.65058	
Alpha virt. eigenvalues --	5.69538	6.86657	7.72278	7.77253	7.90118	
Alpha virt. eigenvalues --	23.69821	23.74564	23.82978	23.85822	23.88200	
Alpha virt. eigenvalues --	23.88913	23.91562	24.05464	24.13510	24.22331	
Alpha virt. eigenvalues --	35.44033	35.56981	48.13437	49.95068	49.95860	
Alpha virt. eigenvalues --	289.93228	289.98362	290.10648	1020.94060		

Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	9.275823	-3.260380	0.675177	-1.114562	-0.652715	0.897564
2	C	-3.260380	8.688903	-0.446289	0.981685	0.819466	-0.905357
3	N	0.675177	-0.446289	6.895546	-0.290571	-0.410723	0.110331
4	C	-1.114562	0.981685	-0.290571	7.879254	0.847497	-0.746066
5	N	-0.652715	0.819466	-0.410723	0.847497	6.970346	-0.253622
6	C	0.897564	-0.905357	0.110331	-0.746066	-0.253622	6.985979
7	C	-0.235063	0.286327	-0.054581	0.078500	0.113743	-0.295845
8	H	0.559195	-0.171086	0.043668	-0.000274	-0.095586	0.017280
9	H	-0.130420	0.526154	-0.077484	-0.003557	0.026510	-0.001475
10	H	0.118696	-0.124400	0.037802	-0.039197	-0.097367	0.521017
11	H	-0.115526	0.116619	-0.006268	0.006200	-0.016767	0.278460
12	H	0.097883	-0.099682	0.019773	-0.065736	-0.046179	0.095268
13	H	-0.166825	0.133285	-0.046200	0.119715	0.063564	-0.195287
14	Br	0.014590	-0.018747	-0.021057	-0.109215	-0.012337	0.024003
15	H	0.006057	-0.137518	0.217565	-1.156038	-0.151999	0.173043

16	C	0.584289	-0.577721	0.259695	-0.333810	-0.131441	-0.038357
17	C	-0.308100	0.199027	-0.030659	-0.161514	-0.047544	-0.057739
18	H	-0.016075	0.029310	-0.091089	0.125531	0.021388	-0.003561
19	H	-0.003500	0.004525	0.023762	-0.008005	-0.000743	0.000185
20	H	-0.011418	0.016688	-0.039391	0.014213	0.002930	-0.002812
21	O	-0.035911	0.022634	-0.008263	0.043434	0.012785	-0.181777
22	H	-0.052915	0.032518	-0.006791	0.083868	0.009658	-0.081188
23	C	0.002877	-0.002957	-0.000309	-0.016853	-0.000427	0.037988
24	C	-0.001892	0.002447	-0.000329	0.034011	0.001088	-0.052959
25	O	-0.001740	-0.000172	-0.000129	-0.017181	-0.001979	-0.006065
26	H	-0.000400	0.000487	0.000108	0.004920	-0.000026	-0.007099
27	H	0.000094	-0.000197	-0.000258	-0.000121	0.000049	0.003028
28	H	-0.000218	0.000171	0.000031	0.000918	-0.000024	-0.003003
29	C	0.000733	-0.000304	0.000133	-0.007711	0.000394	0.009542
30	H	0.000023	-0.000049	-0.000003	-0.000090	0.000006	-0.000653
31	H	0.000096	-0.000039	0.000001	-0.000516	0.000043	0.001247
32	H	0.000036	-0.000124	0.000012	-0.000702	-0.000235	0.002384

		7	8	9	10	11	12
1	C	-0.235063	0.559195	-0.130420	0.118696	-0.115526	0.097883
2	C	0.286327	-0.171086	0.526154	-0.124400	0.116619	-0.099682
3	N	-0.054581	0.043668	-0.077484	0.037802	-0.006268	0.019773
4	C	0.078500	-0.000274	-0.003557	-0.039197	0.006200	-0.065736
5	N	0.113743	-0.095586	0.026510	-0.097367	-0.016767	-0.046179
6	C	-0.295845	0.017280	-0.001475	0.521017	0.278460	0.095268
7	C	5.929496	-0.010479	0.002098	-0.099857	-0.077239	0.396774
8	H	-0.010479	0.491527	-0.010565	0.007754	-0.021947	0.004213
9	H	0.002098	-0.010565	0.503057	-0.000361	0.004041	-0.000297
10	H	-0.099857	0.007754	-0.000361	0.495708	-0.069046	0.024466
11	H	-0.077239	-0.021947	0.004041	-0.069046	0.727817	-0.027232
12	H	0.396774	0.004213	-0.000297	0.024466	-0.027232	0.684011
13	H	0.316718	-0.005863	0.000139	-0.039184	0.032450	-0.118319
14	Br	0.159908	0.000035	-0.002401	-0.015931	0.014828	0.017769
15	H	-0.119804	-0.004605	0.002220	0.002550	0.028639	0.014939
16	C	-0.021487	0.014645	0.001809	0.022825	-0.010964	0.002453
17	C	-0.004324	-0.002713	-0.010554	-0.005551	0.000748	-0.001108
18	H	0.001250	0.000102	0.001204	-0.000068	-0.001717	-0.001032
19	H	0.000155	-0.000194	-0.000377	-0.000065	0.000172	0.000057
20	H	-0.000031	0.000588	0.003691	-0.000024	-0.000526	-0.000186
21	O	0.158645	-0.001628	-0.000131	-0.050271	0.025987	-0.137083
22	H	-0.115347	-0.001343	0.000090	0.009423	0.003922	-0.000006
23	C	0.001627	0.000048	-0.000007	0.003610	0.001449	0.004582
24	C	0.016672	0.000049	-0.000002	0.001136	-0.004010	-0.004952
25	O	-0.047805	-0.000001	-0.000025	-0.002972	-0.000482	-0.005139
26	H	-0.001973	0.000005	0.000003	0.001117	-0.000523	-0.000556

27	H	-0.000489	-0.000001	-0.000004	-0.000860	0.000145	0.000035
28	H	-0.002803	0.000001	0.000000	0.000123	-0.000278	-0.000739
29	C	0.005556	-0.000021	-0.000002	-0.001866	0.001193	0.002457
30	H	-0.000440	0.000005	0.000000	0.001030	-0.000390	0.000121
31	H	0.002919	0.000001	0.000000	-0.000149	0.000251	0.000360
32	H	0.001422	0.000001	-0.000003	-0.000668	0.000521	0.000061
		13	14	15	16	17	18
1	C	-0.166825	0.014590	0.006057	0.584289	-0.308100	-0.016075
2	C	0.133285	-0.018747	-0.137518	-0.577721	0.199027	0.029310
3	N	-0.046200	-0.021057	0.217565	0.259695	-0.030659	-0.091089
4	C	0.119715	-0.109215	-1.156038	-0.333810	-0.161514	0.125531
5	N	0.063564	-0.012337	-0.151999	-0.131441	-0.047544	0.021388
6	C	-0.195287	0.024003	0.173043	-0.038357	-0.057739	-0.003561
7	C	0.316718	0.159908	-0.119804	-0.021487	-0.004324	0.001250
8	H	-0.005863	0.000035	-0.004605	0.014645	-0.002713	0.000102
9	H	0.000139	-0.002401	0.002220	0.001809	-0.010554	0.001204
10	H	-0.039184	-0.015931	0.002550	0.022825	-0.005551	-0.000068
11	H	0.032450	0.014828	0.028639	-0.010964	0.000748	-0.001717
12	H	-0.118319	0.017769	0.014939	0.002453	-0.001108	-0.001032
13	H	0.698161	-0.034197	-0.039618	-0.013010	0.007471	0.001628
14	Br	-0.034197	36.025862	0.045582	0.033753	0.035987	0.000015
15	H	-0.039618	0.045582	2.014248	-0.020833	0.122078	-0.077909
16	C	-0.013010	0.033753	-0.020833	6.185087	-0.391310	0.426771
17	C	0.007471	0.035987	0.122078	-0.391310	6.416582	-0.091314
18	H	0.001628	0.000015	-0.077909	0.426771	-0.091314	0.462773
19	H	-0.000033	-0.000506	0.006430	-0.095525	0.450162	-0.009808
20	H	0.000335	0.001330	-0.002602	0.071814	0.303696	0.004274
21	O	0.050438	-0.146061	-0.003919	0.000958	0.000725	0.000323
22	H	0.001730	0.009684	-0.031855	-0.001172	0.001296	0.000580
23	C	-0.008858	-0.027202	0.004949	-0.002411	-0.000457	0.000155
24	C	0.004821	0.108576	-0.056962	0.001924	0.000157	0.000447
25	O	0.011542	-0.422632	0.054734	0.002208	0.000376	-0.000460
26	H	0.000781	0.000007	-0.003740	0.000776	0.000030	0.000021
27	H	0.000236	0.011516	-0.003869	-0.000761	-0.000041	0.000107
28	H	0.001012	-0.011742	0.000705	0.000251	0.000030	-0.000008
29	C	-0.000846	-0.012232	0.015065	0.000006	0.000016	-0.000144
30	H	-0.000199	-0.005414	-0.000094	-0.000005	0.000000	0.000005
31	H	-0.000163	0.006459	-0.000294	-0.000032	-0.000004	0.000000
32	H	-0.000025	0.000113	0.000506	0.000047	0.000020	-0.000005
		19	20	21	22	23	24
1	C	-0.003500	-0.011418	-0.035911	-0.052915	0.002877	-0.001892
2	C	0.004525	0.016688	0.022634	0.032518	-0.002957	0.002447
3	N	0.023762	-0.039391	-0.008263	-0.006791	-0.000309	-0.000329
4	C	-0.008005	0.014213	0.043434	0.083868	-0.016853	0.034011

5	N	-0.000743	0.002930	0.012785	0.009658	-0.000427	0.001088
6	C	0.000185	-0.002812	-0.181777	-0.081188	0.037988	-0.052959
7	C	0.000155	-0.000031	0.158645	-0.115347	0.001627	0.016672
8	H	-0.000194	0.000588	-0.001628	-0.001343	0.000048	0.000049
9	H	-0.000377	0.003691	-0.000131	0.000090	-0.000007	-0.000002
10	H	-0.000065	-0.000024	-0.050271	0.009423	0.003610	0.001136
11	H	0.000172	-0.000526	0.025987	0.003922	0.001449	-0.004010
12	H	0.000057	-0.000186	-0.137083	-0.000006	0.004582	-0.004952
13	H	-0.000033	0.000335	0.050438	0.001730	-0.008858	0.004821
14	Br	-0.000506	0.001330	-0.146061	0.009684	-0.027202	0.108576
15	H	0.006430	-0.002602	-0.003919	-0.031855	0.004949	-0.056962
16	C	-0.095525	0.071814	0.000958	-0.001172	-0.002411	0.001924
17	C	0.450162	0.303696	0.000725	0.001296	-0.000457	0.000157
18	H	-0.009808	0.004274	0.000323	0.000580	0.000155	0.000447
19	H	0.465687	-0.021696	-0.000015	-0.000045	-0.000006	-0.000002
20	H	-0.021696	0.535649	0.000038	0.000092	-0.000005	0.000010
21	O	-0.000015	0.000038	8.139827	0.250158	-0.005095	-0.012715
22	H	-0.000045	0.000092	0.250158	0.622717	0.018235	0.001050
23	C	-0.000006	-0.000005	-0.005095	0.018235	6.591787	-1.106129
24	C	-0.000002	0.000010	-0.012715	0.001050	-1.106129	6.934027
25	O	-0.000001	0.000008	0.064965	-0.026730	0.093090	-0.104317
26	H	0.000000	0.000002	0.000464	0.004289	0.235773	0.146874
27	H	-0.000003	-0.000001	0.000832	-0.001491	0.434968	-0.071269
28	H	0.000000	0.000001	0.003007	0.004620	0.013592	0.309870
29	C	0.000002	-0.000001	0.006358	-0.012840	0.045173	-0.013090
30	H	0.000000	0.000000	-0.000545	-0.000769	-0.002034	0.001078
31	H	0.000000	0.000000	-0.000289	-0.007573	0.032026	-0.104803
32	H	0.000000	0.000000	-0.002665	-0.005142	-0.001436	-0.066825

		25	26	27	28	29	30
1	C	-0.001740	-0.000400	0.000094	-0.000218	0.000733	0.000023
2	C	-0.000172	0.000487	-0.000197	0.000171	-0.000304	-0.000049
3	N	-0.000129	0.000108	-0.000258	0.000031	0.000133	-0.000003
4	C	-0.017181	0.004920	-0.000121	0.000918	-0.007711	-0.000090
5	N	-0.001979	-0.000026	0.000049	-0.000024	0.000394	0.000006
6	C	-0.006065	-0.007099	0.003028	-0.003003	0.009542	-0.000653
7	C	-0.047805	-0.001973	-0.000489	-0.002803	0.005556	-0.000440
8	H	-0.000001	0.000005	-0.000001	0.000001	-0.000021	0.000005
9	H	-0.000025	0.000003	-0.000004	0.000000	-0.000002	0.000000
10	H	-0.002972	0.001117	-0.000860	0.000123	-0.001866	0.001030
11	H	-0.000482	-0.000523	0.000145	-0.000278	0.001193	-0.000390
12	H	-0.005139	-0.000556	0.000035	-0.000739	0.002457	0.000121
13	H	0.011542	0.000781	0.000236	0.001012	-0.000846	-0.000199
14	Br	-0.422632	0.000007	0.011516	-0.011742	-0.012232	-0.005414
15	H	0.054734	-0.003740	-0.003869	0.000705	0.015065	-0.000094

16	C	0.002208	0.000776	-0.000761	0.000251	0.000006	-0.000005
17	C	0.000376	0.000030	-0.000041	0.000030	0.000016	0.000000
18	H	-0.000460	0.000021	0.000107	-0.000008	-0.000144	0.000005
19	H	-0.000001	0.000000	-0.000003	0.000000	0.000002	0.000000
20	H	0.000008	0.000002	-0.000001	0.000001	-0.000001	0.000000
21	O	0.064965	0.000464	0.000832	0.003007	0.006358	-0.000545
22	H	-0.026730	0.004289	-0.001491	0.004620	-0.012840	-0.000769
23	C	0.093090	0.235773	0.434968	0.013592	0.045173	-0.002034
24	C	-0.104317	0.146874	-0.071269	0.309870	-0.013090	0.001078
25	O	8.608112	-0.054730	-0.046781	0.002128	-0.097576	-0.011128
26	H	-0.054730	0.620358	-0.077319	0.012137	-0.002990	-0.001115
27	H	-0.046781	-0.077319	0.632530	-0.016466	-0.009214	0.000247
28	H	0.002128	0.012137	-0.016466	0.550470	-0.039913	0.005496
29	C	-0.097576	-0.002990	-0.009214	-0.039913	5.428992	0.382979
30	H	-0.011128	-0.001115	0.000247	0.005496	0.382979	0.551656
31	H	0.014450	-0.008712	0.004976	-0.008085	0.391689	-0.043402
32	H	0.022279	-0.005625	0.005207	0.005421	0.390513	-0.024813

		31	32
1	C	0.000096	0.000036
2	C	-0.000039	-0.000124
3	N	0.000001	0.000012
4	C	-0.000516	-0.000702
5	N	0.000043	-0.000235
6	C	0.001247	0.002384
7	C	0.002919	0.001422
8	H	0.000001	0.000001
9	H	0.000000	-0.000003
10	H	-0.000149	-0.000668
11	H	0.000251	0.000521
12	H	0.000360	0.000061
13	H	-0.000163	-0.000025
14	Br	0.006459	0.000113
15	H	-0.000294	0.000506
16	C	-0.000032	0.000047
17	C	-0.000004	0.000020
18	H	0.000000	-0.000005
19	H	0.000000	0.000000
20	H	0.000000	0.000000
21	O	-0.000289	-0.002665
22	H	-0.007573	-0.005142
23	C	0.032026	-0.001436
24	C	-0.104803	-0.066825
25	O	0.014450	0.022279
26	H	-0.008712	-0.005625

27	H	0.004976	0.005207
28	H	-0.008085	0.005421
29	C	0.391689	0.390513
30	H	-0.043402	-0.024813
31	H	0.632989	-0.031527
32	H	-0.031527	0.576628

Mulliken charges:

		1
1	C	-0.125475
2	C	-0.115221
3	N	0.246789
4	C	-0.148026
5	N	0.030245
6	C	-0.324454
7	C	-0.384242
8	H	0.187190
9	H	0.166650
10	H	0.300582
11	H	0.109473
12	H	0.143024
13	H	0.224598
14	Br	-0.670344
15	H	0.102347
16	C	0.029528
17	C	-0.425468
18	H	0.217307
19	H	0.189389
20	H	0.123334
21	O	-0.195211
22	H	0.291277
23	C	-0.347742
24	C	0.036020
25	O	-0.025847
26	H	0.136655
27	H	0.135175
28	H	0.173294
29	C	-0.482049
30	H	0.148496
31	H	0.118082
32	H	0.134624

Sum of Mulliken charges = 0.00000

Mulliken charges with hydrogens summed into heavy atoms:

		1
1	C	0.061715

```
     2    C        0.051429
     3    N        0.246789
     4    C       -0.045679
     5    N        0.030245
     6    C        0.085601
     7    C       -0.016620
    14    Br      -0.670344
    16    C        0.246834
    17    C       -0.112745
    21    O        0.096066
    23    C       -0.075912
    24    C        0.209314
    25    O       -0.025847
    29    C       -0.080847
 Electronic spatial extent (au):  <R**2>=           6175.1399
 Charge=                 0.0000 electrons
 Dipole moment (field-independent basis, Debye):
    X=              -10.8628    Y=                2.7574    Z=              -0.0067
Tot=                11.2073
 Quadrupole moment (field-independent basis, Debye-Ang):
   XX=              -63.7749   YY=             -100.2708   ZZ=             -108.8446
   XY=               -4.0644   XZ=               -2.3549   YZ=               -3.4508
 Traceless Quadrupole moment (field-independent basis, Debye-Ang):
   XX=               27.1885   YY=               -9.3074   ZZ=              -17.8811
   XY=               -4.0644   XZ=               -2.3549   YZ=               -3.4508
 Octapole moment (field-independent basis, Debye-Ang**2):
  XXX=              -103.8812  YYY=              -22.4828  ZZZ=               -4.3231
XYY=               -44.1933
  XXY=              -30.3237  XXZ=               12.6637  XZZ=               24.3888
YZZ=                -2.0538
  YYZ=               -1.2603  XYZ=                6.3136
 Hexadecapole moment (field-independent basis, Debye-Ang**3):
 XXXX=            -5529.1076 YYYY=            -1398.0568 ZZZZ=             -261.0578
XXXY=               -0.4063
 XXXZ=              -74.0919 YYYX=              -70.1130 YYYZ=              -21.0309
ZZZX=               10.8563
 ZZZY=                7.6865 XXYY=            -1189.1591 XXZZ=            -1184.0930
YYZZ=             -300.1282
 XXYZ=              -24.8886 YYXZ=             -10.7561 ZZXY=              -19.7542
 N-N= 1.350461683416D+03 E-N=-1.037553542817D+04  KE= 3.219914379625D+03
 Calling FoFJK, ICntrl=          2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
```

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000372078	-0.000200632	-0.000049186
2	6	-0.000574335	-0.000490478	-0.000005486
3	7	-0.000351604	-0.000230484	0.000026669
4	6	-0.001617928	-0.001604569	-0.000376613
5	7	-0.000307782	0.000151222	0.000051698
6	6	-0.000211996	0.000140158	-0.000190817
7	6	0.000025949	0.000041991	0.000224929
8	1	-0.000070167	-0.000017800	-0.000016928
9	1	-0.000030554	-0.000085639	-0.000019887
10	1	0.000179887	0.000463991	-0.000207254
11	1	-0.000115620	-0.000198051	-0.000032852
12	1	-0.000144350	-0.000242687	-0.000006714
13	1	0.000088880	0.000112724	0.000087191
14	35	-0.059618989	0.004329976	0.018226918
15	1	0.004276536	0.003518553	0.000470684
16	6	0.000490313	-0.000459560	0.000072016
17	6	-0.000259298	0.000069706	-0.000033245
18	1	0.000241010	-0.000094954	0.000054264
19	1	-0.000002259	-0.000000761	0.000008121
20	1	0.000005743	-0.000041507	-0.000004509
21	8	-0.000182307	-0.000139754	0.000140764
22	1	0.001154246	0.001155761	-0.000338844
23	6	-0.011577360	0.003431097	-0.001139389
24	6	0.017279084	-0.021022867	-0.002875664
25	8	0.050983527	0.010124535	-0.009060942
26	1	0.001241654	-0.001875727	-0.012000138
27	1	0.002075603	-0.011520202	0.003246675
28	1	-0.001764962	0.003471758	0.009949297
29	6	-0.011632851	0.026316690	-0.014094424
30	1	-0.000528007	-0.013406446	-0.007737705
31	1	0.017072015	0.001548884	0.002467213
32	1	-0.005752000	-0.003244926	0.013164156

Cartesian Forces: Max 0.059618989 RMS 0.010114262

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.059381023 RMS 0.005723550
Search for a local minimum.

Step number 1 out of a maximum of 177
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Second derivative matrix not updated -- first step.
ITU= 0

Eigenvalues ---	0.00237	0.00257	0.00356	0.00508	0.00810
Eigenvalues ---	0.01240	0.01358	0.01402	0.01507	0.01851
Eigenvalues ---	0.01906	0.02069	0.02144	0.02198	0.02243
Eigenvalues ---	0.02314	0.02390	0.02590	0.02751	0.03062
Eigenvalues ---	0.03062	0.03218	0.03385	0.04008	0.04333
Eigenvalues ---	0.04542	0.05288	0.05720	0.05720	0.05729
Eigenvalues ---	0.05914	0.06893	0.09368	0.10000	0.10415
Eigenvalues ---	0.10996	0.11476	0.12363	0.12885	0.13324
Eigenvalues ---	0.14853	0.15708	0.16000	0.16000	0.16000
Eigenvalues ---	0.16000	0.16000	0.16000	0.16000	0.16000
Eigenvalues ---	0.16294	0.18515	0.19546	0.21313	0.22000
Eigenvalues ---	0.22781	0.23357	0.23765	0.25000	0.26990
Eigenvalues ---	0.27497	0.28519	0.31333	0.32783	0.33053
Eigenvalues ---	0.33053	0.33053	0.34079	0.34289	0.34416
Eigenvalues ---	0.34763	0.34935	0.35686	0.35690	0.35858
Eigenvalues ---	0.36435	0.36656	0.37230	0.37230	0.37230
Eigenvalues ---	0.38103	0.42170	0.42456	0.44625	0.45579
Eigenvalues ---	0.49034	0.50912	0.54371	0.55994	0.60352

RFO step: Lambda=-4.02579373D-02 EMin= 2.36824163D-03
Linear search not attempted -- first point.
Maximum step size (0.300) exceeded in Quadratic search.
-- Step size scaled by 0.509
Iteration 1 RMS(Cart)= 0.03927860 RMS(Int)= 0.00686799
Iteration 2 RMS(Cart)= 0.01601280 RMS(Int)= 0.00004126
Iteration 3 RMS(Cart)= 0.00005621 RMS(Int)= 0.00003546
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00003546

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56641	-0.00022	0.00000	-0.00017	-0.00018	2.56623
R2	2.61600	0.00083	0.00000	0.00093	0.00093	2.61693
R3	2.03406	0.00002	0.00000	0.00002	0.00002	2.03409
R4	2.62834	0.00031	0.00000	0.00021	0.00019	2.62853
R5	2.03068	0.00004	0.00000	0.00006	0.00006	2.03074
R6	2.54667	0.00025	0.00000	0.00013	0.00014	2.54680
R7	2.68707	-0.00068	0.00000	-0.00075	-0.00075	2.68632
R8	2.51929	0.00039	0.00000	0.00052	0.00057	2.51987
R9	2.08919	0.00278	0.00000	0.00285	0.00288	2.09207
R10	2.79405	0.00140	0.00000	0.00305	0.00307	2.79712
R11	2.93166	0.00124	0.00000	0.00277	0.00279	2.93445

R12	2.05780	0.00026	0.00000	0.00034	0.00034	2.05814
R13	2.06061	0.00017	0.00000	0.00022	0.00022	2.06083
R14	2.06633	0.00024	0.00000	0.00032	0.00032	2.06665
R15	2.07198	-0.00001	0.00000	-0.00001	-0.00001	2.07196
R16	2.64958	0.00172	0.00000	0.00279	0.00279	2.65237
R17	4.31672	-0.00324	0.00000	-0.02753	-0.02753	4.28919
R18	4.50099	0.05938	0.00000	0.29003	0.29001	4.79100
R19	2.50663	0.00026	0.00000	0.00020	0.00020	2.50683
R20	2.04576	0.00009	0.00000	0.00012	0.00012	2.04587
R21	2.04304	0.00000	0.00000	0.00000	0.00000	2.04304
R22	2.04570	0.00002	0.00000	0.00003	0.00003	2.04573
R23	1.85092	0.00016	0.00000	0.00026	0.00022	1.85113
R24	4.59201	-0.00040	0.00000	0.00093	0.00090	4.59290
R25	2.75980	-0.00056	0.00000	0.00195	0.00196	2.76176
R26	2.75980	-0.01292	0.00000	-0.02117	-0.02118	2.73862
R27	2.08959	-0.01195	0.00000	-0.01642	-0.01642	2.07316
R28	2.08959	-0.01205	0.00000	-0.01656	-0.01656	2.07303
R29	2.71683	0.01181	0.00000	0.01601	0.01601	2.73284
R30	2.08959	-0.00927	0.00000	-0.01274	-0.01274	2.07684
R31	2.91018	-0.01162	0.00000	-0.01819	-0.01819	2.89199
R32	2.02201	0.01543	0.00000	0.01906	0.01906	2.04107
R33	2.02201	0.01710	0.00000	0.02112	0.02112	2.04313
R34	2.02201	0.01471	0.00000	0.01817	0.01817	2.04017
A1	1.87533	0.00034	0.00000	0.00096	0.00098	1.87631
A2	2.27758	-0.00024	0.00000	-0.00067	-0.00067	2.27691
A3	2.13026	-0.00009	0.00000	-0.00029	-0.00030	2.12996
A4	1.86202	-0.00039	0.00000	-0.00084	-0.00084	1.86117
A5	2.27733	0.00012	0.00000	0.00022	0.00022	2.27755
A6	2.14384	0.00027	0.00000	0.00062	0.00062	2.14446
A7	1.89623	0.00058	0.00000	0.00076	0.00078	1.89701
A8	2.24543	0.00021	0.00000	0.00050	0.00049	2.24592
A9	2.14152	-0.00079	0.00000	-0.00126	-0.00127	2.14025
A10	1.88971	-0.00037	0.00000	-0.00005	-0.00008	1.88964
A11	2.24697	0.00063	0.00000	0.00244	0.00236	2.24933
A12	2.14520	-0.00025	0.00000	-0.00235	-0.00225	2.14295
A13	1.90146	-0.00016	0.00000	-0.00081	-0.00082	1.90063
A14	2.22831	-0.00148	0.00000	-0.00347	-0.00356	2.22475
A15	2.15113	0.00164	0.00000	0.00439	0.00448	2.15561
A16	1.95878	0.00175	0.00000	0.00586	0.00587	1.96465
A17	1.86477	0.00002	0.00000	0.00320	0.00318	1.86795
A18	1.87525	-0.00109	0.00000	-0.00615	-0.00615	1.86911
A19	1.88706	-0.00008	0.00000	0.00121	0.00122	1.88828
A20	1.96601	-0.00098	0.00000	-0.00449	-0.00452	1.96149
A21	1.90904	0.00041	0.00000	0.00073	0.00074	1.90978

A22	1.92965	-0.00146	0.00000	-0.00558	-0.00559	1.92406
A23	1.89283	-0.00010	0.00000	0.00176	0.00174	1.89456
A24	1.92654	0.00293	0.00000	0.00763	0.00764	1.93419
A25	1.89508	0.00035	0.00000	-0.00027	-0.00026	1.89482
A26	1.87659	-0.00132	0.00000	-0.00632	-0.00631	1.87028
A27	1.94319	-0.00048	0.00000	0.00253	0.00249	1.94567
A28	2.66371	-0.00369	0.00000	-0.01883	-0.01888	2.64484
A29	2.66802	-0.00277	0.00000	-0.00976	-0.00962	2.65840
A30	2.17753	0.00013	0.00000	0.00025	0.00025	2.17777
A31	1.95760	-0.00032	0.00000	-0.00077	-0.00077	1.95683
A32	2.14805	0.00019	0.00000	0.00052	0.00052	2.14857
A33	2.07971	0.00002	0.00000	0.00005	0.00005	2.07975
A34	2.15775	-0.00004	0.00000	-0.00010	-0.00010	2.15765
A35	2.04573	0.00002	0.00000	0.00005	0.00005	2.04578
A36	1.85309	0.00419	0.00000	0.01603	0.01595	1.86903
A37	2.61316	-0.00073	0.00000	-0.00143	-0.00135	2.61181
A38	2.11374	-0.00264	0.00000	-0.00568	-0.00569	2.10805
A39	2.11374	-0.00125	0.00000	-0.00222	-0.00223	2.11151
A40	1.99695	-0.00062	0.00000	-0.00099	-0.00100	1.99595
A41	1.99695	-0.00468	0.00000	-0.00475	-0.00472	1.99223
A42	1.99021	0.00275	0.00000	0.00512	0.00511	1.99532
A43	2.11374	-0.00371	0.00000	-0.01309	-0.01307	2.10068
A44	2.11374	0.00497	0.00000	0.00496	0.00498	2.11872
A45	1.98634	-0.00104	0.00000	0.00221	0.00203	1.98838
A46	1.98634	0.00787	0.00000	0.01558	0.01547	2.00181
A47	1.99021	-0.00123	0.00000	0.00338	0.00326	1.99347
A48	1.09283	-0.00282	0.00000	-0.01368	-0.01378	1.07905
A49	1.85412	0.00340	0.00000	0.01094	0.01104	1.86516
A50	2.57173	0.00167	0.00000	0.00169	0.00167	2.57340
A51	2.18139	-0.00049	0.00000	0.00151	0.00159	2.18298
A52	1.91063	0.00100	0.00000	0.00207	0.00206	1.91270
A53	1.91063	0.00353	0.00000	0.00956	0.00955	1.92018
A54	1.91063	0.00016	0.00000	0.00028	0.00028	1.91091
A55	1.91063	-0.00216	0.00000	-0.00527	-0.00529	1.90535
A56	1.91063	-0.00111	0.00000	-0.00398	-0.00398	1.90665
A57	1.91063	-0.00141	0.00000	-0.00267	-0.00268	1.90795
A58	3.27422	-0.00331	0.00000	-0.01216	-0.01219	3.26203
A59	3.38984	-0.00125	0.00000	-0.00506	-0.00508	3.38476
D1	0.00444	-0.00016	0.00000	-0.00101	-0.00102	0.00342
D2	-3.13680	-0.00011	0.00000	-0.00064	-0.00065	-3.13745
D3	3.14022	0.00002	0.00000	-0.00012	-0.00012	3.14010
D4	-0.00102	0.00007	0.00000	0.00024	0.00025	-0.00077
D5	-0.00643	0.00028	0.00000	0.00176	0.00177	-0.00466
D6	-3.07654	0.00012	0.00000	-0.00011	-0.00010	-3.07664

D7	3.14037	0.00012	0.00000	0.00097	0.00097	3.14134
D8	0.07026	-0.00004	0.00000	-0.00090	-0.00090	0.06936
D9	-0.00098	-0.00001	0.00000	-0.00007	-0.00007	-0.00105
D10	3.13888	0.00010	0.00000	0.00054	0.00055	3.13943
D11	3.14029	-0.00006	0.00000	-0.00040	-0.00040	3.13989
D12	-0.00303	0.00005	0.00000	0.00020	0.00021	-0.00282
D13	-0.00302	0.00018	0.00000	0.00116	0.00117	-0.00185
D14	3.08412	0.00039	0.00000	0.00184	0.00187	3.08599
D15	3.14018	0.00008	0.00000	0.00060	0.00060	3.14079
D16	-0.05587	0.00029	0.00000	0.00128	0.00130	-0.05456
D17	0.05324	-0.00007	0.00000	-0.00039	-0.00040	0.05284
D18	-3.08570	-0.00008	0.00000	-0.00048	-0.00048	-3.08618
D19	-3.09031	0.00006	0.00000	0.00029	0.00029	-3.09001
D20	0.05395	0.00005	0.00000	0.00020	0.00021	0.05415
D21	0.00582	-0.00029	0.00000	-0.00181	-0.00182	0.00400
D22	3.07976	-0.00029	0.00000	-0.00042	-0.00043	3.07934
D23	-3.08518	-0.00051	0.00000	-0.00261	-0.00264	-3.08782
D24	-0.01124	-0.00051	0.00000	-0.00122	-0.00125	-0.01249
D25	-2.75347	-0.00085	0.00000	-0.00559	-0.00562	-2.75909
D26	0.32652	-0.00062	0.00000	-0.00473	-0.00474	0.32178
D27	1.68519	-0.00108	0.00000	-0.00810	-0.00816	1.67702
D28	-2.53248	-0.00017	0.00000	-0.00131	-0.00131	-2.53379
D29	-0.48532	-0.00023	0.00000	-0.00192	-0.00193	-0.48725
D30	-1.37554	-0.00117	0.00000	-0.00996	-0.01002	-1.38556
D31	0.68998	-0.00026	0.00000	-0.00316	-0.00317	0.68681
D32	2.73714	-0.00032	0.00000	-0.00378	-0.00379	2.73335
D33	-1.60211	0.00097	0.00000	0.01171	0.01172	-1.59039
D34	0.47379	0.00049	0.00000	0.00918	0.00918	0.48297
D35	2.60690	0.00167	0.00000	0.01824	0.01827	2.62518
D36	2.62877	-0.00003	0.00000	0.00359	0.00358	2.63236
D37	-1.57851	-0.00052	0.00000	0.00106	0.00104	-1.57747
D38	0.55460	0.00067	0.00000	0.01013	0.01013	0.56474
D39	0.51717	0.00012	0.00000	0.00469	0.00468	0.52185
D40	2.59307	-0.00036	0.00000	0.00216	0.00214	2.59521
D41	-1.55700	0.00082	0.00000	0.01122	0.01123	-1.54577
D42	-1.30188	-0.00159	0.00000	-0.01194	-0.01198	-1.31386
D43	2.87510	-0.00072	0.00000	-0.00571	-0.00572	2.86938
D44	0.80133	-0.00006	0.00000	-0.00292	-0.00292	0.79841
D45	0.41869	-0.00091	0.00000	-0.00670	-0.00671	0.41198
D46	-0.48144	0.00048	0.00000	0.00646	0.00642	-0.47502
D47	-3.04362	-0.00047	0.00000	0.00643	0.00647	-3.03716
D48	-3.13556	-0.00001	0.00000	-0.00010	-0.00010	-3.13566
D49	0.00608	-0.00001	0.00000	-0.00011	-0.00011	0.00598
D50	0.00309	0.00000	0.00000	0.00000	0.00000	0.00309

D51	-3.13845	0.00000	0.00000	-0.00001	-0.00001	-3.13846
D52	-2.42438	-0.00033	0.00000	-0.00106	-0.00108	-2.42546
D53	2.83161	-0.00072	0.00000	-0.00030	-0.00033	2.83128
D54	-2.10761	-0.00005	0.00000	-0.00285	-0.00286	-2.11047
D55	-0.55823	0.00054	0.00000	0.00477	0.00475	-0.55348
D56	-2.73799	0.00077	0.00000	0.00911	0.00909	-2.72890
D57	0.00000	0.00058	0.00000	-0.00416	-0.00415	-0.00415
D58	0.00000	-0.00200	0.00000	0.00205	0.00206	0.00206
D59	2.73799	-0.00218	0.00000	-0.01122	-0.01119	2.72680
D60	1.06791	-0.00043	0.00000	0.00025	0.00022	1.06814
D61	-0.05442	0.00022	0.00000	0.00958	0.00960	-0.04482
D62	-1.27442	0.00104	0.00000	-0.00145	-0.00149	-1.27590
D63	-2.39675	0.00170	0.00000	0.00788	0.00789	-2.38886
D64	1.82841	0.00364	0.00000	0.01639	0.01641	1.84482
D65	-0.49179	-0.00145	0.00000	-0.00668	-0.00672	-0.49851
D66	2.57333	-0.00158	0.00000	0.00003	0.00004	2.57336
D67	-1.61546	-0.00146	0.00000	0.00070	0.00072	-1.61475
D68	0.47893	-0.00093	0.00000	0.00346	0.00348	0.48241
D69	1.37305	0.00278	0.00000	0.00658	0.00660	1.37965
D70	-2.81574	0.00291	0.00000	0.00725	0.00728	-2.80846
D71	-0.72134	0.00344	0.00000	0.01001	0.01004	-0.71130
D72	-0.94530	-0.00242	0.00000	-0.01600	-0.01604	-0.96135
D73	1.14909	-0.00229	0.00000	-0.01533	-0.01537	1.13373
D74	-3.03970	-0.00177	0.00000	-0.01257	-0.01260	-3.05230

Item	Value	Threshold	Converged?
Maximum Force	0.059381	0.000450	NO
RMS Force	0.005724	0.000300	NO
Maximum Displacement	0.181644	0.001800	NO
RMS Displacement	0.054779	0.001200	NO

Predicted change in Energy=-1.715787D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.864014	-2.006007	0.249747
2	6	0	-2.871803	-1.127738	0.010704
3	7	0	-2.302936	0.141573	0.013550
4	6	0	-0.981704	0.022181	0.251068
5	7	0	-0.699057	-1.272459	0.399793
6	6	0	0.672681	-1.791748	0.598742
7	6	0	1.474282	-1.881193	-0.728192

8	1	0	-1.877110	-3.079392	0.329068
9	1	0	-3.919824	-1.296776	-0.156282
10	1	0	1.185244	-1.093715	1.259206
11	1	0	0.580566	-2.758815	1.094307
12	1	0	1.343802	-2.867010	-1.183332
13	1	0	1.088729	-1.123321	-1.420399
14	35	0	1.945754	1.520748	0.142197
15	1	0	-0.206226	0.811853	0.277017
16	6	0	-2.934294	1.398594	-0.191546
17	6	0	-4.237152	1.570339	-0.372714
18	1	0	-2.225100	2.216584	-0.186630
19	1	0	-4.620443	2.569479	-0.526488
20	1	0	-4.953940	0.759091	-0.376414
21	8	0	2.847734	-1.711851	-0.493733
22	1	0	2.995955	-0.757848	-0.327963
23	6	0	5.109563	2.306942	-0.036909
24	6	0	5.775438	1.261749	-0.811536
25	8	0	4.338704	1.242616	-0.647815
26	1	0	5.120139	2.285857	1.059909
27	1	0	4.925474	3.298744	-0.468012
28	1	0	6.104059	1.457937	-1.841759
29	6	0	6.512453	0.108771	-0.126332
30	1	0	6.430995	-0.782922	-0.730348
31	1	0	7.556869	0.359080	-0.001905
32	1	0	6.071628	-0.075729	0.841757

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357990	0.000000			
3	N	2.204664	1.390959	0.000000		
4	C	2.211791	2.225435	1.347710	0.000000	
5	N	1.384821	2.212048	2.172809	1.333455	0.000000
6	C	2.569538	3.653774	3.596453	2.479557	1.480171
7	C	3.480828	4.472372	4.348464	3.257860	2.523155
8	H	1.076392	2.213532	3.264276	3.229179	2.158198
9	H	2.212290	1.074620	2.170718	3.246249	3.268509
10	H	3.339051	4.244943	3.904484	2.637656	2.078733
11	H	2.693691	3.969062	4.230233	3.299345	2.080634
12	H	3.617337	4.714034	4.876761	3.976545	3.036800
13	H	3.505312	4.211162	3.893528	2.897010	2.555684
14	Br	5.192677	5.499147	4.468785	3.290526	3.855306
15	H	3.269455	3.307300	2.216953	1.107077	2.145300
16	C	3.596046	2.535185	1.421541	2.429614	3.532774

17	C	4.336991	3.048082	2.435521	3.658393	4.603953
18	H	4.260409	3.411987	2.086097	2.559886	3.853067
19	H	5.397732	4.125012	3.399589	4.509295	5.567383
20	H	4.193506	2.836420	2.749768	4.088451	4.778464
21	O	4.779106	5.771373	5.497446	4.269214	3.683908
22	H	5.050836	5.889151	5.385521	4.094569	3.800996
23	C	8.204539	8.689159	7.722467	6.512034	6.836877
24	C	8.376501	9.008911	8.197297	6.951591	7.057521
25	O	7.059240	7.618637	6.764693	5.532105	5.727313
26	H	8.237405	8.753547	7.797106	6.558272	6.852766
27	H	8.645965	8.978888	7.902502	6.793209	7.299612
28	H	8.936637	9.522784	8.709336	7.526576	7.665638
29	C	8.647480	9.466361	8.816560	7.504153	7.361419
30	H	8.441783	9.338635	8.814172	7.520603	7.235642
31	H	9.716480	10.534133	9.862215	8.548960	8.425176
32	H	8.188459	9.043358	8.418222	7.078699	6.889823

		6	7	8	9	10
6	C	0.000000				
7	C	1.552843	0.000000			
8	H	2.869178	3.712857	0.000000		
9	H	4.680402	5.455732	2.754264	0.000000	
10	H	1.089120	2.157178	3.766442	5.301562	0.000000
11	H	1.090545	2.211436	2.593941	4.894389	1.779153
12	H	2.186866	1.093624	3.564651	5.588044	3.022533
13	H	2.167215	1.096436	3.960183	5.168529	2.681506
14	Br	3.577957	3.543030	5.984187	6.514026	2.943043
15	H	2.766717	3.329722	4.235133	4.292420	2.555792
16	C	4.879867	5.520918	4.630447	2.870110	5.028606
17	C	6.029412	6.682808	5.261397	2.892730	6.258013
18	H	5.008060	5.547116	5.332392	3.900860	4.967793
19	H	6.950079	7.549493	6.337791	3.946624	7.093215
20	H	6.254324	6.958224	4.969763	2.311805	6.617985
21	O	2.435311	1.403573	4.987115	6.788667	2.493744
22	H	2.706536	1.933281	5.437648	6.938871	2.431170
23	C	6.073650	5.588703	8.829503	9.722698	5.352070
24	C	6.111534	5.327754	8.871751	10.048558	5.559322
25	O	4.919450	4.239051	7.633505	8.654097	4.363425
26	H	6.051398	5.818408	8.847684	9.799761	5.190821
27	H	6.718432	6.229781	9.359012	9.972727	6.022151
28	H	6.783536	5.815896	9.433922	10.531263	6.349933
29	C	6.183902	5.450262	8.986464	10.526579	5.634256
30	H	5.995198	5.076929	8.684512	10.379454	5.618970
31	H	7.237325	6.522589	10.046521	11.596559	6.655720
32	H	5.670309	5.182665	8.512771	10.115145	5.008723

		11	12	13	14	15
11	H	0.000000				
12	H	2.404553	0.000000			
13	H	3.042502	1.778121	0.000000		
14	Br	4.591831	4.622964	3.188620	0.000000	
15	H	3.746555	4.250793	2.881497	2.269742	0.000000
16	C	5.593899	6.122183	4.904574	4.892972	2.829517
17	C	6.641094	7.175947	6.059576	6.204508	4.152808
18	H	5.853815	6.290740	4.864012	4.241266	2.502816
19	H	7.620248	8.096856	6.857878	6.682957	4.818732
20	H	6.720821	7.311722	6.414610	6.960952	4.792759
21	O	2.959401	2.017858	2.073445	3.415797	4.036063
22	H	3.443955	2.812442	2.228115	2.552640	3.617171
23	C	6.888639	6.501155	5.463318	3.264945	5.530954
24	C	6.839873	6.068301	5.293818	3.955144	6.096528
25	O	5.759344	5.113242	4.093516	2.535288	4.658032
26	H	6.786576	6.770885	5.833239	3.391800	5.581736
27	H	7.616632	7.166351	5.931468	3.523117	5.751004
28	H	7.543901	6.465194	5.656320	4.607768	6.687775
29	C	6.700768	6.057018	5.710467	4.787539	6.767397
30	H	6.439025	5.516171	5.397392	5.117189	6.900058
31	H	7.719569	7.099691	6.785754	5.731915	7.781288
32	H	6.116738	5.851885	5.571721	4.478946	6.365390

		16	17	18	19	20
16	C	0.000000				
17	C	1.326559	0.000000			
18	H	1.082630	2.121465	0.000000		
19	H	2.079966	1.081128	2.444935	0.000000	
20	H	2.126525	1.082553	3.099495	1.846955	0.000000
21	O	6.572521	7.809163	6.423438	8.608398	8.184463
22	H	6.311632	7.598703	6.010544	8.313846	8.093471
23	C	8.096458	9.381707	7.336747	9.745852	10.187501
24	C	8.732842	10.026951	8.081511	10.481686	10.749955
25	O	7.288964	8.586523	6.651678	9.057681	9.309171
26	H	8.199223	9.493327	7.450583	9.872995	10.289854
27	H	8.090918	9.324708	7.237469	9.573911	10.201031
28	H	9.187956	10.445638	8.525836	10.861878	11.176535
29	C	9.534617	10.851308	8.988401	11.408619	11.487542
30	H	9.631093	10.930467	9.177181	11.550517	11.494339
31	H	10.544242	11.861853	9.958481	12.387412	12.522803
32	H	9.184115	10.509777	8.668793	11.099081	11.124028

		21	22	23	24	25
21	O	0.000000				
22	H	0.979577	0.000000			

23	C	4.634139	3.734298	0.000000		
24	C	4.185062	3.469602	1.461460	0.000000	
25	O	3.312945	2.430460	1.449213	1.446159	0.000000
26	H	4.853791	3.962636	1.097071	2.231707	2.148327
27	H	5.424364	4.494285	1.097001	2.233786	2.145761
28	H	4.740082	4.106286	2.228748	1.099019	2.142042
29	C	4.108505	3.627319	2.609224	1.530377	2.506539
30	H	3.709266	3.458619	3.431370	2.148727	2.913298
31	H	5.167843	4.706992	3.128050	2.154950	3.399179
32	H	3.854078	3.360549	2.715648	2.147080	2.638159

		26	27	28	29	30
26	H	0.000000				
27	H	1.843469	0.000000			
28	H	3.173834	2.581631	0.000000		
29	C	2.843485	3.579271	2.220298	0.000000	
30	H	3.786921	4.358373	2.522612	1.080087	0.000000
31	H	3.282921	3.972797	2.589055	1.081176	1.761360
32	H	2.555388	3.796872	3.091026	1.079613	1.760903

		31	32
31	H	0.000000	
32	H	1.762602	0.000000

Stoichiometry C10H17BrN2O2
Framework group C1[X(C10H17BrN2O2)]
Deg. of freedom 90
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.361787	1.843505	-0.187767
2	6	0	-4.227686	0.831086	0.075599
3	7	0	-3.487682	-0.346058	0.036967
4	6	0	-2.205624	-0.041169	-0.245333
5	7	0	-2.112102	1.281354	-0.387778
6	6	0	-0.834483	1.988976	-0.628336
7	6	0	-0.005274	2.179899	0.670617
8	1	0	-3.527489	2.905050	-0.253215
9	1	0	-5.282236	0.850539	0.281404
10	1	0	-0.253972	1.374462	-1.315040
11	1	0	-1.078744	2.937276	-1.108285
12	1	0	-0.255378	3.134353	1.142294

13	1	0	-0.255700	1.370419	1.366462
14	35	0	0.904372	-1.116030	-0.258070
15	1	0	-1.328973	-0.714320	-0.308344
16	6	0	-3.929457	-1.680555	0.248466
17	6	0	-5.188084	-2.034292	0.473159
18	1	0	-3.113674	-2.391178	0.208451
19	1	0	-5.422264	-3.078353	0.627864
20	1	0	-6.010484	-1.331399	0.512143
21	8	0	1.368876	2.206190	0.385945
22	1	0	1.642668	1.283577	0.203210
23	6	0	4.151364	-1.452991	-0.200061
24	6	0	4.692665	-0.330658	0.563632
25	8	0	3.262315	-0.511584	0.450756
26	1	0	4.118809	-1.422509	-1.296225
27	1	0	4.123410	-2.463962	0.224870
28	1	0	5.082877	-0.486548	1.579149
29	6	0	5.235974	0.919166	-0.132649
30	1	0	5.052958	1.786184	0.484906
31	1	0	6.299855	0.818424	-0.296810
32	1	0	4.738633	1.047320	-1.082277

Rotational constants (GHZ): 0.8606705 0.1990397 0.1664600

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.

475 basis functions, 751 primitive gaussians, 492 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1340.3218048522 Hartrees.

NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 475 RedAO= T EigKep= 4.43D-06 NBF= 475

NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999992 0.002578 -0.000491 0.003118 Ang= 0.47 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3225.48460998 A.U. after 11 cycles
NFock= 11 Conv=0.99D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000090030	-0.000298278	-0.000173259
2	6	-0.000175577	-0.000370907	0.000089298
3	7	-0.000269214	-0.000037779	0.000089476
4	6	-0.000344965	-0.001183951	-0.000272388
5	7	0.000304262	0.000049383	-0.000433740
6	6	0.000328173	-0.000099932	0.000179300
7	6	0.000067265	0.000303612	-0.000136099
8	1	-0.000032724	-0.000018917	-0.000032473
9	1	0.000013182	-0.000029867	-0.000012749
10	1	-0.000111735	0.000550000	-0.000338153
11	1	0.000200472	-0.000142665	0.000121379
12	1	-0.000249388	-0.000078680	-0.000210337
13	1	0.000294491	0.000232962	0.000371821
14	35	-0.037124936	0.003944985	0.011704051
15	1	0.002757714	0.002267947	0.000246553
16	6	0.000256977	-0.000292516	0.000069488
17	6	-0.000132066	0.000092769	-0.000029119
18	1	0.000079827	-0.000043587	0.000022375
19	1	-0.000002459	-0.000006796	-0.000000894
20	1	0.000025210	-0.000031388	-0.000003755
21	8	-0.000687190	0.000470673	0.000925427
22	1	-0.000328478	0.000297635	-0.000641971
23	6	-0.010493534	0.002274142	-0.001239115
24	6	0.008886896	-0.015616120	-0.000041070

25	8	0.037148314	0.004240279	-0.007174674
26	1	0.001425387	-0.001236194	-0.006384139
27	1	0.001718298	-0.006081061	0.001715544
28	1	-0.001813063	0.003101267	0.005983990
29	6	-0.008166206	0.017450444	-0.009288083
30	1	-0.000014202	-0.007823049	-0.003641796
31	1	0.009190311	0.000431873	0.001221689
32	1	-0.002661011	-0.002316286	0.007313422

Cartesian Forces: Max 0.037148314 RMS 0.006660229

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.036517785 RMS 0.003449870
Search for a local minimum.
Step number 2 out of a maximum of 177
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 1 2
DE= -1.63D-02 DEPred=-1.72D-02 R= 9.48D-01
TightC=F SS= 1.41D+00 RLast= 3.05D-01 DXNew= 5.0454D-01 9.1472D-01
Trust test= 9.48D-01 RLast= 3.05D-01 DXMaxT set to 5.05D-01
ITU= 1 0
Use linear search instead of GDIIS.
Linear search step of 0.600 exceeds DXMaxT= 0.505 but not scaled.
Quartic linear search produced a step of 2.00000.
Iteration 1 RMS(Cart)= 0.04496000 RMS(Int)= 0.02900207
Iteration 2 RMS(Cart)= 0.03728201 RMS(Int)= 0.01293401
Iteration 3 RMS(Cart)= 0.02951295 RMS(Int)= 0.00021819
Iteration 4 RMS(Cart)= 0.00019125 RMS(Int)= 0.00020731
Iteration 5 RMS(Cart)= 0.00000004 RMS(Int)= 0.00020731

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56623	-0.00026	-0.00036	0.00000	-0.00044	2.56579
R2	2.61693	0.00038	0.00186	0.00000	0.00189	2.61882
R3	2.03409	0.00001	0.00004	0.00000	0.00004	2.03413
R4	2.62853	0.00019	0.00039	0.00000	0.00031	2.62884
R5	2.03074	-0.00001	0.00011	0.00000	0.00011	2.03085
R6	2.54680	0.00021	0.00028	0.00000	0.00031	2.54712
R7	2.68632	-0.00034	-0.00150	0.00000	-0.00150	2.68483
R8	2.51987	0.00043	0.00115	0.00000	0.00148	2.52134

R9	2.09207	0.00152	0.00576	0.00000	0.00591	2.09798
R10	2.79712	0.00017	0.00614	0.00000	0.00625	2.80337
R11	2.93445	-0.00009	0.00558	0.00000	0.00572	2.94017
R12	2.05814	0.00009	0.00068	0.00000	0.00068	2.05882
R13	2.06083	0.00016	0.00045	0.00000	0.00045	2.06128
R14	2.06665	0.00019	0.00063	0.00000	0.00063	2.06728
R15	2.07196	-0.00018	-0.00002	0.00000	-0.00002	2.07194
R16	2.65237	-0.00035	0.00558	0.00000	0.00558	2.65795
R17	4.28919	-0.00261	-0.05506	0.00000	-0.05503	4.23416
R18	4.79100	0.03652	0.58002	0.00000	0.57990	5.37090
R19	2.50683	0.00012	0.00041	0.00000	0.00041	2.50724
R20	2.04587	0.00002	0.00024	0.00000	0.00024	2.04611
R21	2.04304	0.00000	0.00000	0.00000	0.00000	2.04304
R22	2.04573	0.00000	0.00006	0.00000	0.00006	2.04579
R23	1.85113	-0.00115	0.00043	0.00000	0.00019	1.85132
R24	4.59290	-0.00069	0.00180	0.00000	0.00165	4.59455
R25	2.76176	0.00013	0.00393	0.00000	0.00398	2.76574
R26	2.73862	-0.00866	-0.04236	0.00000	-0.04243	2.69619
R27	2.07316	-0.00634	-0.03285	0.00000	-0.03285	2.04031
R28	2.07303	-0.00646	-0.03311	0.00000	-0.03311	2.03992
R29	2.73284	0.00357	0.03203	0.00000	0.03204	2.76488
R30	2.07684	-0.00560	-0.02549	0.00000	-0.02549	2.05136
R31	2.89199	-0.00858	-0.03637	0.00000	-0.03637	2.85562
R32	2.04107	0.00850	0.03812	0.00000	0.03812	2.07919
R33	2.04313	0.00912	0.04224	0.00000	0.04224	2.08536
R34	2.04017	0.00804	0.03633	0.00000	0.03633	2.07650
A1	1.87631	0.00016	0.00195	0.00000	0.00204	1.87835
A2	2.27691	-0.00012	-0.00135	0.00000	-0.00139	2.27551
A3	2.12996	-0.00004	-0.00059	0.00000	-0.00064	2.12932
A4	1.86117	-0.00013	-0.00169	0.00000	-0.00169	1.85948
A5	2.27755	0.00004	0.00045	0.00000	0.00045	2.27800
A6	2.14446	0.00009	0.00124	0.00000	0.00124	2.14570
A7	1.89701	0.00033	0.00155	0.00000	0.00166	1.89867
A8	2.24592	0.00008	0.00098	0.00000	0.00093	2.24685
A9	2.14025	-0.00041	-0.00253	0.00000	-0.00258	2.13767
A10	1.88964	-0.00037	-0.00015	0.00000	-0.00027	1.88937
A11	2.24933	0.00006	0.00473	0.00000	0.00425	2.25358
A12	2.14295	0.00031	-0.00450	0.00000	-0.00390	2.13904
A13	1.90063	0.00001	-0.00165	0.00000	-0.00173	1.89890
A14	2.22475	-0.00153	-0.00711	0.00000	-0.00762	2.21714
A15	2.15561	0.00153	0.00897	0.00000	0.00955	2.16517
A16	1.96465	0.00005	0.01173	0.00000	0.01176	1.97641
A17	1.86795	0.00023	0.00635	0.00000	0.00622	1.87417
A18	1.86911	-0.00024	-0.01229	0.00000	-0.01227	1.85684

A19	1.88828	0.00034	0.00243	0.00000	0.00243	1.89071
A20	1.96149	-0.00050	-0.00904	0.00000	-0.00917	1.95232
A21	1.90978	0.00016	0.00147	0.00000	0.00152	1.91130
A22	1.92406	-0.00069	-0.01118	0.00000	-0.01121	1.91285
A23	1.89456	0.00017	0.00347	0.00000	0.00332	1.89788
A24	1.93419	0.00086	0.01528	0.00000	0.01537	1.94956
A25	1.89482	0.00017	-0.00052	0.00000	-0.00049	1.89432
A26	1.87028	-0.00052	-0.01263	0.00000	-0.01260	1.85768
A27	1.94567	-0.00003	0.00497	0.00000	0.00472	1.95040
A28	2.64484	-0.00405	-0.03775	0.00000	-0.03798	2.60686
A29	2.65840	-0.00199	-0.01923	0.00000	-0.01838	2.64002
A30	2.17777	0.00010	0.00049	0.00000	0.00049	2.17827
A31	1.95683	-0.00014	-0.00154	0.00000	-0.00154	1.95530
A32	2.14857	0.00004	0.00104	0.00000	0.00104	2.14962
A33	2.07975	0.00003	0.00010	0.00000	0.00010	2.07985
A34	2.15765	-0.00005	-0.00020	0.00000	-0.00020	2.15745
A35	2.04578	0.00002	0.00010	0.00000	0.00010	2.04588
A36	1.86903	0.00204	0.03189	0.00000	0.03142	1.90045
A37	2.61181	-0.00134	-0.00271	0.00000	-0.00226	2.60955
A38	2.10805	-0.00150	-0.01139	0.00000	-0.01148	2.09657
A39	2.11151	-0.00075	-0.00446	0.00000	-0.00448	2.10704
A40	1.99595	0.00023	-0.00199	0.00000	-0.00202	1.99393
A41	1.99223	-0.00215	-0.00943	0.00000	-0.00925	1.98298
A42	1.99532	0.00149	0.01022	0.00000	0.01013	2.00545
A43	2.10068	-0.00320	-0.02613	0.00000	-0.02598	2.07470
A44	2.11872	0.00327	0.00995	0.00000	0.01007	2.12879
A45	1.98838	-0.00128	0.00407	0.00000	0.00301	1.99139
A46	2.00181	0.00465	0.03094	0.00000	0.03030	2.03211
A47	1.99347	-0.00004	0.00651	0.00000	0.00576	1.99923
A48	1.07905	-0.00101	-0.02756	0.00000	-0.02816	1.05089
A49	1.86516	0.00079	0.02207	0.00000	0.02267	1.88782
A50	2.57340	0.00083	0.00335	0.00000	0.00326	2.57666
A51	2.18298	-0.00087	0.00318	0.00000	0.00362	2.18659
A52	1.91270	0.00147	0.00413	0.00000	0.00408	1.91678
A53	1.92018	0.00186	0.01910	0.00000	0.01901	1.93919
A54	1.91091	0.00097	0.00055	0.00000	0.00051	1.91142
A55	1.90535	-0.00171	-0.01057	0.00000	-0.01066	1.89468
A56	1.90665	-0.00143	-0.00796	0.00000	-0.00795	1.89871
A57	1.90795	-0.00119	-0.00536	0.00000	-0.00544	1.90251
A58	3.26203	-0.00188	-0.02438	0.00000	-0.02455	3.23748
A59	3.38476	-0.00061	-0.01016	0.00000	-0.01025	3.37451
D1	0.00342	-0.00010	-0.00204	0.00000	-0.00209	0.00133
D2	-3.13745	-0.00006	-0.00129	0.00000	-0.00132	-3.13877
D3	3.14010	0.00001	-0.00025	0.00000	-0.00025	3.13985

D4	-0.00077	0.00005	0.00050	0.00000	0.00053	-0.00024
D5	-0.00466	0.00016	0.00355	0.00000	0.00362	-0.00104
D6	-3.07664	0.00004	-0.00019	0.00000	-0.00013	-3.07677
D7	3.14134	0.00007	0.00194	0.00000	0.00197	-3.13987
D8	0.06936	-0.00006	-0.00179	0.00000	-0.00178	0.06758
D9	-0.00105	0.00000	-0.00013	0.00000	-0.00012	-0.00117
D10	3.13943	0.00008	0.00109	0.00000	0.00114	3.14057
D11	3.13989	-0.00003	-0.00081	0.00000	-0.00083	3.13907
D12	-0.00282	0.00005	0.00042	0.00000	0.00044	-0.00238
D13	-0.00185	0.00010	0.00234	0.00000	0.00238	0.00054
D14	3.08599	0.00033	0.00375	0.00000	0.00393	3.08992
D15	3.14079	0.00002	0.00120	0.00000	0.00121	-3.14119
D16	-0.05456	0.00026	0.00261	0.00000	0.00275	-0.05181
D17	0.05284	-0.00006	-0.00080	0.00000	-0.00082	0.05202
D18	-3.08618	-0.00006	-0.00097	0.00000	-0.00099	-3.08717
D19	-3.09001	0.00003	0.00058	0.00000	0.00061	-3.08941
D20	0.05415	0.00003	0.00041	0.00000	0.00043	0.05458
D21	0.00400	-0.00016	-0.00364	0.00000	-0.00370	0.00030
D22	3.07934	-0.00019	-0.00085	0.00000	-0.00090	3.07843
D23	-3.08782	-0.00037	-0.00528	0.00000	-0.00542	-3.09324
D24	-0.01249	-0.00040	-0.00249	0.00000	-0.00262	-0.01510
D25	-2.75909	-0.00072	-0.01124	0.00000	-0.01143	-2.77052
D26	0.32178	-0.00047	-0.00948	0.00000	-0.00954	0.31223
D27	1.67702	-0.00091	-0.01633	0.00000	-0.01666	1.66036
D28	-2.53379	-0.00032	-0.00262	0.00000	-0.00264	-2.53643
D29	-0.48725	-0.00014	-0.00387	0.00000	-0.00396	-0.49121
D30	-1.38556	-0.00097	-0.02005	0.00000	-0.02040	-1.40596
D31	0.68681	-0.00038	-0.00634	0.00000	-0.00637	0.68044
D32	2.73335	-0.00020	-0.00759	0.00000	-0.00769	2.72566
D33	-1.59039	0.00067	0.02345	0.00000	0.02354	-1.56685
D34	0.48297	0.00058	0.01836	0.00000	0.01839	0.50136
D35	2.62518	0.00122	0.03655	0.00000	0.03675	2.66192
D36	2.63236	0.00014	0.00716	0.00000	0.00709	2.63945
D37	-1.57747	0.00005	0.00208	0.00000	0.00195	-1.57553
D38	0.56474	0.00068	0.02027	0.00000	0.02030	0.58504
D39	0.52185	0.00002	0.00936	0.00000	0.00932	0.53117
D40	2.59521	-0.00007	0.00428	0.00000	0.00417	2.59938
D41	-1.54577	0.00057	0.02247	0.00000	0.02253	-1.52324
D42	-1.31386	-0.00120	-0.02396	0.00000	-0.02419	-1.33805
D43	2.86938	-0.00054	-0.01144	0.00000	-0.01151	2.85787
D44	0.79841	-0.00041	-0.00584	0.00000	-0.00580	0.79261
D45	0.41198	-0.00068	-0.01343	0.00000	-0.01351	0.39846
D46	-0.47502	0.00062	0.01283	0.00000	0.01260	-0.46242
D47	-3.03716	-0.00021	0.01293	0.00000	0.01316	-3.02399

D48	-3.13566	0.00000	-0.00019	0.00000	-0.00019	-3.13585
D49	0.00598	-0.00001	-0.00021	0.00000	-0.00021	0.00577
D50	0.00309	0.00000	0.00000	0.00000	0.00000	0.00309
D51	-3.13846	-0.00001	-0.00002	0.00000	-0.00002	-3.13848
D52	-2.42546	-0.00009	-0.00216	0.00000	-0.00230	-2.42776
D53	2.83128	0.00010	-0.00066	0.00000	-0.00085	2.83043
D54	-2.11047	-0.00078	-0.00572	0.00000	-0.00579	-2.11626
D55	-0.55348	0.00071	0.00950	0.00000	0.00940	-0.54408
D56	-2.72890	0.00038	0.01819	0.00000	0.01812	-2.71078
D57	-0.00415	0.00042	-0.00830	0.00000	-0.00823	-0.01239
D58	0.00206	-0.00143	0.00412	0.00000	0.00416	0.00622
D59	2.72680	-0.00139	-0.02237	0.00000	-0.02219	2.70461
D60	1.06814	0.00009	0.00045	0.00000	0.00029	1.06843
D61	-0.04482	0.00113	0.01921	0.00000	0.01934	-0.02548
D62	-1.27590	-0.00014	-0.00298	0.00000	-0.00318	-1.27909
D63	-2.38886	0.00090	0.01578	0.00000	0.01587	-2.37299
D64	1.84482	0.00275	0.03283	0.00000	0.03295	1.87778
D65	-0.49851	-0.00077	-0.01344	0.00000	-0.01367	-0.51219
D66	2.57336	-0.00071	0.00008	0.00000	0.00013	2.57349
D67	-1.61475	-0.00075	0.00143	0.00000	0.00151	-1.61324
D68	0.48241	-0.00045	0.00696	0.00000	0.00706	0.48947
D69	1.37965	0.00153	0.01320	0.00000	0.01331	1.39296
D70	-2.80846	0.00149	0.01455	0.00000	0.01470	-2.79376
D71	-0.71130	0.00179	0.02008	0.00000	0.02024	-0.69106
D72	-0.96135	-0.00145	-0.03209	0.00000	-0.03233	-0.99368
D73	1.13373	-0.00148	-0.03074	0.00000	-0.03095	1.10278
D74	-3.05230	-0.00119	-0.02521	0.00000	-0.02540	-3.07770

Item	Value	Threshold	Converged?
Maximum Force	0.036518	0.000450	NO
RMS Force	0.003450	0.000300	NO
Maximum Displacement	0.351321	0.001800	NO
RMS Displacement	0.108086	0.001200	NO

Predicted change in Energy=-9.148240D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.882482	-2.005638	0.226116
2	6	0	-2.921272	-1.164391	-0.012047
3	7	0	-2.400659	0.125358	0.015078
4	6	0	-1.078226	0.054451	0.265893

5	7	0	-0.746098	-1.231109	0.397095
6	6	0	0.641440	-1.713784	0.603198
7	6	0	1.466873	-1.789990	-0.713460
8	1	0	-1.855682	-3.079794	0.290439
9	1	0	-3.960253	-1.371498	-0.192495
10	1	0	1.133534	-1.012218	1.275964
11	1	0	0.559768	-2.687354	1.088271
12	1	0	1.341884	-2.777031	-1.168296
13	1	0	1.087597	-1.034090	-1.411249
14	35	0	1.784025	1.610464	0.226222
15	1	0	-0.329848	0.872979	0.315842
16	6	0	-3.075433	1.360657	-0.177908
17	6	0	-4.381919	1.487852	-0.370906
18	1	0	-2.395680	2.203061	-0.152414
19	1	0	-4.799841	2.474673	-0.513616
20	1	0	-5.068424	0.651118	-0.394970
21	8	0	2.843987	-1.633722	-0.473755
22	1	0	3.032555	-0.685689	-0.314253
23	6	0	5.265796	2.272921	-0.057003
24	6	0	5.916604	1.208094	-0.821607
25	8	0	4.464506	1.250753	-0.647557
26	1	0	5.284060	2.253826	1.022361
27	1	0	5.111385	3.248810	-0.491829
28	1	0	6.247988	1.417140	-1.833963
29	6	0	6.641723	0.066937	-0.146716
30	1	0	6.544491	-0.846813	-0.751844
31	1	0	7.714546	0.294698	-0.024452
32	1	0	6.199522	-0.115059	0.842617

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357756	0.000000			
3	N	2.203222	1.391124	0.000000		
4	C	2.211872	2.227026	1.347875	0.000000	
5	N	1.385821	2.214324	2.173365	1.334236	0.000000
6	C	2.568570	3.656948	3.603151	2.489513	1.483480
7	C	3.485324	4.487668	4.376886	3.292206	2.538291
8	H	1.076414	2.212633	3.262794	3.229324	2.158748
9	H	2.212351	1.074679	2.171634	3.248004	3.270797
10	H	3.344461	4.257179	3.921025	2.655166	2.086465
11	H	2.678177	3.955724	4.222230	3.298002	2.074526
12	H	3.596661	4.702342	4.881687	3.991380	3.033149
13	H	3.527923	4.248032	3.942926	2.947629	2.582899

14	Br	5.149705	5.467761	4.445414	3.258102	3.808576
15	H	3.271874	3.312683	2.222084	1.110204	2.146405
16	C	3.594205	2.535181	1.420749	2.427339	3.531810
17	C	4.336829	3.049043	2.435315	3.657122	4.604537
18	H	4.256736	3.411112	2.084449	2.554837	3.849234
19	H	5.397348	4.125940	3.399245	4.507275	5.567319
20	H	4.194559	2.837775	2.749824	4.088330	4.780445
21	O	4.792458	5.802728	5.553344	4.333677	3.716071
22	H	5.117798	5.980680	5.503279	4.216977	3.883519
23	C	8.335713	8.879482	7.961894	6.728483	6.973327
24	C	8.500091	9.186519	8.429071	7.172251	7.199066
25	O	7.186908	7.796571	6.988283	5.743466	5.865265
26	H	8.374746	8.948837	8.037407	6.774081	6.992749
27	H	8.777177	9.177696	8.151301	7.006379	7.427648
28	H	9.058911	9.698402	8.937939	7.742074	7.804362
29	C	8.780470	9.642882	9.044019	7.730977	7.520675
30	H	8.562311	9.499938	9.030449	7.742989	7.390564
31	H	9.872045	10.735442	10.116700	8.800843	8.607455
32	H	8.323050	9.220652	8.643249	7.302531	7.048808

		6	7	8	9	10
6	C	0.000000				
7	C	1.555872	0.000000			
8	H	2.863463	3.702807	0.000000		
9	H	4.682505	5.468110	2.753310	0.000000	
10	H	1.089479	2.161909	3.765839	5.313390	0.000000
11	H	1.090782	2.207790	2.573897	4.878773	1.780594
12	H	2.181584	1.093959	3.527606	5.571388	3.021982
13	H	2.172335	1.096424	3.967813	5.203844	2.687695
14	Br	3.535284	3.542129	5.937180	6.485687	2.898889
15	H	2.778006	3.373288	4.237126	4.298363	2.572410
16	C	4.886457	5.553912	4.628688	2.871896	5.045759
17	C	6.036015	6.713416	5.261429	2.895775	6.275567
18	H	5.013653	5.583775	5.328816	3.902174	4.983336
19	H	6.956865	7.582809	6.337719	3.949817	7.110973
20	H	6.260323	6.983592	4.971036	2.315171	6.634983
21	O	2.453050	1.406528	4.976144	6.815096	2.524565
22	H	2.759734	1.957092	5.476519	7.027412	2.498338
23	C	6.141201	5.600893	8.915589	9.920691	5.444679
24	C	6.196354	5.366593	8.946009	10.227530	5.675152
25	O	4.996870	4.270395	7.718696	8.835148	4.462774
26	H	6.121401	5.825500	8.941987	10.003808	5.287554
27	H	6.768075	6.222628	9.444744	10.184864	6.091367
28	H	6.868465	5.865174	9.508152	10.708832	6.459958
29	C	6.303709	5.527066	9.071876	10.699209	5.790401

30	H	6.118317	5.164617	8.754169	10.532702	5.780815
31	H	7.379483	6.622241	10.152616	11.794294	6.834386
32	H	5.788396	5.255925	8.601214	10.289369	5.163034

		11	12	13	14	15
11	H	0.000000				
12	H	2.389946	0.000000			
13	H	3.042940	1.778069	0.000000		
14	Br	4.551172	4.624962	3.187474	0.000000	
15	H	3.750205	4.280179	2.937500	2.240619	0.000000
16	C	5.586080	6.133028	4.958505	4.882628	2.831935
17	C	6.631878	7.182407	6.112128	6.196003	4.155595
18	H	5.847233	6.308940	4.919048	4.238452	2.501209
19	H	7.611699	8.107391	6.912242	6.681430	4.820193
20	H	6.709840	7.310424	6.462922	6.947106	4.796726
21	O	2.961034	2.011431	2.079268	3.483995	4.120708
22	H	3.476840	2.821608	2.260010	2.668943	3.759284
23	C	6.932725	6.491076	5.497968	3.555530	5.780145
24	C	6.893319	6.076963	5.356713	4.282296	6.358007
25	O	5.811090	5.122986	4.148162	2.842158	4.904761
26	H	6.836559	6.756423	5.860303	3.646642	5.824249
27	H	7.645389	7.139853	5.948061	3.777711	5.991988
28	H	7.598826	6.488762	5.728599	4.920233	6.941591
29	C	6.789808	6.100826	5.801691	5.110654	7.033240
30	H	6.526142	5.564737	5.499780	5.445811	7.166183
31	H	7.830813	7.166220	6.899662	6.079897	8.072328
32	H	6.203537	5.892921	5.661829	4.780584	6.624680

		16	17	18	19	20
16	C	0.000000				
17	C	1.326774	0.000000			
18	H	1.082755	2.122359	0.000000		
19	H	2.080219	1.081130	2.446268	0.000000	
20	H	2.126635	1.082586	3.100149	1.847043	0.000000
21	O	6.640284	7.872008	6.502174	8.678052	8.236076
22	H	6.443108	7.726701	6.151163	8.448317	8.210934
23	C	8.391838	9.684692	7.662389	10.078008	10.466163
24	C	9.016339	10.312176	8.398324	10.795428	11.007411
25	O	7.555352	8.853925	6.943646	9.345804	9.555110
26	H	8.492322	9.795870	7.769240	10.202601	10.571255
27	H	8.407595	9.656004	7.587148	9.941436	10.506469
28	H	9.469524	10.730351	8.840717	11.176592	11.433227
29	C	9.802950	11.117101	9.286427	11.697914	11.727338
30	H	9.886621	11.179544	9.465078	11.822981	11.714562
31	H	10.843591	12.160103	10.289553	12.712256	12.793305
32	H	9.446905	10.770740	8.957749	11.381215	11.361570

		21	22	23	24	25
21	O	0.000000				
22	H	0.979676	0.000000			
23	C	4.615268	3.715765	0.000000		
24	C	4.199750	3.487343	1.463566	0.000000	
25	O	3.313078	2.431334	1.426760	1.463113	0.000000
26	H	4.827561	3.936567	1.079688	2.212213	2.113398
27	H	5.383357	4.453465	1.079479	2.218480	2.105929
28	H	4.769187	4.131635	2.203326	1.085532	2.148499
29	C	4.173967	3.690611	2.601459	1.511130	2.528346
30	H	3.793454	3.542759	3.442471	2.149826	2.955841
31	H	5.257663	4.792304	3.148143	2.168489	3.444569
32	H	3.911367	3.419597	2.717280	2.144859	2.663896

		26	27	28	29	30
26	H	0.000000				
27	H	1.820050	0.000000			
28	H	3.128544	2.539332	0.000000		
29	C	2.827096	3.547584	2.196560	0.000000	
30	H	3.788199	4.346899	2.526732	1.100261	0.000000
31	H	3.292607	3.965056	2.585536	1.103527	1.789183
32	H	2.545976	3.778942	3.084487	1.098838	1.787953

		31	32
31	H	0.000000	
32	H	1.793044	0.000000

Stoichiometry C10H17BrN2O2
Framework group C1[X(C10H17BrN2O2)]
Deg. of freedom 90
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.325380	1.894440	-0.180845
2	6	0	-4.235469	0.926676	0.099637
3	7	0	-3.551262	-0.283907	0.059924
4	6	0	-2.259436	-0.042741	-0.239727
5	7	0	-2.103961	1.273905	-0.389581
6	6	0	-0.800124	1.932240	-0.649036
7	6	0	0.054755	2.128966	0.635961
8	1	0	-3.442227	2.962155	-0.251560
9	1	0	-5.285519	0.997574	0.317132

10	1	0	-0.244545	1.294634	-1.335880
11	1	0	-1.026284	2.881874	-1.135710
12	1	0	-0.182437	3.095542	1.090073
13	1	0	-0.196716	1.336789	1.351058
14	35	0	0.781972	-1.209673	-0.297484
15	1	0	-1.412298	-0.756561	-0.313019
16	6	0	-4.050583	-1.595034	0.283869
17	6	0	-5.321286	-1.890477	0.525442
18	1	0	-3.267419	-2.341276	0.237661
19	1	0	-5.600585	-2.922111	0.688436
20	1	0	-6.110446	-1.150756	0.570499
21	8	0	1.430990	2.152203	0.346553
22	1	0	1.736620	1.235542	0.185035
23	6	0	4.328480	-1.407195	-0.139179
24	6	0	4.860735	-0.258761	0.595552
25	8	0	3.421530	-0.493108	0.475257
26	1	0	4.305421	-1.396513	-1.218568
27	1	0	4.319261	-2.390569	0.305979
28	1	0	5.252738	-0.412572	1.596079
29	6	0	5.405044	0.960889	-0.111340
30	1	0	5.210359	1.859931	0.492310
31	1	0	6.493417	0.874527	-0.271831
32	1	0	4.907633	1.073588	-1.084647

Rotational constants (GHZ): 0.8602395 0.1904933 0.1606718

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.

475 basis functions, 751 primitive gaussians, 492 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1322.2801640434 Hartrees.

NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 475 RedAO= T EigKep= 4.43D-06 NBF= 475

NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999960 0.006262 -0.001098 0.006357 Ang= 1.03 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3225.49940141 A.U. after 12 cycles
NFock= 12 Conv=0.73D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000444896	-0.000555426	-0.000429121
2	6	0.000516180	-0.000140179	0.000288251
3	7	-0.000089095	0.000245810	0.000250799
4	6	0.001492793	-0.000762191	-0.000132175
5	7	0.001365910	-0.000020793	-0.001399346
6	6	0.001365000	-0.000561623	0.000974947
7	6	-0.000132037	0.000643081	-0.000965279
8	1	0.000030471	-0.000028131	-0.000062402
9	1	0.000059326	0.000038829	0.000010245
10	1	-0.000780210	0.000741378	-0.000628773
11	1	0.000825955	-0.000025571	0.000447591
12	1	-0.000449683	0.000256536	-0.000641681
13	1	0.000657141	0.000490555	0.000970936
14	35	-0.013833373	0.003550807	0.005011135
15	1	0.000696763	0.000260227	-0.000191085
16	6	-0.000129762	-0.000018556	0.000076628
17	6	0.000078644	0.000148480	-0.000018568
18	1	-0.000213857	0.000044896	-0.000030215
19	1	-0.000007405	-0.000017404	-0.000019940
20	1	0.000067616	-0.000008248	0.000008158
21	8	-0.001406508	0.001339927	0.002424405

22	1	-0.003272927	-0.001055601	-0.001164393
23	6	-0.005887473	-0.000612744	-0.002204591
24	6	-0.003078094	-0.004199321	0.004723377
25	8	0.022885896	-0.008282715	-0.008360802
26	1	0.001845591	-0.000047442	0.005660032
27	1	0.001315919	0.005519770	-0.001872397
28	1	-0.001574058	0.002757554	-0.002487280
29	6	-0.001608778	-0.000415487	0.000537090
30	1	0.001171091	0.002513536	0.003678463
31	1	-0.005299398	-0.001033456	-0.000951976
32	1	0.002943467	-0.000766497	-0.003502031

Cartesian Forces: Max 0.022885896 RMS 0.003512681

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.012939079 RMS 0.001830458

Search for a local minimum.

Step number 3 out of a maximum of 177

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 2 3

ITU= 0 1 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00237	0.00260	0.00356	0.00519	0.00803
Eigenvalues ---	0.01254	0.01347	0.01402	0.01508	0.01850
Eigenvalues ---	0.01902	0.02069	0.02094	0.02144	0.02241
Eigenvalues ---	0.02316	0.02389	0.02564	0.02673	0.03062
Eigenvalues ---	0.03062	0.03190	0.03450	0.03874	0.04247
Eigenvalues ---	0.04317	0.04704	0.05231	0.05512	0.05682
Eigenvalues ---	0.05764	0.06292	0.09500	0.09992	0.10473
Eigenvalues ---	0.10855	0.11585	0.12307	0.12951	0.13476
Eigenvalues ---	0.14614	0.15590	0.15971	0.16000	0.16000
Eigenvalues ---	0.16000	0.16000	0.16000	0.16000	0.16056
Eigenvalues ---	0.16225	0.18677	0.19652	0.21468	0.22000
Eigenvalues ---	0.22780	0.23386	0.23763	0.25001	0.27003
Eigenvalues ---	0.27801	0.28403	0.31434	0.32795	0.33044
Eigenvalues ---	0.33053	0.33815	0.34082	0.34319	0.34416
Eigenvalues ---	0.34763	0.34936	0.35686	0.35690	0.35858
Eigenvalues ---	0.36435	0.36656	0.37227	0.37230	0.37835
Eigenvalues ---	0.38297	0.42170	0.42469	0.44693	0.45601

Eigenvalues --- 0.49053 0.51019 0.54372 0.56006 0.60352

RFO step: Lambda=-8.13149240D-03 EMin= 2.36841589D-03

Quartic linear search produced a step of 0.77028.

Iteration 1 RMS(Cart)= 0.06673376 RMS(Int)= 0.03098657

Iteration 2 RMS(Cart)= 0.03620013 RMS(Int)= 0.01483510

Iteration 3 RMS(Cart)= 0.03272963 RMS(Int)= 0.00045408

Iteration 4 RMS(Cart)= 0.00024085 RMS(Int)= 0.00044627

Iteration 5 RMS(Cart)= 0.00000008 RMS(Int)= 0.00044627

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56579	-0.00038	-0.00034	-0.00063	-0.00116	2.56462
R2	2.61882	-0.00040	0.00145	-0.00218	-0.00066	2.61816
R3	2.03413	0.00002	0.00003	0.00008	0.00012	2.03424
R4	2.62884	0.00004	0.00024	0.00055	0.00061	2.62945
R5	2.03085	-0.00007	0.00009	-0.00028	-0.00019	2.03066
R6	2.54712	0.00011	0.00024	0.00017	0.00049	2.54761
R7	2.68483	0.00024	-0.00115	0.00136	0.00020	2.68503
R8	2.52134	0.00039	0.00114	-0.00071	0.00107	2.52241
R9	2.09798	-0.00022	0.00455	-0.00241	0.00249	2.10047
R10	2.80337	-0.00202	0.00482	-0.01225	-0.00733	2.79604
R11	2.94017	-0.00237	0.00441	-0.01585	-0.01154	2.92863
R12	2.05882	-0.00026	0.00052	-0.00138	-0.00086	2.05796
R13	2.06128	0.00016	0.00034	0.00050	0.00084	2.06212
R14	2.06728	0.00009	0.00049	0.00012	0.00061	2.06790
R15	2.07194	-0.00051	-0.00002	-0.00214	-0.00216	2.06978
R16	2.65795	-0.00366	0.00430	-0.01449	-0.01024	2.64772
R17	4.23416	-0.00171	-0.04239	-0.03294	-0.07513	4.15902
R18	5.37090	0.01294	0.44669	0.16217	0.60885	5.97975
R19	2.50724	-0.00012	0.00031	-0.00044	-0.00013	2.50711
R20	2.04611	-0.00010	0.00018	-0.00047	-0.00029	2.04582
R21	2.04304	-0.00001	0.00000	-0.00003	-0.00003	2.04301
R22	2.04579	-0.00004	0.00005	-0.00019	-0.00014	2.04565
R23	1.85132	-0.00332	0.00014	-0.00896	-0.00922	1.84210
R24	4.59455	-0.00079	0.00127	-0.03706	-0.03615	4.55840
R25	2.76574	0.00139	0.00307	0.00742	0.01030	2.77604
R26	2.69619	0.00143	-0.03268	0.02502	-0.00775	2.68844
R27	2.04031	0.00569	-0.02530	0.03815	0.01285	2.05316
R28	2.03992	0.00555	-0.02551	0.03766	0.01216	2.05208
R29	2.76488	-0.00784	0.02468	-0.04290	-0.01795	2.74693
R30	2.05136	0.00237	-0.01963	0.02061	0.00098	2.05234
R31	2.85562	-0.00166	-0.02802	0.00621	-0.02181	2.83382
R32	2.07919	-0.00421	0.02937	-0.03038	-0.00102	2.07817
R33	2.08536	-0.00547	0.03254	-0.03675	-0.00422	2.08115
R34	2.07650	-0.00421	0.02798	-0.02974	-0.00175	2.07475

A1	1.87835	-0.00020	0.00157	-0.00353	-0.00176	1.87659
A2	2.27551	0.00011	-0.00107	0.00201	0.00084	2.27635
A3	2.12932	0.00008	-0.00049	0.00150	0.00090	2.13022
A4	1.85948	0.00032	-0.00130	0.00275	0.00142	1.86090
A5	2.27800	-0.00013	0.00035	-0.00102	-0.00066	2.27735
A6	2.14570	-0.00019	0.00095	-0.00173	-0.00076	2.14493
A7	1.89867	-0.00008	0.00128	-0.00147	0.00004	1.89871
A8	2.24685	-0.00015	0.00071	-0.00099	-0.00039	2.24646
A9	2.13767	0.00024	-0.00199	0.00246	0.00035	2.13802
A10	1.88937	-0.00040	-0.00020	-0.00173	-0.00219	1.88718
A11	2.25358	-0.00077	0.00327	-0.00246	-0.00042	2.25316
A12	2.13904	0.00118	-0.00301	0.00443	0.00288	2.14192
A13	1.89890	0.00036	-0.00133	0.00398	0.00246	1.90136
A14	2.21714	-0.00190	-0.00587	-0.00264	-0.00949	2.20765
A15	2.16517	0.00153	0.00736	-0.00131	0.00721	2.17237
A16	1.97641	-0.00300	0.00906	-0.02499	-0.01481	1.96160
A17	1.87417	0.00068	0.00479	-0.00313	0.00145	1.87562
A18	1.85684	0.00115	-0.00945	0.01268	0.00263	1.85946
A19	1.89071	0.00123	0.00187	0.00529	0.00657	1.89728
A20	1.95232	0.00026	-0.00707	0.00586	-0.00130	1.95102
A21	1.91130	-0.00028	0.00117	0.00454	0.00586	1.91716
A22	1.91285	0.00046	-0.00863	0.01035	0.00239	1.91524
A23	1.89788	0.00066	0.00256	0.00311	0.00560	1.90348
A24	1.94956	-0.00239	0.01184	-0.03018	-0.01985	1.92971
A25	1.89432	-0.00011	-0.00038	0.00581	0.00528	1.89961
A26	1.85768	0.00057	-0.00971	0.00965	0.00019	1.85787
A27	1.95040	0.00085	0.00364	0.00253	0.00674	1.95714
A28	2.60686	-0.00568	-0.02925	-0.03567	-0.06556	2.54130
A29	2.64002	-0.00100	-0.01416	-0.00450	-0.01713	2.62289
A30	2.17827	0.00003	0.00038	-0.00002	0.00036	2.17863
A31	1.95530	0.00019	-0.00118	0.00223	0.00104	1.95634
A32	2.14962	-0.00022	0.00080	-0.00221	-0.00141	2.14821
A33	2.07985	0.00005	0.00008	0.00046	0.00053	2.08039
A34	2.15745	-0.00008	-0.00016	-0.00068	-0.00084	2.15661
A35	2.04588	0.00003	0.00008	0.00022	0.00030	2.04618
A36	1.90045	-0.00031	0.02420	-0.02106	0.00235	1.90280
A37	2.60955	-0.00341	-0.00174	-0.01546	-0.01520	2.59435
A38	2.09657	0.00040	-0.00884	-0.00791	-0.01700	2.07956
A39	2.10704	0.00014	-0.00345	-0.01067	-0.01443	2.09260
A40	1.99393	0.00139	-0.00156	0.02089	0.01886	2.01278
A41	1.98298	0.00229	-0.00712	0.03403	0.02663	2.00962
A42	2.00545	-0.00069	0.00780	-0.00063	0.00565	2.01111
A43	2.07470	-0.00229	-0.02001	-0.01511	-0.03497	2.03973
A44	2.12879	-0.00013	0.00776	0.00240	0.01016	2.13895

A45	1.99139	-0.00147	0.00232	-0.01819	-0.01661	1.97477
A46	2.03211	-0.00132	0.02334	-0.01587	0.00710	2.03922
A47	1.99923	0.00240	0.00444	0.01872	0.02278	2.02201
A48	1.05089	0.00053	-0.02169	0.00379	-0.01891	1.03198
A49	1.88782	-0.00168	0.01746	-0.02310	-0.00473	1.88310
A50	2.57666	-0.00024	0.00251	-0.00223	-0.00032	2.57633
A51	2.18659	-0.00093	0.00278	0.00854	0.01176	2.19835
A52	1.91678	0.00237	0.00314	0.01993	0.02288	1.93965
A53	1.93919	-0.00132	0.01464	-0.02071	-0.00607	1.93313
A54	1.91142	0.00259	0.00039	0.02423	0.02442	1.93584
A55	1.89468	-0.00084	-0.00821	-0.00662	-0.01482	1.87986
A56	1.89871	-0.00206	-0.00612	-0.01083	-0.01734	1.88137
A57	1.90251	-0.00081	-0.00419	-0.00638	-0.01058	1.89192
A58	3.23748	-0.00040	-0.01891	0.01233	-0.00715	3.23034
A59	3.37451	-0.00007	-0.00790	0.01280	0.00476	3.37927
D1	0.00133	0.00001	-0.00161	0.00545	0.00389	0.00522
D2	-3.13877	0.00004	-0.00101	0.00388	0.00293	-3.13583
D3	3.13985	-0.00001	-0.00019	-0.00028	-0.00056	3.13929
D4	-0.00024	0.00001	0.00041	-0.00185	-0.00152	-0.00176
D5	-0.00104	-0.00005	0.00279	-0.00966	-0.00701	-0.00805
D6	-3.07677	-0.00012	-0.00010	-0.01004	-0.01043	-3.08720
D7	-3.13987	-0.00002	0.00152	-0.00452	-0.00302	3.14029
D8	0.06758	-0.00010	-0.00137	-0.00489	-0.00644	0.06115
D9	-0.00117	0.00003	-0.00010	0.00054	0.00049	-0.00068
D10	3.14057	0.00007	0.00088	-0.00087	-0.00003	3.14054
D11	3.13907	0.00000	-0.00064	0.00196	0.00136	3.14043
D12	-0.00238	0.00005	0.00034	0.00055	0.00084	-0.00154
D13	0.00054	-0.00006	0.00184	-0.00657	-0.00486	-0.00433
D14	3.08992	0.00026	0.00303	-0.00130	0.00149	3.09141
D15	-3.14119	-0.00010	0.00093	-0.00526	-0.00438	3.13761
D16	-0.05181	0.00022	0.00212	0.00001	0.00197	-0.04984
D17	0.05202	-0.00006	-0.00063	-0.00113	-0.00171	0.05030
D18	-3.08717	-0.00003	-0.00076	0.00001	-0.00070	-3.08788
D19	-3.08941	-0.00001	0.00047	-0.00272	-0.00230	-3.09171
D20	0.05458	0.00001	0.00033	-0.00158	-0.00129	0.05330
D21	0.00030	0.00007	-0.00285	0.00999	0.00731	0.00761
D22	3.07843	-0.00002	-0.00070	0.01028	0.00988	3.08831
D23	-3.09324	-0.00016	-0.00417	0.00537	0.00156	-3.09167
D24	-0.01510	-0.00025	-0.00202	0.00566	0.00413	-0.01098
D25	-2.77052	-0.00060	-0.00880	-0.02584	-0.03389	-2.80441
D26	0.31223	-0.00029	-0.00735	-0.02009	-0.02686	0.28537
D27	1.66036	-0.00074	-0.01284	-0.01328	-0.02575	1.63461
D28	-2.53643	-0.00057	-0.00203	-0.02387	-0.02552	-2.56195
D29	-0.49121	0.00002	-0.00305	-0.01378	-0.01667	-0.50788

D30	-1.40596	-0.00075	-0.01571	-0.01387	-0.02936	-1.43532
D31	0.68044	-0.00058	-0.00491	-0.02447	-0.02913	0.65130
D32	2.72566	0.00000	-0.00593	-0.01438	-0.02029	2.70537
D33	-1.56685	0.00034	0.01813	0.05630	0.07448	-1.49238
D34	0.50136	0.00086	0.01417	0.07116	0.08563	0.58699
D35	2.66192	0.00080	0.02831	0.05622	0.08474	2.74666
D36	2.63945	0.00052	0.00546	0.07206	0.07740	2.71684
D37	-1.57553	0.00104	0.00150	0.08692	0.08855	-1.48698
D38	0.58504	0.00098	0.01564	0.07198	0.08766	0.67269
D39	0.53117	-0.00011	0.00718	0.05923	0.06650	0.59767
D40	2.59938	0.00041	0.00321	0.07410	0.07765	2.67703
D41	-1.52324	0.00035	0.01735	0.05915	0.07676	-1.44648
D42	-1.33805	-0.00084	-0.01863	-0.02767	-0.04545	-1.38350
D43	2.85787	-0.00041	-0.00886	-0.02922	-0.03740	2.82047
D44	0.79261	-0.00109	-0.00447	-0.04355	-0.04768	0.74493
D45	0.39846	-0.00039	-0.01041	-0.04441	-0.05474	0.34372
D46	-0.46242	0.00088	0.00971	0.06737	0.07641	-0.38602
D47	-3.02399	0.00040	0.01014	0.05848	0.06835	-2.95564
D48	-3.13585	0.00003	-0.00015	0.00134	0.00119	-3.13465
D49	0.00577	0.00001	-0.00016	0.00064	0.00048	0.00625
D50	0.00309	0.00000	0.00000	0.00008	0.00008	0.00317
D51	-3.13848	-0.00001	-0.00002	-0.00062	-0.00064	-3.13912
D52	-2.42776	0.00027	-0.00177	-0.03080	-0.03352	-2.46127
D53	2.83043	0.00099	-0.00066	0.02802	0.02718	2.85761
D54	-2.11626	-0.00138	-0.00446	-0.01174	-0.01627	-2.13252
D55	-0.54408	0.00107	0.00724	0.01522	0.02242	-0.52166
D56	-2.71078	-0.00015	0.01395	0.01016	0.02384	-2.68694
D57	-0.01239	0.00037	-0.00634	0.03034	0.02375	0.01137
D58	0.00622	-0.00070	0.00320	-0.04234	-0.03880	-0.03258
D59	2.70461	-0.00018	-0.01709	-0.02216	-0.03889	2.66572
D60	1.06843	0.00083	0.00023	0.02274	0.02318	1.09161
D61	-0.02548	0.00241	0.01490	0.05158	0.06717	0.04169
D62	-1.27909	-0.00202	-0.00245	-0.03446	-0.03761	-1.31670
D63	-2.37299	-0.00044	0.01222	-0.00563	0.00638	-2.36661
D64	1.87778	0.00096	0.02538	0.00425	0.02960	1.90738
D65	-0.51219	0.00037	-0.01053	0.01453	0.00405	-0.50814
D66	2.57349	0.00091	0.00010	-0.00643	-0.00620	2.56729
D67	-1.61324	0.00057	0.00116	-0.01490	-0.01372	-1.62695
D68	0.48947	0.00041	0.00544	-0.02019	-0.01482	0.47465
D69	1.39296	-0.00072	0.01025	-0.02087	-0.01039	1.38258
D70	-2.79376	-0.00107	0.01132	-0.02934	-0.01790	-2.81166
D71	-0.69106	-0.00122	0.01559	-0.03462	-0.01900	-0.71006
D72	-0.99368	0.00034	-0.02490	0.00518	-0.01977	-1.01344
D73	1.10278	-0.00001	-0.02384	-0.00329	-0.02728	1.07550

D74 -3.07770 -0.00016 -0.01956 -0.00857 -0.02839 -3.10608

Item	Value	Threshold	Converged?
Maximum Force	0.012939	0.000450	NO
RMS Force	0.001830	0.000300	NO
Maximum Displacement	0.439082	0.001800	NO
RMS Displacement	0.123452	0.001200	NO

Predicted change in Energy=-2.244255D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.842404	-1.998549	0.208363
2	6	0	-2.924953	-1.211632	-0.016759
3	7	0	-2.474630	0.104452	0.018635
4	6	0	-1.148490	0.103217	0.261165
5	7	0	-0.750097	-1.164728	0.384824
6	6	0	0.653300	-1.585076	0.592185
7	6	0	1.453128	-1.646839	-0.733799
8	1	0	-1.757847	-3.070272	0.263676
9	1	0	-3.952195	-1.472402	-0.194218
10	1	0	1.120558	-0.851981	1.248097
11	1	0	0.616602	-2.556153	1.088614
12	1	0	1.302057	-2.619699	-1.211477
13	1	0	1.090987	-0.862302	-1.406849
14	35	0	1.604970	1.760535	0.252229
15	1	0	-0.444979	0.962076	0.315146
16	6	0	-3.216874	1.302745	-0.160254
17	6	0	-4.529101	1.360436	-0.347033
18	1	0	-2.584983	2.181305	-0.130720
19	1	0	-5.001015	2.323977	-0.480066
20	1	0	-5.168501	0.487412	-0.375724
21	8	0	2.827543	-1.536135	-0.485124
22	1	0	3.049236	-0.598395	-0.337735
23	6	0	5.409606	2.229828	-0.076253
24	6	0	6.028226	1.119132	-0.812238
25	8	0	4.586241	1.231330	-0.667045
26	1	0	5.438014	2.225921	1.009856
27	1	0	5.343737	3.212344	-0.533994
28	1	0	6.373506	1.330118	-1.820093
29	6	0	6.690252	-0.036283	-0.122664
30	1	0	6.567801	-0.964938	-0.698851

31	1	0	7.770137	0.145538	-0.005859
32	1	0	6.256634	-0.199365	0.872720

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357141	0.000000			
3	N	2.204159	1.391446	0.000000		
4	C	2.213984	2.227531	1.348136	0.000000	
5	N	1.385472	2.212119	2.172309	1.334801	0.000000
6	C	2.558676	3.648859	3.601029	2.491255	1.479599
7	C	3.445562	4.457707	4.365828	3.289539	2.517528
8	H	1.076475	2.212538	3.263846	3.231463	2.159012
9	H	2.211361	1.074578	2.171399	3.248186	3.268545
10	H	3.342874	4.253865	3.918126	2.652360	2.083842
11	H	2.670669	3.946162	4.216561	3.297342	2.073462
12	H	3.505625	4.612767	4.816382	3.948180	2.979338
13	H	3.536205	4.264054	3.959828	2.954615	2.586724
14	Br	5.100688	5.424604	4.409117	3.213770	3.757803
15	H	3.275591	3.314429	2.223268	1.111522	2.149709
16	C	3.594939	2.535330	1.420857	2.427896	3.531363
17	C	4.337002	3.049247	2.435582	3.657737	4.603579
18	H	4.258824	3.411831	2.085139	2.556470	3.850783
19	H	5.397684	4.126163	3.399650	4.508121	5.566813
20	H	4.193338	2.837096	2.749386	4.088243	4.778106
21	O	4.743749	5.780648	5.573001	4.365004	3.700576
22	H	5.117304	6.014152	5.579793	4.297888	3.908677
23	C	8.399513	9.017320	8.166235	6.902531	7.048229
24	C	8.526921	9.285724	8.603400	7.327314	7.252216
25	O	7.247478	7.925211	7.183029	5.917884	5.943402
26	H	8.455355	9.099996	8.251853	6.960491	7.083776
27	H	8.907588	9.392036	8.431562	7.242096	7.558954
28	H	9.093726	9.806827	9.119906	7.900465	7.863310
29	C	8.761638	9.687355	9.167052	7.849373	7.542528
30	H	8.521909	9.520425	9.133670	7.848804	7.400398
31	H	9.851088	10.780862	10.244878	8.922723	8.629241
32	H	8.323032	9.279947	8.778197	7.436492	7.089728

		6	7	8	9	10
6	C	0.000000				
7	C	1.549765	0.000000			
8	H	2.850852	3.651229	0.000000		
9	H	4.673512	5.434987	2.752820	0.000000	
10	H	1.089026	2.161091	3.764985	5.310180	0.000000
11	H	1.091228	2.201775	2.565706	4.867656	1.784266

12	H	2.178194	1.094283	3.426675	5.473414	3.034349
13	H	2.170278	1.095281	3.972611	5.222679	2.655130
14	Br	3.494904	3.550423	5.886031	6.444631	2.837542
15	H	2.787642	3.392570	4.241002	4.299616	2.571401
16	C	4.887118	5.553190	4.629444	2.871113	5.043770
17	C	6.034522	6.706740	5.261558	2.895021	6.273585
18	H	5.019432	5.596850	5.330925	3.901650	4.983271
19	H	6.957133	7.582066	6.337919	3.948953	7.109635
20	H	6.255032	6.966292	4.969759	2.313702	6.631970
21	O	2.426999	1.401111	4.892860	6.786275	2.527038
22	H	2.752962	1.950298	5.438742	7.057232	2.509775
23	C	6.133737	5.578049	8.920705	10.067955	5.444941
24	C	6.178590	5.346800	8.906831	10.329898	5.675868
25	O	4.998582	4.254963	7.721235	8.968758	4.474250
26	H	6.131201	5.823909	8.965871	10.163828	5.307605
27	H	6.803213	6.228035	9.515252	10.415212	6.126159
28	H	6.858440	5.852558	9.477575	10.822093	6.462880
29	C	6.273321	5.513152	8.984694	10.739145	5.793604
30	H	6.085446	5.160047	8.641487	10.544310	5.785830
31	H	7.348608	6.606596	10.059649	11.834959	6.839909
32	H	5.778948	5.267804	8.534925	10.343073	5.190963

		11	12	13	14	15
11	H	0.000000				
12	H	2.400897	0.000000			
13	H	3.053114	1.780777	0.000000		
14	Br	4.506684	4.628244	3.145789	0.000000	
15	H	3.755414	4.267531	2.941566	2.200860	0.000000
16	C	5.580887	6.075473	4.979869	4.861059	2.832926
17	C	6.624123	7.112745	6.135891	6.176246	4.156588
18	H	5.846403	6.271105	4.940121	4.228404	2.502985
19	H	7.604870	8.043856	6.937131	6.670289	4.821266
20	H	6.698880	7.226392	6.485841	6.920627	4.797319
21	O	2.899198	2.007189	2.078282	3.592549	4.194150
22	H	3.432928	2.811002	2.246640	2.828165	3.882121
23	C	6.872802	6.455897	5.475602	3.847517	6.003045
24	C	6.812241	6.039448	5.353128	4.594528	6.572522
25	O	5.760677	5.090452	4.140943	3.164348	5.133261
26	H	6.791203	6.746888	5.854419	3.934820	6.057188
27	H	7.632445	7.127895	5.954032	4.087086	6.268490
28	H	7.530314	6.456862	5.734326	5.217156	7.154470
29	C	6.686267	6.073895	5.803724	5.406403	7.218027
30	H	6.414340	5.543381	5.523340	5.741293	7.343068
31	H	7.724640	7.136953	6.898518	6.378409	8.261834
32	H	6.116455	5.894890	5.685053	5.085686	6.824328

		16	17	18	19	20
16	C	0.000000				
17	C	1.326707	0.000000			
18	H	1.082602	2.121370	0.000000		
19	H	2.080470	1.081116	2.445324	0.000000	
20	H	2.126039	1.082510	3.099011	1.847136	0.000000
21	O	6.685788	7.907554	6.575744	8.728506	8.248845
22	H	6.550571	7.827407	6.286017	8.565458	8.289248
23	C	8.676560	9.980333	7.994921	10.418875	10.724833
24	C	9.269881	10.570326	8.705174	11.099827	11.223027
25	O	7.819881	9.121871	7.253726	9.651130	9.787404
26	H	8.782284	10.096216	8.103788	10.545274	10.836993
27	H	8.778970	10.046763	8.005640	10.382967	10.860822
28	H	9.732997	11.001712	9.156038	11.496224	11.662517
29	C	9.997278	11.308185	9.536653	11.932489	11.873009
30	H	10.058446	11.343384	9.695105	12.029228	11.830237
31	H	11.048863	12.363803	10.554072	12.964289	12.948437
32	H	9.647318	10.965986	9.211334	11.616022	11.513644

		21	22	23	24	25
21	O	0.000000				
22	H	0.974796	0.000000			
23	C	4.584397	3.693042	0.000000		
24	C	4.171549	3.471230	1.469017	0.000000	
25	O	3.284049	2.412203	1.422660	1.453613	0.000000
26	H	4.816907	3.936880	1.086488	2.212094	2.127610
27	H	5.374167	4.452526	1.085912	2.219793	2.125069
28	H	4.750937	4.119141	2.186221	1.086050	2.129225
29	C	4.159502	3.690423	2.603357	1.499591	2.515961
30	H	3.789653	3.555988	3.454790	2.155770	2.958241
31	H	5.242800	4.790666	3.149813	2.152297	3.428309
32	H	3.922928	3.451352	2.742076	2.151671	2.684768

		26	27	28	29	30
26	H	0.000000				
27	H	1.834501	0.000000			
28	H	3.112270	2.501450	0.000000		
29	C	2.822812	3.540603	2.201964	0.000000	
30	H	3.791791	4.356053	2.561683	1.099721	0.000000
31	H	3.286102	3.946092	2.577838	1.101296	1.777359
32	H	2.563388	3.801576	3.099067	1.097911	1.775602

		31	32
31	H	0.000000	
32	H	1.783690	0.000000

Stoichiometry C10H17BrN2O2

Framework group C1[X(C10H17BrN2O2)]

Deg. of freedom 90

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.227487	1.964874	-0.196060
2	6	0	-4.197858	1.059919	0.089015
3	7	0	-3.592956	-0.192947	0.065781
4	6	0	-2.286375	-0.038869	-0.228458
5	7	0	-2.049289	1.263946	-0.396261
6	6	0	-0.715585	1.844185	-0.667869
7	6	0	0.118262	2.037674	0.624042
8	1	0	-3.275470	3.037087	-0.278861
9	1	0	-5.242039	1.200017	0.300622
10	1	0	-0.186953	1.155035	-1.324831
11	1	0	-0.887598	2.789954	-1.184310
12	1	0	-0.132216	2.997932	1.085151
13	1	0	-0.121584	1.233868	1.328323
14	35	0	0.646127	-1.352254	-0.289880
15	1	0	-1.486392	-0.808061	-0.290513
16	6	0	-4.177578	-1.466481	0.300647
17	6	0	-5.465530	-1.676427	0.539924
18	1	0	-3.445369	-2.263171	0.266264
19	1	0	-5.812095	-2.685744	0.713087
20	1	0	-6.204548	-0.886157	0.573884
21	8	0	1.486072	2.086304	0.324305
22	1	0	1.814286	1.178364	0.189589
23	6	0	4.488961	-1.351607	-0.100107
24	6	0	4.994631	-0.155004	0.585788
25	8	0	3.572567	-0.443664	0.499746
26	1	0	4.477414	-1.373828	-1.186306
27	1	0	4.559218	-2.322111	0.381961
28	1	0	5.399130	-0.295481	1.583862
29	6	0	5.486417	1.052457	-0.155130
30	1	0	5.273245	1.974965	0.404266
31	1	0	6.575443	0.998684	-0.309990
32	1	0	5.000544	1.135112	-1.136203

Rotational constants (GHZ): 0.8548864 0.1849270 0.1565346

Standard basis: 6-311++G(d,p) (5D, 7F)

```
 There are      492 symmetry adapted cartesian basis functions of A      symmetry.
 There are      475 symmetry adapted basis functions of A      symmetry.
    475 basis functions,      751 primitive gaussians,      492 cartesian basis functions
     71 alpha electrons              71 beta electrons
          nuclear repulsion energy          1310.1824125098 Hartrees.
 NAtoms=       32 NActive=       32 NUniq=       32 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      475 RedAO= T EigKep=    4.35D-06    NBF=      475
 NBsUse=      475 1.00D-06 EigRej= -1.00D+00 NBFU=      475
 Initial guess from the checkpoint file:    "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"
 B after Tr=          0.000000        0.000000        0.000000
             Rot=       0.999918       0.010111      -0.000749       0.007854 Ang=      1.47 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn=                5 AccDes=
0.00D+00
 Harris functional with IExCor=    402 and IRadAn=             5 diagonalized for initial guess.
 HarFok:    IExCor=    402 AccDes= 0.00D+00 IRadAn=                5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=    3500011 ScaDFX=    1.000000    1.000000    1.000000    1.000000
 FoFCou: FMM=F IPFlag=                  0 FMFlag=           100000 FMFlg1=                  0
             NFxFlg=                  0 DoJE=T BraDBF=F KetDBF=T FulRan=T
             wScrn=     0.000000  ICntrl=             500  IOpCl=      0  I1Cent=        200000004  NGrid=
0
             NMat0=        1 NMatS0=            1 NMatT0=        0 NMatD0=        1 NMtDS0=        0
NMtDT0=        0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                       energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3225.50616232          A.U. after      12 cycles
                  NFock= 12    Conv=0.32D-08         -V/T= 2.0018
 Calling FoFJK, ICntrl=             2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center         Atomic                             Forces (Hartrees/Bohr)
 Number         Number                       X                      Y                      Z
 -------------------------------------------------------------------
        1              6               -0.000035421        0.000375268        0.000240891
        2              6               -0.000470950        0.000224486       -0.000200566
        3              7               -0.000395429       -0.000182898       -0.000118680
```

4	6	0.000331839	-0.001200452	0.000761598
5	7	-0.000258173	-0.000157741	-0.000886304
6	6	-0.000402457	-0.000754113	-0.000055486
7	6	-0.001352624	-0.001379691	0.000391646
8	1	0.000084094	0.000078698	0.000004116
9	1	-0.000052981	0.000019968	-0.000065776
10	1	-0.000432254	0.000761065	-0.000715723
11	1	0.001089427	0.000287932	0.000413688
12	1	-0.001062929	0.000291415	-0.000964482
13	1	0.000588727	0.000640608	0.000782109
14	35	-0.003524499	0.004146187	0.002232698
15	1	0.000262045	-0.000956155	-0.000108720
16	6	0.000031325	-0.000263974	-0.000080219
17	6	-0.000040261	0.000047929	-0.000042594
18	1	-0.000057900	0.000015511	0.000030944
19	1	-0.000006699	-0.000008987	0.000034130
20	1	-0.000032307	-0.000009762	0.000006292
21	8	0.003420617	0.000624382	0.000866100
22	1	-0.001662758	0.001336800	-0.000567329
23	6	0.001088693	0.000728418	0.001436294
24	6	-0.006478485	0.002977709	0.001769181
25	8	0.010010088	-0.006756256	-0.004690187
26	1	-0.000910460	0.000182287	0.001009439
27	1	-0.000681786	0.001052236	-0.000120015
28	1	0.000085043	-0.000169024	-0.002335763
29	6	0.003171992	-0.006026804	0.003083354
30	1	0.000038869	0.003228915	0.001555712
31	1	-0.003642491	-0.000257504	-0.000581688
32	1	0.001298107	0.001103547	-0.003084663

Cartesian Forces: Max 0.010010088 RMS 0.002034537

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.004966943 RMS 0.001009625
Search for a local minimum.
Step number 4 out of a maximum of 177
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 3 4
DE= -6.76D-03 DEPred=-2.24D-03 R= 3.01D+00

TightC=F SS= 1.41D+00 RLast= 7.01D-01 DXNew= 8.4853D-01 2.1040D+00
Trust test= 3.01D+00 RLast= 7.01D-01 DXMaxT set to 8.49D-01
ITU= 1 0 1 0
Use linear search instead of GDIIS.
Linear search step of 1.253 exceeds DXMaxT= 0.849 but not scaled.
Quartic linear search produced a step of 2.00000.
Iteration 1 RMS(Cart)= 0.12158761 RMS(Int)= 0.07683171
Iteration 2 RMS(Cart)= 0.03835391 RMS(Int)= 0.05931836
Iteration 3 RMS(Cart)= 0.03608290 RMS(Int)= 0.04239193
Iteration 4 RMS(Cart)= 0.03450437 RMS(Int)= 0.02597464
Iteration 5 RMS(Cart)= 0.03307617 RMS(Int)= 0.01016660
Iteration 6 RMS(Cart)= 0.02011576 RMS(Int)= 0.00244668
Iteration 7 RMS(Cart)= 0.00010207 RMS(Int)= 0.00244643
Iteration 8 RMS(Cart)= 0.00000013 RMS(Int)= 0.00244643

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56462	0.00012	-0.00232	0.00000	-0.00312	2.56151
R2	2.61816	0.00002	-0.00132	0.00000	-0.00105	2.61711
R3	2.03424	-0.00007	0.00023	0.00000	0.00023	2.03447
R4	2.62945	-0.00035	0.00122	0.00000	0.00045	2.62990
R5	2.03066	0.00006	-0.00038	0.00000	-0.00038	2.03027
R6	2.54761	0.00079	0.00098	0.00000	0.00130	2.54891
R7	2.68503	-0.00011	0.00041	0.00000	0.00041	2.68544
R8	2.52241	-0.00032	0.00213	0.00000	0.00482	2.52722
R9	2.10047	0.00139	0.00498	0.00000	0.00647	2.10694
R10	2.79604	-0.00003	-0.01467	0.00000	-0.01424	2.78180
R11	2.92863	-0.00069	-0.02308	0.00000	-0.02410	2.90453
R12	2.05796	-0.00010	-0.00171	0.00000	-0.00171	2.05625
R13	2.06212	-0.00010	0.00169	0.00000	0.00169	2.06381
R14	2.06790	0.00031	0.00122	0.00000	0.00122	2.06912
R15	2.06978	-0.00022	-0.00432	0.00000	-0.00432	2.06547
R16	2.64772	0.00158	-0.02047	0.00000	-0.02035	2.62737
R17	4.15902	0.00136	-0.15027	0.00000	-0.14938	4.00964
R18	5.97975	0.00495	1.21770	0.00000	1.21765	7.19741
R19	2.50711	0.00008	-0.00025	0.00000	-0.00025	2.50686
R20	2.04582	-0.00002	-0.00058	0.00000	-0.00058	2.04524
R21	2.04301	-0.00001	-0.00005	0.00000	-0.00005	2.04296
R22	2.04565	0.00002	-0.00029	0.00000	-0.00029	2.04536
R23	1.84210	-0.00093	-0.01844	0.00000	-0.02000	1.82210
R24	4.55840	-0.00152	-0.07230	0.00000	-0.07371	4.48469
R25	2.77604	0.00055	0.02060	0.00000	0.01928	2.79532
R26	2.68844	0.00085	-0.01550	0.00000	-0.01579	2.67264
R27	2.05316	0.00099	0.02570	0.00000	0.02570	2.07886
R28	2.05208	0.00104	0.02431	0.00000	0.02431	2.07639

R29	2.74693	-0.00497	-0.03590	0.00000	-0.03426	2.71267
R30	2.05234	0.00216	0.00196	0.00000	0.00196	2.05430
R31	2.83382	0.00234	-0.04361	0.00000	-0.04361	2.79021
R32	2.07817	-0.00354	-0.00204	0.00000	-0.00204	2.07613
R33	2.08115	-0.00368	-0.00843	0.00000	-0.00843	2.07271
R34	2.07475	-0.00347	-0.00350	0.00000	-0.00350	2.07125
A1	1.87659	0.00031	-0.00353	0.00000	-0.00274	1.87385
A2	2.27635	-0.00006	0.00168	0.00000	0.00123	2.27758
A3	2.13022	-0.00024	0.00181	0.00000	0.00140	2.13162
A4	1.86090	-0.00031	0.00284	0.00000	0.00274	1.86365
A5	2.27735	0.00020	-0.00131	0.00000	-0.00126	2.27609
A6	2.14493	0.00012	-0.00153	0.00000	-0.00148	2.14345
A7	1.89871	0.00025	0.00008	0.00000	0.00103	1.89974
A8	2.24646	-0.00039	-0.00078	0.00000	-0.00126	2.24520
A9	2.13802	0.00013	0.00071	0.00000	0.00023	2.13825
A10	1.88718	-0.00026	-0.00438	0.00000	-0.00542	1.88177
A11	2.25316	-0.00058	-0.00084	0.00000	-0.00612	2.24704
A12	2.14192	0.00084	0.00576	0.00000	0.01193	2.15385
A13	1.90136	0.00001	0.00492	0.00000	0.00410	1.90546
A14	2.20765	0.00025	-0.01898	0.00000	-0.02292	2.18473
A15	2.17237	-0.00026	0.01442	0.00000	0.01921	2.19159
A16	1.96160	-0.00047	-0.02962	0.00000	-0.02200	1.93960
A17	1.87562	-0.00009	0.00291	0.00000	0.00185	1.87747
A18	1.85946	0.00066	0.00525	0.00000	0.00129	1.86075
A19	1.89728	-0.00003	0.01315	0.00000	0.00921	1.90649
A20	1.95102	-0.00009	-0.00260	0.00000	-0.00275	1.94827
A21	1.91716	0.00003	0.01172	0.00000	0.01265	1.92980
A22	1.91524	0.00021	0.00477	0.00000	0.00925	1.92448
A23	1.90348	-0.00035	0.01119	0.00000	0.01044	1.91392
A24	1.92971	-0.00008	-0.03969	0.00000	-0.04835	1.88136
A25	1.89961	-0.00005	0.01057	0.00000	0.00960	1.90921
A26	1.85787	0.00054	0.00037	0.00000	0.00146	1.85933
A27	1.95714	-0.00025	0.01349	0.00000	0.01758	1.97472
A28	2.54130	-0.00466	-0.13111	0.00000	-0.13392	2.40739
A29	2.62289	0.00165	-0.03426	0.00000	-0.02852	2.59437
A30	2.17863	0.00005	0.00072	0.00000	0.00072	2.17935
A31	1.95634	0.00003	0.00209	0.00000	0.00209	1.95843
A32	2.14821	-0.00007	-0.00281	0.00000	-0.00282	2.14540
A33	2.08039	-0.00001	0.00107	0.00000	0.00107	2.08146
A34	2.15661	0.00003	-0.00167	0.00000	-0.00167	2.15494
A35	2.04618	-0.00002	0.00060	0.00000	0.00060	2.04679
A36	1.90280	-0.00093	0.00469	0.00000	0.00255	1.90535
A37	2.59435	-0.00233	-0.03039	0.00000	-0.01959	2.57476
A38	2.07956	0.00106	-0.03400	0.00000	-0.03510	2.04447

A39	2.09260	0.00031	-0.02887	0.00000	-0.03035	2.06225
A40	2.01278	0.00050	0.03771	0.00000	0.03467	2.04745
A41	2.00962	0.00039	0.05327	0.00000	0.05068	2.06030
A42	2.01111	-0.00058	0.01131	0.00000	0.00243	2.01354
A43	2.03973	0.00055	-0.06995	0.00000	-0.06941	1.97031
A44	2.13895	-0.00086	0.02032	0.00000	0.01985	2.15880
A45	1.97477	-0.00026	-0.03323	0.00000	-0.03442	1.94036
A46	2.03922	-0.00068	0.01421	0.00000	0.01404	2.05326
A47	2.02201	0.00026	0.04557	0.00000	0.04552	2.06753
A48	1.03198	0.00119	-0.03781	0.00000	-0.04292	0.98906
A49	1.88310	-0.00225	-0.00946	0.00000	-0.00565	1.87745
A50	2.57633	-0.00108	-0.00065	0.00000	-0.00438	2.57196
A51	2.19835	-0.00037	0.02352	0.00000	0.02529	2.22365
A52	1.93965	-0.00050	0.04575	0.00000	0.04468	1.98433
A53	1.93313	-0.00037	-0.01214	0.00000	-0.01179	1.92133
A54	1.93584	-0.00051	0.04883	0.00000	0.04770	1.98353
A55	1.87986	0.00049	-0.02965	0.00000	-0.02927	1.85059
A56	1.88137	0.00058	-0.03468	0.00000	-0.03686	1.84451
A57	1.89192	0.00037	-0.02117	0.00000	-0.02093	1.87100
A58	3.23034	0.00082	-0.01429	0.00000	-0.01763	3.21271
A59	3.37927	0.00060	0.00952	0.00000	0.00963	3.38889
D1	0.00522	-0.00013	0.00778	0.00000	0.00833	0.01355
D2	-3.13583	-0.00010	0.00586	0.00000	0.00641	-3.12943
D3	3.13929	0.00002	-0.00112	0.00000	-0.00176	3.13753
D4	-0.00176	0.00004	-0.00304	0.00000	-0.00369	-0.00545
D5	-0.00805	0.00018	-0.01403	0.00000	-0.01528	-0.02334
D6	-3.08720	0.00013	-0.02086	0.00000	-0.02319	-3.11039
D7	3.14029	0.00005	-0.00604	0.00000	-0.00622	3.13407
D8	0.06115	0.00000	-0.01287	0.00000	-0.01413	0.04702
D9	-0.00068	0.00003	0.00099	0.00000	0.00129	0.00061
D10	3.14054	0.00005	-0.00006	0.00000	-0.00049	3.14005
D11	3.14043	0.00001	0.00272	0.00000	0.00303	-3.13973
D12	-0.00154	0.00002	0.00168	0.00000	0.00126	-0.00029
D13	-0.00433	0.00008	-0.00972	0.00000	-0.01073	-0.01506
D14	3.09141	0.00005	0.00297	0.00000	0.00071	3.09211
D15	3.13761	0.00007	-0.00876	0.00000	-0.00909	3.12852
D16	-0.04984	0.00003	0.00394	0.00000	0.00235	-0.04749
D17	0.05030	0.00000	-0.00343	0.00000	-0.00302	0.04728
D18	-3.08788	-0.00004	-0.00141	0.00000	-0.00099	-3.08887
D19	-3.09171	0.00002	-0.00460	0.00000	-0.00501	-3.09672
D20	0.05330	-0.00002	-0.00258	0.00000	-0.00299	0.05031
D21	0.00761	-0.00017	0.01463	0.00000	0.01604	0.02365
D22	3.08831	-0.00009	0.01976	0.00000	0.02212	3.11043
D23	-3.09167	-0.00009	0.00313	0.00000	0.00589	-3.08579

D24	-0.01098	-0.00002	0.00826	0.00000	0.01197	0.00100
D25	-2.80441	-0.00008	-0.06777	0.00000	-0.06158	-2.86599
D26	0.28537	-0.00015	-0.05373	0.00000	-0.04902	0.23635
D27	1.63461	0.00001	-0.05150	0.00000	-0.04784	1.58677
D28	-2.56195	-0.00036	-0.05103	0.00000	-0.04832	-2.61027
D29	-0.50788	-0.00003	-0.03334	0.00000	-0.03199	-0.53987
D30	-1.43532	-0.00006	-0.05873	0.00000	-0.05615	-1.49148
D31	0.65130	-0.00044	-0.05826	0.00000	-0.05664	0.59467
D32	2.70537	-0.00011	-0.04057	0.00000	-0.04031	2.66506
D33	-1.49238	0.00040	0.14895	0.00000	0.14905	-1.34332
D34	0.58699	0.00026	0.17126	0.00000	0.17301	0.76000
D35	2.74666	-0.00034	0.16947	0.00000	0.17008	2.91674
D36	2.71684	0.00082	0.15479	0.00000	0.15427	2.87111
D37	-1.48698	0.00068	0.17710	0.00000	0.17823	-1.30875
D38	0.67269	0.00007	0.17531	0.00000	0.17530	0.84799
D39	0.59767	0.00086	0.13300	0.00000	0.13384	0.73151
D40	2.67703	0.00072	0.15530	0.00000	0.15780	2.83483
D41	-1.44648	0.00012	0.15351	0.00000	0.15487	-1.29162
D42	-1.38350	0.00011	-0.09089	0.00000	-0.08379	-1.46729
D43	2.82047	-0.00043	-0.07481	0.00000	-0.07000	2.75047
D44	0.74493	-0.00057	-0.09536	0.00000	-0.09288	0.65204
D45	0.34372	-0.00031	-0.10948	0.00000	-0.10752	0.23620
D46	-0.38602	0.00019	0.15281	0.00000	0.14903	-0.23699
D47	-2.95564	0.00053	0.13670	0.00000	0.13384	-2.82181
D48	-3.13465	-0.00005	0.00239	0.00000	0.00238	-3.13227
D49	0.00625	-0.00001	0.00096	0.00000	0.00096	0.00720
D50	0.00317	-0.00001	0.00016	0.00000	0.00016	0.00333
D51	-3.13912	0.00003	-0.00127	0.00000	-0.00127	-3.14039
D52	-2.46127	-0.00004	-0.06704	0.00000	-0.07039	-2.53167
D53	2.85761	0.00085	0.05436	0.00000	0.05529	2.91289
D54	-2.13252	-0.00069	-0.03254	0.00000	-0.03197	-2.16450
D55	-0.52166	0.00025	0.04484	0.00000	0.04566	-0.47600
D56	-2.68694	-0.00103	0.04768	0.00000	0.04589	-2.64105
D57	0.01137	-0.00106	0.04751	0.00000	0.04554	0.05691
D58	-0.03258	0.00061	-0.07761	0.00000	-0.07552	-0.10810
D59	2.66572	0.00058	-0.07778	0.00000	-0.07587	2.58985
D60	1.09161	-0.00016	0.04636	0.00000	0.04739	1.13900
D61	0.04169	0.00063	0.13435	0.00000	0.13823	0.17993
D62	-1.31670	-0.00029	-0.07523	0.00000	-0.07898	-1.39568
D63	-2.36661	0.00050	0.01276	0.00000	0.01186	-2.35475
D64	1.90738	-0.00031	0.05921	0.00000	0.05883	1.96621
D65	-0.50814	0.00040	0.00810	0.00000	0.00922	-0.49892
D66	2.56729	0.00020	-0.01240	0.00000	-0.01180	2.55549
D67	-1.62695	0.00025	-0.02743	0.00000	-0.02751	-1.65446

D68	0.47465	0.00013	-0.02964	0.00000	-0.03029	0.44437
D69	1.38258	-0.00072	-0.02077	0.00000	-0.01980	1.36278
D70	-2.81166	-0.00067	-0.03580	0.00000	-0.03551	-2.84717
D71	-0.71006	-0.00079	-0.03801	0.00000	-0.03828	-0.74834
D72	-1.01344	0.00024	-0.03954	0.00000	-0.03918	-1.05263
D73	1.07550	0.00029	-0.05456	0.00000	-0.05489	1.02061
D74	-3.10608	0.00017	-0.05677	0.00000	-0.05767	3.11944

Item	Value	Threshold	Converged?
Maximum Force	0.004967	0.000450	NO
RMS Force	0.001010	0.000300	NO
Maximum Displacement	0.815811	0.001800	NO
RMS Displacement	0.244336	0.001200	NO

Predicted change in Energy=-6.579672D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.740008	-1.957737	0.185005
2	6	0	-2.904520	-1.290955	-0.006480
3	7	0	-2.600499	0.066673	0.028159
4	6	0	-1.275684	0.211350	0.236162
5	7	0	-0.743806	-1.010228	0.351734
6	6	0	0.684382	-1.307096	0.549525
7	6	0	1.430241	-1.361074	-0.793304
8	1	0	-1.538772	-3.014363	0.230898
9	1	0	-3.901245	-1.660554	-0.162097
10	1	0	1.103870	-0.510612	1.160792
11	1	0	0.734676	-2.262293	1.076589
12	1	0	1.222697	-2.306761	-1.304649
13	1	0	1.110123	-0.528874	-1.425451
14	35	0	1.229515	2.084744	0.228850
15	1	0	-0.674285	1.149239	0.278417
16	6	0	-3.475486	1.176103	-0.123546
17	6	0	-4.789807	1.089379	-0.281142
18	1	0	-2.946643	2.120151	-0.102074
19	1	0	-5.368939	1.994847	-0.397281
20	1	0	-5.327715	0.150399	-0.302864
21	8	0	2.793936	-1.348632	-0.522683
22	1	0	3.085192	-0.436928	-0.405740
23	6	0	5.661531	2.124258	-0.109148
24	6	0	6.219746	0.929355	-0.778999

25	8	0	4.806299	1.169154	-0.706314
26	1	0	5.701991	2.148240	0.989932
27	1	0	5.775445	3.097767	-0.605750
28	1	0	6.603586	1.142684	-1.773442
29	6	0	6.754177	-0.240987	-0.054585
30	1	0	6.586759	-1.195173	-0.572770
31	1	0	7.840574	-0.146980	0.063512
32	1	0	6.329133	-0.369481	0.947498

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.355490	0.000000			
3	N	2.205285	1.391684	0.000000		
4	C	2.218817	2.229104	1.348826	0.000000	
5	N	1.384915	2.208124	2.170652	1.337350	0.000000
6	C	2.536509	3.631752	3.598543	2.499147	1.472064
7	C	3.370990	4.406151	4.354324	3.294594	2.482073
8	H	1.076597	2.211731	3.265143	3.236428	2.159428
9	H	2.209015	1.074374	2.170588	3.249031	3.264410
10	H	3.336761	4.247194	3.916436	2.653008	2.078003
11	H	2.647968	3.919220	4.200795	3.296479	2.068571
12	H	3.334442	4.444213	4.693229	3.867414	2.879537
13	H	3.571899	4.325692	4.029439	3.000161	2.612879
14	Br	5.016138	5.342376	4.333809	3.128208	3.672594
15	H	3.285999	3.318081	2.223708	1.114945	2.161829
16	C	3.595558	2.534972	1.421073	2.428841	3.531007
17	C	4.336299	3.048891	2.436116	3.658907	4.602066
18	H	4.262342	3.412706	2.086516	2.559303	3.854570
19	H	5.397325	4.125843	3.400457	4.509639	5.566269
20	H	4.189737	2.834999	2.748507	4.088180	4.773655
21	O	4.629091	5.722080	5.604146	4.423935	3.659883
22	H	5.093564	6.063450	5.724419	4.455283	3.945081
23	C	8.457658	9.222335	8.515495	7.204403	7.146031
24	C	8.521871	9.422251	8.899015	7.597866	7.316529
25	O	7.309311	8.123955	7.524333	6.228657	6.055810
26	H	8.537581	9.321638	8.613319	7.280636	7.206352
27	H	9.092054	9.744835	8.930051	7.665419	7.764859
28	H	9.113928	9.972404	9.440273	8.184668	7.945789
29	C	8.669245	9.715719	9.360100	8.047846	7.548283
30	H	8.395878	9.508640	9.292959	8.028118	7.390946
31	H	9.750956	10.806046	10.443319	9.124932	8.632488
32	H	8.259236	9.328426	8.987422	7.660066	7.126847

	6	7	8	9	10

6	C	0.000000				
7	C	1.537013	0.000000			
8	H	2.821117	3.549281	0.000000		
9	H	4.653957	5.377068	2.751095	0.000000	
10	H	1.088120	2.155990	3.757264	5.303167	0.000000
11	H	1.092120	2.189179	2.539561	4.836134	1.792144
12	H	2.174184	1.094930	3.237950	5.289404	3.052650
13	H	2.165044	1.092997	3.992217	5.290612	2.586315
14	Br	3.450301	3.599826	5.802096	6.364338	2.760466
15	H	2.820117	3.446634	4.252667	4.301425	2.587572
16	C	4.891197	5.563452	4.629957	2.868689	5.046289
17	C	6.033229	6.704926	5.260429	2.892377	6.274917
18	H	5.035370	5.635055	5.334437	3.899821	4.992234
19	H	6.960026	7.592621	6.336953	3.946060	7.113520
20	H	6.244692	6.942266	4.965553	2.309585	6.629066
21	O	2.366764	1.390343	4.702649	6.712137	2.528377
22	H	2.726465	1.934713	5.331935	7.096966	2.526873
23	C	6.081122	5.524439	8.852425	10.284663	5.415493
24	C	6.116122	5.309014	8.761702	10.465308	5.657604
25	O	4.969823	4.219880	7.657683	9.171955	4.473889
26	H	6.108166	5.808877	8.925091	10.395010	5.314264
27	H	6.830549	6.228743	9.568484	10.792441	6.161549
28	H	6.814291	5.830349	9.359296	10.991181	6.449030
29	C	6.192249	5.490410	8.749064	10.750105	5.785828
30	H	6.009169	5.163897	8.365380	10.506353	5.791021
31	H	7.265890	6.580314	9.809284	11.841121	6.835162
32	H	5.735914	5.292710	8.331437	10.371051	5.231518

		11	12	13	14	15
11	H	0.000000				
12	H	2.431139	0.000000			
13	H	3.066905	1.785538	0.000000		
14	Br	4.456485	4.651557	3.095475	0.000000	
15	H	3.776347	4.248361	2.983846	2.121811	0.000000
16	C	5.566718	5.966428	5.062580	4.804878	2.830022
17	C	6.602806	6.980798	6.223934	6.122343	4.153819
18	H	5.843558	6.198962	5.022550	4.189399	2.500211
19	H	7.586148	7.923181	7.028836	6.628704	4.817820
20	H	6.669075	7.067468	6.570188	6.857236	4.794787
21	O	2.762789	1.999569	2.078995	3.847114	4.348526
22	H	3.324783	2.788046	2.224672	3.194538	4.137350
23	C	6.702366	6.384857	5.430201	4.445061	6.422105
24	C	6.611794	5.976559	5.352811	5.220449	6.978119
25	O	5.615308	5.028140	4.130639	3.808703	5.568384
26	H	6.643382	6.721325	5.838344	4.537214	6.493162

27	H	7.547838	7.101049	5.965708	4.731623	6.795405
28	H	7.359392	6.408775	5.752681	5.811823	7.561585
29	C	6.449778	6.035508	5.815282	6.000937	7.564765
30	H	6.173006	5.526702	5.582522	6.332496	7.677470
31	H	7.482959	7.094563	6.903755	6.979543	8.615637
32	H	5.907398	5.907699	5.735360	5.704890	7.197364

		16	17	18	19	20
16	C	0.000000				
17	C	1.326573	0.000000			
18	H	1.082296	2.119389	0.000000		
19	H	2.080970	1.081089	2.443433	0.000000	
20	H	2.124847	1.082359	3.096731	1.847323	0.000000
21	O	6.770469	7.969655	6.720388	8.821967	8.261758
22	H	6.761953	8.022515	6.558499	8.796927	8.434011
23	C	9.186092	10.503858	8.608178	11.034991	11.166789
24	C	9.720496	11.021966	9.268167	11.643822	11.583494
25	O	8.302267	9.605852	7.834387	10.213361	10.193080
26	H	9.295750	10.621424	8.717347	11.158556	11.283488
27	H	9.460711	10.759347	8.791146	11.200767	11.491688
28	H	10.213274	11.490831	9.744526	12.081446	12.062470
29	C	10.327580	11.622598	9.984145	12.332329	12.090780
30	H	10.347633	11.607346	10.104389	12.375206	11.993252
31	H	11.394681	12.695429	11.024126	13.389958	13.176741
32	H	9.983312	11.281341	9.661257	12.010135	11.735237

		21	22	23	24	25
21	O	0.000000				
22	H	0.964214	0.000000			
23	C	4.522728	3.644882	0.000000		
24	C	4.122025	3.439692	1.479222	0.000000	
25	O	3.228400	2.373195	1.414303	1.435486	0.000000
26	H	4.793005	3.934289	1.100086	2.209721	2.153630
27	H	5.354134	4.446519	1.098776	2.220231	2.160765
28	H	4.720644	4.092051	2.149611	1.087087	2.090383
29	C	4.138780	3.690956	2.606000	1.476514	2.491481
30	H	3.796256	3.586614	3.477012	2.165836	2.962754
31	H	5.220742	4.787267	3.152231	2.120237	3.395830
32	H	3.951934	3.515530	2.789432	2.163269	2.724245

		26	27	28	29	30
26	H	0.000000				
27	H	1.858279	0.000000			
28	H	3.075752	2.423153	0.000000		
29	C	2.811853	3.522637	2.211717	0.000000	
30	H	3.795163	4.369055	2.628207	1.098643	0.000000
31	H	3.271059	3.903978	2.562767	1.096833	1.753744

32 H 2.595000 3.839395 3.124977 1.096058 1.749100

31 32

31 H 0.000000

32 H 1.765048 0.000000

Stoichiometry C10H17BrN2O2

Framework group C1[X(C10H17BrN2O2)]

Deg. of freedom 90

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.995978	2.093575	-0.230781
2	6	0	-4.081656	1.328372	0.039627
3	7	0	-3.648180	0.005975	0.051777
4	6	0	-2.324545	-0.021070	-0.206273
5	7	0	-1.919227	1.238844	-0.398205
6	6	0	-0.535477	1.661188	-0.669932
7	6	0	0.252597	1.850630	0.636000
8	1	0	-2.900709	3.161187	-0.331727
9	1	0	-5.102968	1.607931	0.221421
10	1	0	-0.064076	0.880106	-1.262972
11	1	0	-0.598910	2.590433	-1.240202
12	1	0	-0.026425	2.795547	1.113652
13	1	0	0.039729	1.022895	1.317311
14	35	0	0.349909	-1.643621	-0.223937
15	1	0	-1.636576	-0.898048	-0.232953
16	6	0	-4.404268	-1.173536	0.289550
17	6	0	-5.713750	-1.205524	0.499390
18	1	0	-3.787056	-2.062584	0.286996
19	1	0	-6.196880	-2.155638	0.679999
20	1	0	-6.339473	-0.322371	0.502805
21	8	0	1.599590	1.955777	0.307963
22	1	0	1.973701	1.071574	0.218882
23	6	0	4.774333	-1.242584	-0.074886
24	6	0	5.238622	0.030997	0.517165
25	8	0	3.853572	-0.346167	0.515782
26	1	0	4.774680	-1.315267	-1.172569
27	1	0	5.001683	-2.175782	0.458744
28	1	0	5.679368	-0.096683	1.502659
29	6	0	5.628084	1.211014	-0.280313

```
      30        1        0        5.388399        2.168549        0.202071
      31        1        0        6.713126        1.215844       -0.440634
      32        1        0        5.154344        1.250038       -1.267931
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.8247900           0.1759470           0.1488064
 Standard basis: 6-311++G(d,p) (5D, 7F)
 There are     492 symmetry adapted cartesian basis functions of A      symmetry.
 There are     475 symmetry adapted basis functions of A      symmetry.
   475 basis functions,      751 primitive gaussians,      492 cartesian basis functions
    71 alpha electrons              71 beta electrons
         nuclear repulsion energy           1291.1060625503 Hartrees.
 NAtoms=       32 NActive=       32 NUniq=       32 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      475 RedAO= T EigKep=    4.17D-06    NBF=      475
 NBsUse=      475 1.00D-06 EigRej= -1.00D+00 NBFU=      475
 Initial guess from the checkpoint file:    "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"
 B after Tr=          0.000000        0.000000        0.000000
             Rot=        0.999669        0.019096       -0.001315        0.017212 Ang=      2.95 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn=                5 AccDes=
0.00D+00
 Harris functional with IExCor=    402 and IRadAn=             5 diagonalized for initial guess.
 HarFok:    IExCor=    402 AccDes= 0.00D+00 IRadAn=                5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=    3500011 ScaDFX=    1.000000    1.000000    1.000000    1.000000
 FoFCou: FMM=F IPFlag=                  0 FMFlag=           100000 FMFlg1=                  0
             NFxFlg=                    0 DoJE=T BraDBF=F KetDBF=T FulRan=T
             wScrn=      0.000000 ICntrl=             500 IOpCl=      0 I1Cent=        200000004 NGrid=
0
             NMat0=        1 NMatS0=            1 NMatT0=        0 NMatD0=        1 NMtDS0=        0
NMtDT0=        0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                    energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3225.50645471          A.U. after      13 cycles
                  NFock= 13    Conv=0.61D-08         -V/T= 2.0018
 Calling FoFJK, ICntrl=             2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 ---------------------------------------------------------------------
```

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.001014399	0.001841418	0.001728383
2	6	-0.003005360	0.000458568	-0.001145816
3	7	-0.000800566	-0.000987043	-0.000834962
4	6	-0.002351774	-0.003869445	0.002502497
5	7	-0.004423735	0.000686782	-0.000451313
6	6	-0.004992731	-0.000577178	-0.001573094
7	6	-0.004684623	-0.005035786	0.003254815
8	1	0.000124492	0.000258219	0.000132417
9	1	-0.000258342	-0.000020606	-0.000243914
10	1	0.000454868	0.000696396	-0.000425052
11	1	0.001944566	0.001030198	0.000107937
12	1	-0.002486419	0.000535940	-0.001216230
13	1	0.000663562	0.001351155	0.000226163
14	35	0.004650041	0.007030873	0.000442050
15	1	-0.000042295	-0.003456182	0.000433586
16	6	0.000386842	-0.000607384	-0.000464351
17	6	-0.000259282	-0.000201304	-0.000105854
18	1	0.000339549	0.000026008	0.000144466
19	1	0.000010108	0.000009351	0.000171385
20	1	-0.000176532	-0.000055854	-0.000019922
21	8	0.013640073	-0.003428683	-0.002844815
22	1	0.003092335	0.007204252	0.000516678
23	6	0.016665913	0.002180395	0.009533308
24	6	-0.008522918	0.017762031	-0.006308286
25	8	-0.007597682	-0.002543658	-0.001400607
26	1	-0.006177720	0.000750915	-0.007556820
27	1	-0.006632641	-0.006117978	0.002806931
28	1	0.003336587	-0.006434833	-0.002058755
29	6	0.011655642	-0.018829313	0.009485993
30	1	-0.001961694	0.004407291	-0.002945982
31	1	-0.000087364	0.000810586	0.000139206
32	1	-0.001488503	0.005124872	-0.002030042

Cartesian Forces: Max 0.018829313 RMS 0.004869347

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.013966608 RMS 0.002716994
Search for a local minimum.

Step number 5 out of a maximum of 177

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 4 5

ITU= 0 1 0 1 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00234	0.00242	0.00317	0.00431	0.00570
Eigenvalues ---	0.00932	0.01282	0.01343	0.01402	0.01550
Eigenvalues ---	0.01857	0.01894	0.01948	0.02106	0.02146
Eigenvalues ---	0.02250	0.02300	0.02313	0.02389	0.02540
Eigenvalues ---	0.03062	0.03062	0.03161	0.03574	0.04226
Eigenvalues ---	0.04614	0.04993	0.05170	0.05287	0.05350
Eigenvalues ---	0.05756	0.06552	0.09194	0.09901	0.10645
Eigenvalues ---	0.10932	0.11250	0.12293	0.13017	0.13535
Eigenvalues ---	0.14090	0.15387	0.15996	0.16000	0.16000
Eigenvalues ---	0.16000	0.16000	0.16000	0.16007	0.16225
Eigenvalues ---	0.16662	0.19147	0.20212	0.21789	0.22000
Eigenvalues ---	0.22794	0.23507	0.24291	0.25000	0.27144
Eigenvalues ---	0.27799	0.28974	0.31746	0.32881	0.33053
Eigenvalues ---	0.33094	0.34026	0.34097	0.34416	0.34759
Eigenvalues ---	0.34929	0.35328	0.35687	0.35690	0.35858
Eigenvalues ---	0.36435	0.36656	0.37230	0.37234	0.37760
Eigenvalues ---	0.38792	0.42174	0.42460	0.45479	0.46487
Eigenvalues ---	0.49131	0.51735	0.54433	0.56034	0.60353

RFO step: Lambda=-2.80650034D-03 EMin= 2.34383587D-03

Quartic linear search produced a step of -0.50853.

Iteration 1 RMS(Cart)= 0.05147494 RMS(Int)= 0.01437236

Iteration 2 RMS(Cart)= 0.02906664 RMS(Int)= 0.00073075

Iteration 3 RMS(Cart)= 0.00022103 RMS(Int)= 0.00072734

Iteration 4 RMS(Cart)= 0.00000016 RMS(Int)= 0.00072734

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56151	0.00141	0.00159	0.00087	0.00271	2.56422
R2	2.61711	0.00111	0.00053	0.00069	0.00111	2.61822
R3	2.03447	-0.00022	-0.00012	-0.00033	-0.00044	2.03403
R4	2.62990	-0.00097	-0.00023	-0.00099	-0.00096	2.62894
R5	2.03027	0.00028	0.00020	0.00034	0.00053	2.03081
R6	2.54891	0.00205	-0.00066	0.00249	0.00173	2.55064
R7	2.68544	-0.00081	-0.00021	-0.00086	-0.00107	2.68437
R8	2.52722	-0.00304	-0.00245	-0.00180	-0.00510	2.52212
R9	2.10694	0.00485	-0.00329	0.00875	0.00503	2.11197
R10	2.78180	0.00502	0.00724	0.00427	0.01135	2.79315
R11	2.90453	0.00359	0.01226	0.00079	0.01342	2.91795
R12	2.05625	0.00044	0.00087	0.00005	0.00092	2.05717

R13	2.06381	-0.00076	-0.00086	-0.00078	-0.00164	2.06217
R14	2.06912	0.00058	-0.00062	0.00141	0.00078	2.06990
R15	2.06547	0.00071	0.00220	-0.00025	0.00194	2.06741
R16	2.62737	0.01397	0.01035	0.01182	0.02212	2.64949
R17	4.00964	0.00776	0.07596	0.07106	0.14677	4.15641
R18	7.19741	0.00184	-0.61921	0.23316	-0.38605	6.81135
R19	2.50686	0.00043	0.00013	0.00032	0.00045	2.50731
R20	2.04524	0.00019	0.00029	0.00009	0.00038	2.04563
R21	2.04296	-0.00002	0.00003	-0.00004	-0.00001	2.04295
R22	2.04536	0.00014	0.00015	0.00015	0.00029	2.04565
R23	1.82210	0.00603	0.01017	0.00067	0.01130	1.83340
R24	4.48469	-0.00247	0.03749	-0.07361	-0.03569	4.44900
R25	2.79532	-0.00013	-0.00981	0.00203	-0.00781	2.78751
R26	2.67264	0.00102	0.00803	0.00218	0.01007	2.68272
R27	2.07886	-0.00776	-0.01307	-0.00331	-0.01637	2.06249
R28	2.07639	-0.00738	-0.01236	-0.00297	-0.01533	2.06105
R29	2.71267	0.00389	0.01742	-0.00934	0.00825	2.72092
R30	2.05430	0.00180	-0.00100	0.00649	0.00549	2.05979
R31	2.79021	0.01194	0.02218	0.01467	0.03685	2.82705
R32	2.07613	-0.00214	0.00104	-0.00842	-0.00739	2.06875
R33	2.07271	0.00000	0.00429	-0.00739	-0.00310	2.06961
R34	2.07125	-0.00188	0.00178	-0.00826	-0.00648	2.06477
A1	1.87385	0.00126	0.00139	0.00287	0.00389	1.87774
A2	2.27758	-0.00043	-0.00063	-0.00054	-0.00103	2.27655
A3	2.13162	-0.00083	-0.00071	-0.00216	-0.00274	2.12889
A4	1.86365	-0.00187	-0.00139	-0.00316	-0.00455	1.85909
A5	2.27609	0.00102	0.00064	0.00196	0.00259	2.27868
A6	2.14345	0.00085	0.00075	0.00121	0.00196	2.14541
A7	1.89974	0.00081	-0.00052	0.00223	0.00138	1.90112
A8	2.24520	-0.00065	0.00064	-0.00225	-0.00144	2.24375
A9	2.13825	-0.00016	-0.00012	0.00002	0.00007	2.13832
A10	1.88177	0.00047	0.00275	-0.00052	0.00242	1.88419
A11	2.24704	0.00013	0.00311	-0.00142	0.00336	2.25040
A12	2.15385	-0.00063	-0.00607	0.00154	-0.00649	2.14736
A13	1.90546	-0.00066	-0.00208	-0.00094	-0.00283	1.90263
A14	2.18473	0.00445	0.01166	0.00401	0.01699	2.20172
A15	2.19159	-0.00378	-0.00977	-0.00263	-0.01393	2.17766
A16	1.93960	0.00517	0.01119	0.00514	0.01395	1.95354
A17	1.87747	-0.00162	-0.00094	-0.00514	-0.00569	1.87177
A18	1.86075	-0.00034	-0.00065	0.01084	0.01131	1.87206
A19	1.90649	-0.00238	-0.00468	-0.00779	-0.01125	1.89524
A20	1.94827	-0.00132	0.00140	-0.00186	-0.00062	1.94765
A21	1.92980	0.00059	-0.00643	-0.00088	-0.00764	1.92216
A22	1.92448	-0.00136	-0.00470	0.00144	-0.00502	1.91946

A23	1.91392	-0.00268	-0.00531	-0.00984	-0.01484	1.89907
A24	1.88136	0.00744	0.02459	0.01132	0.03842	1.91979
A25	1.90921	0.00051	-0.00488	-0.00361	-0.00826	1.90096
A26	1.85933	-0.00025	-0.00074	0.01316	0.01181	1.87114
A27	1.97472	-0.00354	-0.00894	-0.01152	-0.02149	1.95323
A28	2.40739	-0.00228	0.06810	-0.05173	0.01729	2.42467
A29	2.59437	0.00686	0.01450	0.00661	0.01950	2.61388
A30	2.17935	0.00003	-0.00037	0.00030	-0.00007	2.17928
A31	1.95843	-0.00032	-0.00106	-0.00031	-0.00137	1.95705
A32	2.14540	0.00029	0.00143	0.00003	0.00146	2.14685
A33	2.08146	-0.00012	-0.00054	-0.00016	-0.00070	2.08075
A34	2.15494	0.00019	0.00085	0.00030	0.00114	2.15609
A35	2.04679	-0.00007	-0.00031	-0.00013	-0.00044	2.04634
A36	1.90535	-0.00075	-0.00130	-0.00055	-0.00121	1.90413
A37	2.57476	0.00003	0.00996	-0.01160	-0.00479	2.56997
A38	2.04447	0.00198	0.01785	0.01927	0.03632	2.08079
A39	2.06225	0.00050	0.01543	0.01594	0.03062	2.09288
A40	2.04745	-0.00114	-0.01763	-0.01534	-0.03323	2.01422
A41	2.06030	-0.00304	-0.02577	-0.01646	-0.04252	2.01778
A42	2.01354	0.00051	-0.00124	-0.00026	-0.00388	2.00966
A43	1.97031	0.00631	0.03530	0.01533	0.05061	2.02092
A44	2.15880	-0.00214	-0.01010	-0.00062	-0.01055	2.14825
A45	1.94036	0.00258	0.01750	-0.00910	0.00829	1.94864
A46	2.05326	0.00061	-0.00714	0.00080	-0.00638	2.04689
A47	2.06753	-0.00431	-0.02315	-0.00735	-0.03081	2.03672
A48	0.98906	0.00162	0.02183	-0.00052	0.02278	1.01184
A49	1.87745	-0.00217	0.00287	-0.01655	-0.01464	1.86280
A50	2.57196	-0.00213	0.00223	-0.00538	-0.00205	2.56990
A51	2.22365	0.00121	-0.01286	0.00863	-0.00470	2.21894
A52	1.98433	-0.00581	-0.02272	-0.00900	-0.03172	1.95261
A53	1.92133	0.00157	0.00600	0.00197	0.00796	1.92929
A54	1.98353	-0.00611	-0.02425	-0.01100	-0.03526	1.94827
A55	1.85059	0.00285	0.01488	0.00720	0.02209	1.87268
A56	1.84451	0.00619	0.01874	0.00918	0.02792	1.87243
A57	1.87100	0.00238	0.01064	0.00357	0.01419	1.88519
A58	3.21271	0.00283	0.00897	0.00811	0.01808	3.23078
A59	3.38889	0.00151	-0.00490	0.01696	0.01204	3.40094
D1	0.01355	-0.00045	-0.00424	-0.01138	-0.01581	-0.00226
D2	-3.12943	-0.00042	-0.00326	-0.00914	-0.01258	3.14118
D3	3.13753	0.00005	0.00090	0.00034	0.00143	3.13896
D4	-0.00545	0.00008	0.00187	0.00258	0.00466	-0.00079
D5	-0.02334	0.00069	0.00777	0.01769	0.02588	0.00254
D6	-3.11039	0.00054	0.01179	0.00922	0.02169	-3.08870
D7	3.13407	0.00023	0.00316	0.00714	0.01040	-3.13872

D8	0.04702	0.00009	0.00718	-0.00132	0.00621	0.05323
D9	0.00061	0.00004	-0.00065	0.00138	0.00063	0.00124
D10	3.14005	-0.00003	0.00025	0.00193	0.00231	-3.14082
D11	-3.13973	0.00002	-0.00154	-0.00066	-0.00230	3.14116
D12	-0.00029	-0.00006	-0.00064	-0.00011	-0.00061	-0.00090
D13	-0.01506	0.00037	0.00546	0.00958	0.01539	0.00033
D14	3.09211	-0.00046	-0.00036	-0.00341	-0.00309	3.08903
D15	3.12852	0.00044	0.00462	0.00907	0.01383	-3.14083
D16	-0.04749	-0.00039	-0.00120	-0.00391	-0.00465	-0.05214
D17	0.04728	0.00011	0.00154	0.00022	0.00163	0.04891
D18	-3.08887	-0.00005	0.00051	-0.00281	-0.00243	-3.09130
D19	-3.09672	0.00002	0.00255	0.00084	0.00352	-3.09320
D20	0.05031	-0.00013	0.00152	-0.00219	-0.00054	0.04977
D21	0.02365	-0.00068	-0.00815	-0.01683	-0.02540	-0.00175
D22	3.11043	-0.00021	-0.01125	-0.00807	-0.02010	3.09034
D23	-3.08579	0.00008	-0.00299	-0.00463	-0.00849	-3.09427
D24	0.00100	0.00055	-0.00609	0.00413	-0.00318	-0.00218
D25	-2.86599	0.00131	0.03131	0.02158	0.05090	-2.81508
D26	0.23635	0.00038	0.02493	0.00672	0.03013	0.26648
D27	1.58677	0.00124	0.02433	0.00013	0.02337	1.61015
D28	-2.61027	0.00034	0.02457	-0.00959	0.01415	-2.59612
D29	-0.53987	0.00001	0.01627	-0.00758	0.00819	-0.53169
D30	-1.49148	0.00091	0.02856	-0.00980	0.01800	-1.47348
D31	0.59467	0.00002	0.02880	-0.01952	0.00878	0.60344
D32	2.66506	-0.00031	0.02050	-0.01751	0.00281	2.66787
D33	-1.34332	0.00103	-0.07580	0.06137	-0.01451	-1.35783
D34	0.76000	-0.00091	-0.08798	0.05152	-0.03698	0.72302
D35	2.91674	-0.00216	-0.08649	0.03848	-0.04837	2.86836
D36	2.87111	0.00138	-0.07845	0.06949	-0.00877	2.86235
D37	-1.30875	-0.00056	-0.09063	0.05963	-0.03124	-1.33999
D38	0.84799	-0.00181	-0.08914	0.04659	-0.04263	0.80536
D39	0.73151	0.00317	-0.06806	0.07725	0.00892	0.74043
D40	2.83483	0.00123	-0.08024	0.06740	-0.01354	2.82128
D41	-1.29162	-0.00001	-0.07875	0.05436	-0.02494	-1.31655
D42	-1.46729	0.00130	0.04261	-0.01410	0.02664	-1.44064
D43	2.75047	-0.00077	0.03560	-0.02846	0.00540	2.75587
D44	0.65204	0.00085	0.04723	-0.02595	0.02049	0.67253
D45	0.23620	-0.00014	0.05468	-0.05233	0.00151	0.23771
D46	-0.23699	-0.00143	-0.07579	0.04756	-0.02747	-0.26445
D47	-2.82181	0.00044	-0.06806	0.04204	-0.02523	-2.84704
D48	-3.13227	-0.00024	-0.00121	-0.00392	-0.00513	-3.13740
D49	0.00720	-0.00009	-0.00049	-0.00154	-0.00203	0.00517
D50	0.00333	-0.00007	-0.00008	-0.00057	-0.00065	0.00267
D51	-3.14039	0.00009	0.00064	0.00180	0.00244	-3.13794

D52	-2.53167	-0.00143	0.03580	-0.03202	0.00459	-2.52708
D53	2.91289	0.00004	-0.02811	0.01544	-0.01302	2.89987
D54	-2.16450	0.00100	0.01626	-0.01605	0.00009	-2.16441
D55	-0.47600	-0.00147	-0.02322	-0.00152	-0.02507	-0.50107
D56	-2.64105	-0.00221	-0.02334	-0.04803	-0.07217	-2.71322
D57	0.05691	-0.00343	-0.02316	-0.03172	-0.05523	0.00168
D58	-0.10810	0.00295	0.03840	0.01021	0.04895	-0.05915
D59	2.58985	0.00172	0.03858	0.02652	0.06590	2.65575
D60	1.13900	-0.00236	-0.02410	-0.03515	-0.05824	1.08076
D61	0.17993	-0.00342	-0.07029	-0.01003	-0.08013	0.09979
D62	-1.39568	0.00362	0.04016	0.01865	0.05861	-1.33707
D63	-2.35475	0.00256	-0.00603	0.04377	0.03671	-2.31804
D64	1.96621	-0.00292	-0.02992	-0.01988	-0.04978	1.91643
D65	-0.49892	0.00024	-0.00469	0.00362	-0.00124	-0.50016
D66	2.55549	-0.00134	0.00600	-0.02522	-0.01917	2.53632
D67	-1.65446	-0.00043	0.01399	-0.02057	-0.00655	-1.66101
D68	0.44437	-0.00038	0.01540	-0.02203	-0.00658	0.43779
D69	1.36278	-0.00064	0.01007	-0.02825	-0.01807	1.34471
D70	-2.84717	0.00026	0.01806	-0.02360	-0.00544	-2.85261
D71	-0.74834	0.00031	0.01947	-0.02506	-0.00547	-0.75382
D72	-1.05263	-0.00012	0.01993	-0.00267	0.01710	-1.03553
D73	1.02061	0.00079	0.02791	0.00198	0.02973	1.05034
D74	3.11944	0.00084	0.02933	0.00052	0.02970	-3.13405

Item	Value	Threshold	Converged?
Maximum Force	0.013967	0.000450	NO
RMS Force	0.002717	0.000300	NO
Maximum Displacement	0.300403	0.001800	NO
RMS Displacement	0.072462	0.001200	NO

Predicted change in Energy=-2.820706D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.782162	-1.978828	0.203189
2	6	0	-2.922150	-1.275213	-0.012677
3	7	0	-2.570621	0.070150	0.029772
4	6	0	-1.245222	0.169104	0.264988
5	7	0	-0.752780	-1.066820	0.371195
6	6	0	0.675831	-1.390965	0.567902
7	6	0	1.447683	-1.429988	-0.768888
8	1	0	-1.616047	-3.041189	0.251654

9	1	0	-3.928078	-1.610858	-0.186862
10	1	0	1.101693	-0.607057	1.191756
11	1	0	0.721840	-2.350109	1.086322
12	1	0	1.242247	-2.369986	-1.292319
13	1	0	1.113926	-0.596013	-1.393373
14	35	0	1.380489	2.023773	0.255390
15	1	0	-0.607858	1.085590	0.318565
16	6	0	-3.403676	1.208628	-0.136741
17	6	0	-4.717495	1.167183	-0.317285
18	1	0	-2.842199	2.133455	-0.101504
19	1	0	-5.262991	2.092663	-0.438361
20	1	0	-5.287840	0.247712	-0.350673
21	8	0	2.827924	-1.382927	-0.527105
22	1	0	3.095868	-0.459791	-0.395574
23	6	0	5.599993	2.152984	-0.108338
24	6	0	6.173826	0.980714	-0.795643
25	8	0	4.751316	1.185022	-0.706799
26	1	0	5.586411	2.177070	0.982733
27	1	0	5.616479	3.129767	-0.593276
28	1	0	6.543080	1.157055	-1.805910
29	6	0	6.744499	-0.194708	-0.067104
30	1	0	6.560784	-1.133261	-0.599842
31	1	0	7.829099	-0.089343	0.042379
32	1	0	6.312597	-0.298201	0.931186

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.356926	0.000000			
3	N	2.202283	1.391177	0.000000		
4	C	2.214890	2.230525	1.349742	0.000000	
5	N	1.385501	2.212906	2.171133	1.334649	0.000000
6	C	2.553493	3.646360	3.600540	2.493194	1.478070
7	C	3.417317	4.437483	4.362916	3.298140	2.504738
8	H	1.076362	2.212341	3.262035	3.231668	2.158160
9	H	2.211899	1.074657	2.171498	3.251177	3.269545
10	H	3.342998	4.253046	3.910844	2.639949	2.079367
11	H	2.681007	3.954980	4.220693	3.300054	2.081523
12	H	3.396557	4.492017	4.715946	3.880681	2.906140
13	H	3.584483	4.319438	4.005621	2.983479	2.611504
14	Br	5.101559	5.428432	4.413482	3.214692	3.757128
15	H	3.283742	3.322508	2.228668	1.117609	2.157926
16	C	3.592317	2.533125	1.420507	2.429182	3.530286
17	C	4.334104	3.046530	2.435774	3.659492	4.602580

18	H	4.257627	3.410762	2.085238	2.557993	3.851088
19	H	5.394886	4.123509	3.399789	4.509684	5.565943
20	H	4.189752	2.833731	2.749463	4.089986	4.776596
21	O	4.705456	5.774045	5.618348	4.430206	3.705172
22	H	5.144042	6.085069	5.707088	4.435867	3.970958
23	C	8.465526	9.186328	8.433043	7.136674	7.138264
24	C	8.547180	9.404202	8.830390	7.538296	7.316541
25	O	7.316035	8.088056	7.442865	6.159133	6.043834
26	H	8.495590	9.236055	8.478468	7.156695	7.147177
27	H	9.026184	9.625442	8.762309	7.522305	7.688238
28	H	9.120301	9.935904	9.360055	8.119255	7.931895
29	C	8.715509	9.727002	9.319389	8.004891	7.560547
30	H	8.424048	9.502155	9.231856	7.961018	7.378044
31	H	9.796548	10.816593	10.400951	9.080729	8.643623
32	H	8.299374	9.334130	8.936431	7.601501	7.129089

		6	7	8	9	10
6	C	0.000000				
7	C	1.544113	0.000000			
8	H	2.841823	3.608866	0.000000		
9	H	4.670546	5.410201	2.753839	0.000000	
10	H	1.088606	2.154309	3.767612	5.311007	0.000000
11	H	1.091253	2.194373	2.576816	4.877420	1.787074
12	H	2.177092	1.095345	3.317260	5.341401	3.049312
13	H	2.161128	1.094025	4.017183	5.282744	2.585181
14	Br	3.500663	3.603071	5.884989	6.448799	2.806381
15	H	2.800599	3.425775	4.248674	4.306989	2.559312
16	C	4.888434	5.558560	4.626815	2.868277	5.035868
17	C	6.034537	6.705122	5.258619	2.890969	6.268020
18	H	5.024557	5.616637	5.329645	3.899525	4.973651
19	H	6.958293	7.586268	6.335042	3.944783	7.103166
20	H	6.252553	6.953909	4.966058	2.308694	6.628412
21	O	2.414665	1.402048	4.806785	6.768403	2.556625
22	H	2.766216	1.948630	5.411531	7.120698	2.553045
23	C	6.104445	5.524101	8.898330	10.244843	5.435327
24	C	6.141015	5.305528	8.829194	10.446785	5.674267
25	O	4.986998	4.213802	7.702130	9.133409	4.487294
26	H	6.084140	5.762648	8.924131	10.307369	5.282779
27	H	6.796717	6.180701	9.544844	10.664768	6.126458
28	H	6.822902	5.807863	9.403732	10.951155	6.458078
29	C	6.217958	5.484039	8.837579	10.766788	5.796208
30	H	6.005224	5.124493	8.439538	10.507848	5.769609
31	H	7.289694	6.570993	9.897877	11.857435	6.844493
32	H	5.753194	5.276228	8.417193	10.384822	5.226549

		11	12	13	14	15

11	H	0.000000					
12	H	2.434985	0.000000				
13	H	3.062592	1.781476	0.000000			
14	Br	4.500568	4.660433	3.106888	0.000000		
15	H	3.763187	4.237787	2.953482	2.199478	0.000000	
16	C	5.583939	5.977160	5.024399	4.868929	2.835321	
17	C	6.627806	6.998626	6.186461	6.184425	4.159336	
18	H	5.849415	6.195298	4.976932	4.239163	2.503350	
19	H	7.607962	7.934897	6.986136	6.679960	4.822593	
20	H	6.702976	7.097963	6.540773	6.927361	4.801266	
21	O	2.823858	2.018467	2.075438	3.783249	4.314317	
22	H	3.377177	2.808720	2.223118	3.087778	4.076246	
23	C	6.745475	6.391324	5.416003	4.237123	6.313398	
24	C	6.660354	5.982838	5.333473	5.016843	6.873404	
25	O	5.652355	5.029362	4.107806	3.604412	5.457289	
26	H	6.646061	6.687551	5.773992	4.271101	6.324667	
27	H	7.537081	7.061859	5.898692	4.459492	6.614566	
28	H	7.385935	6.387693	5.720064	5.626055	7.460188	
29	C	6.499890	6.042166	5.798567	5.813627	7.472955	
30	H	6.198156	5.504167	5.530514	6.126478	7.560172	
31	H	7.530870	7.097139	6.885611	6.789345	8.522851	
32	H	5.957429	5.911406	5.702494	5.493082	7.083987	

		16	17	18	19	20
16	C	0.000000				
17	C	1.326813	0.000000			
18	H	1.082498	2.120607	0.000000		
19	H	2.080755	1.081082	2.444457	0.000000	
20	H	2.125841	1.082514	3.098269	1.847201	0.000000
21	O	6.760280	7.967460	6.685535	8.806277	8.279839
22	H	6.715259	7.981342	6.486297	8.739988	8.413629
23	C	9.053103	10.366582	8.442218	10.868164	11.055935
24	C	9.602845	10.903415	9.115884	11.496298	11.493697
25	O	8.174927	9.476836	7.676417	10.058937	10.089105
26	H	9.111135	10.434577	8.498173	10.942402	11.124286
27	H	9.233764	10.522306	8.531337	10.929888	11.281369
28	H	10.085967	11.358549	9.588629	11.921781	11.954718
29	C	10.244983	11.545330	9.865410	12.229052	12.043809
30	H	10.246432	11.513968	9.966738	12.257011	11.931432
31	H	11.308937	12.614485	10.901291	13.281381	13.127155
32	H	9.890246	11.196828	9.528363	11.898997	11.683806

		21	22	23	24	25
21	O	0.000000				
22	H	0.970193	0.000000			
23	C	4.512472	3.630391	0.000000		

24	C	4.105359	3.421832	1.475089	0.000000	
25	O	3.213424	2.354311	1.419633	1.439850	0.000000
26	H	4.749994	3.880151	1.091421	2.222373	2.129803
27	H	5.305170	4.390615	1.090662	2.229353	2.131532
28	H	4.678593	4.060358	2.182438	1.089992	2.102199
29	C	4.118620	3.672965	2.612135	1.496012	2.507118
30	H	3.741907	3.535665	3.458916	2.158000	2.942796
31	H	5.197059	4.767862	3.165384	2.141783	3.414385
32	H	3.930164	3.483353	2.756215	2.153328	2.705651

		26	27	28	29	30
26	H	0.000000				
27	H	1.841831	0.000000			
28	H	3.119643	2.494126	0.000000		
29	C	2.840537	3.549848	2.211623	0.000000	
30	H	3.796345	4.366367	2.588524	1.094734	0.000000
31	H	3.324235	3.957577	2.573621	1.095192	1.763756
32	H	2.580110	3.815696	3.108470	1.092627	1.761525

		31	32
31	H	0.000000	
32	H	1.770135	0.000000

Stoichiometry C10H17BrN2O2
Framework group C1[X(C10H17BrN2O2)]
Deg. of freedom 90
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.094107	2.061940	-0.234315
2	6	0	-4.143433	1.253122	0.058901
3	7	0	-3.652053	-0.048384	0.057712
4	6	0	-2.333506	-0.018252	-0.229219
5	7	0	-1.980277	1.256373	-0.407682
6	6	0	-0.602927	1.719428	-0.678198
7	6	0	0.210296	1.900736	0.621833
8	1	0	-3.044381	3.132517	-0.334049
9	1	0	-5.172156	1.488877	0.261477
10	1	0	-0.119639	0.956754	-1.286330
11	1	0	-0.679264	2.653246	-1.237652
12	1	0	-0.074456	2.837011	1.113857
13	1	0	-0.008625	1.065905	1.294159

14	35	0	0.473783	-1.584385	-0.253743
15	1	0	-1.604367	-0.864192	-0.271533
16	6	0	-4.351832	-1.259219	0.306768
17	6	0	-5.654795	-1.347778	0.541031
18	1	0	-3.696508	-2.120575	0.286330
19	1	0	-6.093338	-2.318896	0.723642
20	1	0	-6.318429	-0.492759	0.560224
21	8	0	1.577539	1.987880	0.323856
22	1	0	1.937402	1.092938	0.219683
23	6	0	4.693658	-1.252719	-0.064373
24	6	0	5.164536	0.003698	0.548469
25	8	0	3.769656	-0.352795	0.528683
26	1	0	4.641510	-1.328229	-1.151930
27	1	0	4.832706	-2.199035	0.459742
28	1	0	5.588422	-0.086243	1.548626
29	6	0	5.578441	1.197831	-0.252020
30	1	0	5.315777	2.135380	0.248430
31	1	0	6.663174	1.202077	-0.402953
32	1	0	5.100544	1.209375	-1.234525

Rotational constants (GHZ): 0.8259601 0.1776631 0.1503100

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.

475 basis functions, 751 primitive gaussians, 492 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1292.4415371916 Hartrees.

NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 475 RedAO= T EigKep= 4.32D-06 NBF= 475

NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999968 -0.004406 0.000431 -0.006634 Ang= -0.91 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3225.50991994 A.U. after 12 cycles
NFock= 12 Conv=0.64D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000013433	0.000110410	-0.000786849
2	6	0.000099281	0.000415035	0.000332981
3	7	-0.000085843	0.000524649	-0.000055484
4	6	0.000579732	0.001096955	-0.000333261
5	7	-0.001101821	-0.001343790	0.000862442
6	6	0.000115379	0.000153585	-0.000305388
7	6	-0.002145339	-0.000809140	-0.000022552
8	1	0.000096081	-0.000002819	-0.000037502
9	1	0.000027777	0.000073749	0.000069880
10	1	0.000115914	0.000775707	-0.000063180
11	1	0.000297797	0.000453841	0.000327238
12	1	-0.000122235	0.000381471	-0.000386526
13	1	0.000323605	0.000710202	0.000286042
14	35	-0.000315641	0.003483335	0.000905963
15	1	-0.001041552	-0.004099635	-0.000176619
16	6	-0.000102279	0.000074214	0.000067820
17	6	0.000061256	-0.000096511	0.000044980
18	1	0.000049641	0.000043511	-0.000003268
19	1	0.000019319	0.000004026	-0.000035889
20	1	-0.000081815	0.000014143	-0.000020505
21	8	0.002993952	-0.001956199	0.000129492
22	1	0.000427630	0.003174753	-0.000188743
23	6	0.004350007	0.002150368	0.003581783
24	6	-0.004577208	0.007341117	-0.002676852
25	8	-0.002265209	-0.006578010	-0.002077580

26	1	-0.000756060	-0.000080315	-0.002409059
27	1	-0.001070793	-0.002014581	0.000833607
28	1	0.001978086	-0.001913667	0.000663361
29	6	0.003756854	-0.005840271	0.003177469
30	1	-0.000990242	0.001381054	-0.001393588
31	1	0.000169362	0.000657165	-0.000155416
32	1	-0.000792200	0.001715647	-0.000154799

Cartesian Forces: Max 0.007341117 RMS 0.001845077

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.003277238 RMS 0.000856644

Search for a local minimum.

Step number 6 out of a maximum of 177

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 5 6

DE= -3.47D-03 DEPred=-2.82D-03 R= 1.23D+00

TightC=F SS= 1.41D+00 RLast= 4.97D-01 DXNew= 1.4270D+00 1.4921D+00

Trust test= 1.23D+00 RLast= 4.97D-01 DXMaxT set to 1.43D+00

ITU= 1 0 1 0 1 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00235	0.00244	0.00316	0.00435	0.00572
Eigenvalues ---	0.00918	0.01274	0.01329	0.01402	0.01541
Eigenvalues ---	0.01856	0.01907	0.02041	0.02099	0.02162
Eigenvalues ---	0.02248	0.02315	0.02358	0.02390	0.02488
Eigenvalues ---	0.03062	0.03062	0.03152	0.03642	0.04009
Eigenvalues ---	0.04491	0.05061	0.05287	0.05323	0.05433
Eigenvalues ---	0.05853	0.06443	0.09294	0.09987	0.10711
Eigenvalues ---	0.10937	0.11439	0.11918	0.13133	0.13536
Eigenvalues ---	0.14037	0.14804	0.15828	0.16000	0.16000
Eigenvalues ---	0.16000	0.16000	0.16000	0.16001	0.16094
Eigenvalues ---	0.16275	0.18964	0.20120	0.21982	0.22000
Eigenvalues ---	0.22775	0.23564	0.23986	0.25001	0.27033
Eigenvalues ---	0.27706	0.28643	0.31723	0.32921	0.33053
Eigenvalues ---	0.33292	0.33949	0.34085	0.34416	0.34761
Eigenvalues ---	0.34929	0.35266	0.35686	0.35690	0.35858
Eigenvalues ---	0.36436	0.36658	0.37225	0.37241	0.37767
Eigenvalues ---	0.38649	0.42177	0.42477	0.45478	0.46141
Eigenvalues ---	0.49067	0.51479	0.54477	0.56035	0.60354

RFO step: Lambda=-1.49222661D-03 EMin= 2.34535060D-03
Quartic linear search produced a step of 0.13848.
Iteration 1 RMS(Cart)= 0.07142014 RMS(Int)= 0.00108170
Iteration 2 RMS(Cart)= 0.00290422 RMS(Int)= 0.00024710
Iteration 3 RMS(Cart)= 0.00000381 RMS(Int)= 0.00024709
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00024709

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56422	0.00031	0.00038	0.00065	0.00099	2.56521
R2	2.61822	-0.00014	0.00015	-0.00051	-0.00034	2.61788
R3	2.03403	0.00002	-0.00006	0.00008	0.00002	2.03405
R4	2.62894	-0.00022	-0.00013	-0.00016	-0.00033	2.62861
R5	2.03081	-0.00006	0.00007	-0.00024	-0.00017	2.03064
R6	2.55064	-0.00027	0.00024	-0.00052	-0.00027	2.55037
R7	2.68437	0.00005	-0.00015	0.00019	0.00004	2.68441
R8	2.52212	-0.00038	-0.00071	-0.00090	-0.00146	2.52066
R9	2.11197	-0.00183	0.00070	-0.00550	-0.00476	2.10721
R10	2.79315	0.00045	0.00157	-0.00086	0.00078	2.79393
R11	2.91795	0.00007	0.00186	-0.00358	-0.00181	2.91614
R12	2.05717	0.00057	0.00013	0.00162	0.00174	2.05891
R13	2.06217	-0.00023	-0.00023	-0.00052	-0.00075	2.06142
R14	2.06990	-0.00012	0.00011	-0.00017	-0.00006	2.06984
R15	2.06741	0.00028	0.00027	0.00026	0.00053	2.06794
R16	2.64949	0.00212	0.00306	0.00247	0.00559	2.65508
R17	4.15641	0.00157	0.02032	0.02525	0.04558	4.20199
R18	6.81135	0.00156	-0.05346	0.23674	0.18325	6.99461
R19	2.50731	0.00000	0.00006	-0.00002	0.00004	2.50735
R20	2.04563	0.00006	0.00005	0.00011	0.00017	2.04579
R21	2.04295	0.00000	0.00000	-0.00002	-0.00002	2.04293
R22	2.04565	0.00003	0.00004	0.00006	0.00010	2.04576
R23	1.83340	0.00112	0.00156	-0.00026	0.00127	1.83466
R24	4.44900	-0.00216	-0.00494	-0.11183	-0.11681	4.33219
R25	2.78751	-0.00120	-0.00108	-0.00539	-0.00655	2.78097
R26	2.68272	0.00219	0.00139	0.00847	0.00981	2.69253
R27	2.06249	-0.00240	-0.00227	-0.00433	-0.00659	2.05589
R28	2.06105	-0.00219	-0.00212	-0.00383	-0.00595	2.05510
R29	2.72092	0.00054	0.00114	-0.00308	-0.00180	2.71912
R30	2.05979	-0.00026	0.00076	-0.00044	0.00032	2.06011
R31	2.82705	0.00317	0.00510	0.00620	0.01130	2.83836
R32	2.06875	-0.00034	-0.00102	-0.00150	-0.00252	2.06623
R33	2.06961	0.00022	-0.00043	-0.00077	-0.00120	2.06841
R34	2.06477	0.00001	-0.00090	-0.00065	-0.00155	2.06321
A1	1.87774	-0.00017	0.00054	-0.00138	-0.00082	1.87692
A2	2.27655	0.00017	-0.00014	0.00132	0.00115	2.27770

A3	2.12889	0.00000	-0.00038	0.00005	-0.00036	2.12853
A4	1.85909	0.00017	-0.00063	0.00176	0.00110	1.86019
A5	2.27868	-0.00003	0.00036	-0.00043	-0.00007	2.27861
A6	2.14541	-0.00014	0.00027	-0.00131	-0.00104	2.14438
A7	1.90112	-0.00034	0.00019	-0.00213	-0.00192	1.89920
A8	2.24375	0.00017	-0.00020	0.00092	0.00071	2.24447
A9	2.13832	0.00017	0.00001	0.00121	0.00121	2.13952
A10	1.88419	0.00048	0.00034	0.00170	0.00198	1.88617
A11	2.25040	-0.00073	0.00046	-0.00104	-0.00087	2.24953
A12	2.14736	0.00026	-0.00090	-0.00032	-0.00091	2.14645
A13	1.90263	-0.00014	-0.00039	0.00010	-0.00041	1.90222
A14	2.20172	0.00130	0.00235	0.00505	0.00719	2.20891
A15	2.17766	-0.00117	-0.00193	-0.00557	-0.00720	2.17046
A16	1.95354	0.00013	0.00193	-0.00292	0.00000	1.95354
A17	1.87177	0.00008	-0.00079	-0.00123	-0.00220	1.86957
A18	1.87206	-0.00012	0.00157	0.00263	0.00374	1.87580
A19	1.89524	-0.00023	-0.00156	-0.00270	-0.00473	1.89051
A20	1.94765	0.00012	-0.00009	0.00277	0.00262	1.95027
A21	1.92216	0.00001	-0.00106	0.00140	0.00047	1.92264
A22	1.91946	0.00033	-0.00070	0.00636	0.00609	1.92555
A23	1.89907	-0.00030	-0.00206	-0.00220	-0.00428	1.89480
A24	1.91979	0.00025	0.00532	-0.00659	-0.00230	1.91748
A25	1.90096	0.00007	-0.00114	0.00281	0.00157	1.90253
A26	1.87114	-0.00018	0.00164	0.00248	0.00427	1.87541
A27	1.95323	-0.00016	-0.00298	-0.00248	-0.00502	1.94821
A28	2.42467	-0.00328	0.00239	-0.05020	-0.04841	2.37626
A29	2.61388	0.00299	0.00270	0.00414	0.00676	2.62064
A30	2.17928	0.00001	-0.00001	0.00017	0.00016	2.17943
A31	1.95705	-0.00002	-0.00019	0.00015	-0.00004	1.95702
A32	2.14685	0.00002	0.00020	-0.00032	-0.00012	2.14673
A33	2.08075	-0.00007	-0.00010	-0.00036	-0.00046	2.08029
A34	2.15609	0.00012	0.00016	0.00058	0.00074	2.15682
A35	2.04634	-0.00004	-0.00006	-0.00021	-0.00027	2.04607
A36	1.90413	-0.00117	-0.00017	-0.00972	-0.00989	1.89424
A37	2.56997	-0.00114	-0.00066	-0.00892	-0.00873	2.56124
A38	2.08079	0.00037	0.00503	0.00131	0.00612	2.08691
A39	2.09288	-0.00006	0.00424	0.00330	0.00724	2.10011
A40	2.01422	-0.00063	-0.00460	-0.00376	-0.00855	2.00566
A41	2.01778	-0.00007	-0.00589	-0.00284	-0.00891	2.00887
A42	2.00966	0.00009	-0.00054	0.00053	-0.00100	2.00865
A43	2.02092	0.00225	0.00701	0.00419	0.01126	2.03218
A44	2.14825	-0.00128	-0.00146	-0.00247	-0.00404	2.14422
A45	1.94864	0.00159	0.00115	0.00993	0.01098	1.95962
A46	2.04689	-0.00103	-0.00088	-0.00045	-0.00133	2.04555

A47	2.03672	-0.00126	-0.00427	-0.00696	-0.01127	2.02545
A48	1.01184	0.00094	0.00315	0.00291	0.00572	1.01756
A49	1.86280	-0.00131	-0.00203	-0.01875	-0.02054	1.84226
A50	2.56990	-0.00066	-0.00028	-0.00454	-0.00499	2.56492
A51	2.21894	0.00116	-0.00065	0.01011	0.00959	2.22853
A52	1.95261	-0.00252	-0.00439	-0.01138	-0.01589	1.93673
A53	1.92929	0.00003	0.00110	-0.00029	0.00083	1.93012
A54	1.94827	-0.00204	-0.00488	-0.00814	-0.01314	1.93513
A55	1.87268	0.00146	0.00306	0.00775	0.01084	1.88352
A56	1.87243	0.00226	0.00387	0.00827	0.01190	1.88433
A57	1.88519	0.00110	0.00197	0.00511	0.00708	1.89227
A58	3.23078	0.00210	0.00250	0.01302	0.01531	3.24609
A59	3.40094	0.00133	0.00167	0.02537	0.02705	3.42798
D1	-0.00226	0.00021	-0.00219	0.01320	0.01109	0.00883
D2	3.14118	0.00014	-0.00174	0.00789	0.00621	-3.13579
D3	3.13896	0.00005	0.00020	0.00255	0.00269	-3.14154
D4	-0.00079	-0.00002	0.00065	-0.00276	-0.00219	-0.00297
D5	0.00254	-0.00027	0.00358	-0.01811	-0.01466	-0.01213
D6	-3.08870	-0.00008	0.00300	-0.00883	-0.00606	-3.09476
D7	-3.13872	-0.00013	0.00144	-0.00855	-0.00714	3.13733
D8	0.05323	0.00006	0.00086	0.00073	0.00146	0.05470
D9	0.00124	-0.00008	0.00009	-0.00399	-0.00388	-0.00264
D10	-3.14082	-0.00004	0.00032	-0.00371	-0.00345	3.13891
D11	3.14116	-0.00001	-0.00032	0.00082	0.00053	-3.14150
D12	-0.00090	0.00003	-0.00009	0.00109	0.00096	0.00006
D13	0.00033	-0.00009	0.00213	-0.00720	-0.00519	-0.00486
D14	3.08903	0.00010	-0.00043	-0.00002	-0.00072	3.08830
D15	-3.14083	-0.00013	0.00191	-0.00746	-0.00559	3.13676
D16	-0.05214	0.00006	-0.00064	-0.00028	-0.00112	-0.05325
D17	0.04891	-0.00003	0.00023	-0.00139	-0.00112	0.04779
D18	-3.09130	-0.00002	-0.00034	-0.00029	-0.00058	-3.09189
D19	-3.09320	0.00001	0.00049	-0.00108	-0.00064	-3.09385
D20	0.04977	0.00003	-0.00008	0.00002	-0.00011	0.04966
D21	-0.00175	0.00022	-0.00352	0.01552	0.01219	0.01043
D22	3.09034	0.00012	-0.00278	0.00678	0.00432	3.09466
D23	-3.09427	0.00009	-0.00118	0.00889	0.00804	-3.08623
D24	-0.00218	-0.00001	-0.00044	0.00015	0.00018	-0.00200
D25	-2.81508	-0.00015	0.00705	-0.00934	-0.00154	-2.81663
D26	0.26648	0.00005	0.00417	-0.00114	0.00360	0.27008
D27	1.61015	-0.00011	0.00324	-0.01611	-0.01243	1.59772
D28	-2.59612	-0.00026	0.00196	-0.02188	-0.01960	-2.61571
D29	-0.53169	-0.00027	0.00113	-0.01952	-0.01825	-0.54994
D30	-1.47348	0.00006	0.00249	-0.00565	-0.00285	-1.47633
D31	0.60344	-0.00009	0.00122	-0.01142	-0.01002	0.59343

D32	2.66787	-0.00010	0.00039	-0.00906	-0.00867	2.65920
D33	-1.35783	0.00031	-0.00201	0.06993	0.06791	-1.28992
D34	0.72302	0.00040	-0.00512	0.07579	0.07084	0.79385
D35	2.86836	0.00017	-0.00670	0.06704	0.06039	2.92876
D36	2.86235	0.00027	-0.00121	0.07492	0.07362	2.93597
D37	-1.33999	0.00037	-0.00433	0.08077	0.07655	-1.26344
D38	0.80536	0.00014	-0.00590	0.07202	0.06610	0.87146
D39	0.74043	0.00032	0.00124	0.07321	0.07454	0.81498
D40	2.82128	0.00042	-0.00188	0.07907	0.07747	2.89875
D41	-1.31655	0.00019	-0.00345	0.07032	0.06702	-1.24953
D42	-1.44064	0.00011	0.00369	-0.01574	-0.01140	-1.45204
D43	2.75587	-0.00032	0.00075	-0.02115	-0.01997	2.73590
D44	0.67253	-0.00019	0.00284	-0.02473	-0.02168	0.65086
D45	0.23771	-0.00024	0.00021	-0.07086	-0.07030	0.16741
D46	-0.26445	0.00008	-0.00380	0.07822	0.07402	-0.19043
D47	-2.84704	0.00040	-0.00349	0.07207	0.06828	-2.77876
D48	-3.13740	0.00004	-0.00071	0.00182	0.00111	-3.13629
D49	0.00517	0.00000	-0.00028	0.00035	0.00007	0.00524
D50	0.00267	0.00002	-0.00009	0.00061	0.00052	0.00319
D51	-3.13794	-0.00002	0.00034	-0.00086	-0.00052	-3.13847
D52	-2.52708	-0.00015	0.00064	-0.03448	-0.03445	-2.56153
D53	2.89987	0.00055	-0.00180	0.00357	0.00176	2.90163
D54	-2.16441	0.00023	0.00001	-0.02704	-0.02694	-2.19135
D55	-0.50107	-0.00078	-0.00347	-0.02181	-0.02529	-0.52636
D56	-2.71322	0.00023	-0.00999	0.00596	-0.00423	-2.71746
D57	0.00168	-0.00076	-0.00765	-0.00934	-0.01721	-0.01553
D58	-0.05915	0.00118	0.00678	0.01782	0.02482	-0.03434
D59	2.65575	0.00019	0.00913	0.00252	0.01184	2.66759
D60	1.08076	-0.00024	-0.00806	-0.01236	-0.02020	1.06057
D61	0.09979	-0.00035	-0.01110	0.01013	-0.00059	0.09920
D62	-1.33707	0.00048	0.00812	-0.00493	0.00285	-1.33422
D63	-2.31804	0.00037	0.00508	0.01756	0.02245	-2.29559
D64	1.91643	-0.00077	-0.00689	0.00548	-0.00137	1.91506
D65	-0.50016	0.00053	-0.00017	0.00520	0.00515	-0.49501
D66	2.53632	0.00000	-0.00265	-0.01045	-0.01306	2.52325
D67	-1.66101	0.00021	-0.00091	-0.00835	-0.00928	-1.67029
D68	0.43779	0.00027	-0.00091	-0.00750	-0.00850	0.42929
D69	1.34471	-0.00041	-0.00250	-0.01596	-0.01836	1.32636
D70	-2.85261	-0.00020	-0.00075	-0.01385	-0.01458	-2.86718
D71	-0.75382	-0.00014	-0.00076	-0.01300	-0.01379	-0.76760
D72	-1.03553	-0.00021	0.00237	-0.02336	-0.02093	-1.05646
D73	1.05034	0.00000	0.00412	-0.02125	-0.01715	1.03319
D74	-3.13405	0.00006	0.00411	-0.02040	-0.01636	3.13277

Item	Value	Threshold	Converged?

Maximum Force	0.003277	0.000450	NO
RMS Force	0.000857	0.000300	NO
Maximum Displacement	0.216035	0.001800	NO
RMS Displacement	0.072151	0.001200	NO

Predicted change in Energy=-9.135644D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.745849	-1.973117	0.198214
2	6	0	-2.907391	-1.296690	0.008653
3	7	0	-2.588306	0.056837	0.040762
4	6	0	-1.261186	0.186373	0.249060
5	7	0	-0.737730	-1.035940	0.354771
6	6	0	0.703668	-1.313998	0.530761
7	6	0	1.453911	-1.342597	-0.817442
8	1	0	-1.552065	-3.030996	0.242051
9	1	0	-3.908262	-1.656347	-0.144966
10	1	0	1.114880	-0.505535	1.134387
11	1	0	0.791799	-2.262427	1.062439
12	1	0	1.218242	-2.261739	-1.364568
13	1	0	1.134058	-0.481692	-1.412457
14	35	0	1.333346	2.123674	0.183867
15	1	0	-0.645923	1.115584	0.287006
16	6	0	-3.451574	1.174692	-0.111113
17	6	0	-4.767334	1.101601	-0.265773
18	1	0	-2.911742	2.112818	-0.088855
19	1	0	-5.336470	2.013788	-0.378526
20	1	0	-5.316841	0.169099	-0.286606
21	8	0	2.840723	-1.329962	-0.592414
22	1	0	3.123067	-0.410926	-0.457398
23	6	0	5.630231	2.112085	-0.124915
24	6	0	6.202737	0.921387	-0.773107
25	8	0	4.781904	1.146117	-0.739221
26	1	0	5.566294	2.154135	0.960323
27	1	0	5.665060	3.078431	-0.622556
28	1	0	6.620202	1.064911	-1.769891
29	6	0	6.730779	-0.252878	0.000365
30	1	0	6.528543	-1.190257	-0.524936
31	1	0	7.813773	-0.169335	0.135263
32	1	0	6.263922	-0.311481	0.985581

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357448	0.000000			
3	N	2.203461	1.391001	0.000000		
4	C	2.213794	2.228736	1.349598	0.000000	
5	N	1.385322	2.212513	2.171956	1.333877	0.000000
6	C	2.558351	3.648649	3.599496	2.488196	1.478485
7	C	3.415783	4.439087	4.362848	3.293467	2.504279
8	H	1.076374	2.213414	3.263285	3.230499	2.157799
9	H	2.212272	1.074567	2.170663	3.249290	3.269084
10	H	3.348729	4.251101	3.902033	2.628351	2.078772
11	H	2.696339	3.965743	4.224680	3.297417	2.084353
12	H	3.363247	4.453976	4.673388	3.839871	2.878287
13	H	3.621116	4.360858	4.032103	2.990676	2.633226
14	Br	5.124973	5.451004	4.435273	3.238670	3.781762
15	H	3.279908	3.318250	2.225855	1.115087	2.154547
16	C	3.593589	2.533419	1.420527	2.429876	3.531131
17	C	4.335730	3.047376	2.435911	3.660023	4.603462
18	H	4.258706	3.410905	2.085298	2.559240	3.851987
19	H	5.396351	4.124270	3.399686	4.510127	5.566594
20	H	4.192389	2.835695	2.750396	4.090914	4.778257
21	O	4.698445	5.779550	5.639014	4.453426	3.713346
22	H	5.155251	6.112954	5.752108	4.480795	3.994498
23	C	8.438000	9.193942	8.473243	7.165183	7.119768
24	C	8.514790	9.408796	8.870866	7.569361	7.298858
25	O	7.295202	8.102584	7.490988	6.198124	6.035276
26	H	8.431042	9.198761	8.470050	7.140901	7.091121
27	H	9.006297	9.645052	8.814083	7.556229	7.673261
28	H	9.115583	9.975740	9.438818	8.183169	7.941469
29	C	8.651682	9.694531	9.324318	8.007890	7.517807
30	H	8.342744	9.451608	9.219121	7.948211	7.320958
31	H	9.728513	10.781016	10.404966	9.082641	8.598104
32	H	8.218116	9.275668	8.910123	7.577439	7.067242

		6	7	8	9	10
6	C	0.000000				
7	C	1.543157	0.000000			
8	H	2.849520	3.606814	0.000000		
9	H	4.673725	5.413276	2.755197	0.000000	
10	H	1.089528	2.150640	3.779790	5.309714	0.000000
11	H	1.090856	2.195093	2.599506	4.890372	1.787800
12	H	2.180659	1.095312	3.293567	5.304241	3.056095
13	H	2.157328	1.094306	4.056058	5.330229	2.547028

14	Br	3.512039	3.610012	5.907589	6.470792	2.804275
15	H	2.789924	3.416395	4.244672	4.302680	2.538997
16	C	4.885858	5.558725	4.628247	2.867838	5.022642
17	C	6.033361	6.706887	5.260628	2.891172	6.256499
18	H	5.019778	5.615127	5.330764	3.899077	4.956387
19	H	6.955877	7.587307	6.336930	3.945152	7.089133
20	H	6.254134	6.957736	4.969268	2.310067	6.621283
21	O	2.414287	1.405007	4.783976	6.771671	2.576831
22	H	2.765048	1.945180	5.404707	7.147606	2.564283
23	C	6.036471	5.464071	8.841455	10.255941	5.369001
24	C	6.077564	5.261078	8.762924	10.453305	5.617912
25	O	4.929202	4.156363	7.650512	9.150187	4.436826
26	H	5.988122	5.683245	8.835867	10.271741	5.188375
27	H	6.725993	6.108784	9.495237	10.690870	6.052752
28	H	6.779202	5.778738	9.360037	10.995189	6.419478
29	C	6.142749	5.449921	8.739672	10.732197	5.734821
30	H	5.921063	5.085338	8.323029	10.454115	5.703504
31	H	7.212508	6.536974	9.793846	11.819299	6.781331
32	H	5.668186	5.239304	8.308926	10.322797	5.154847

		11	12	13	14	15
11	H	0.000000				
12	H	2.464187	0.000000			
13	H	3.068106	1.782680	0.000000		
14	Br	4.505891	4.652176	3.062009	0.000000	
15	H	3.752239	4.196322	2.933905	2.223599	0.000000
16	C	5.585448	5.931896	5.046298	4.887028	2.834373
17	C	6.632104	6.953167	6.216763	6.202025	4.158340
18	H	5.846748	6.149874	4.985168	4.253853	2.503933
19	H	7.610393	7.887754	7.011717	6.694386	4.821922
20	H	6.711761	7.055373	6.580667	6.947425	4.800244
21	O	2.793943	2.024073	2.074786	3.847389	4.348652
22	H	3.342570	2.806567	2.207555	3.168363	4.133964
23	C	6.629977	6.335039	5.347991	4.307981	6.368109
24	C	6.540960	5.943678	5.298009	5.106100	6.932943
25	O	5.548431	4.970334	4.050899	3.701386	5.524073
26	H	6.504787	6.618959	5.676476	4.303680	6.334319
27	H	7.423789	6.988718	5.816218	4.508394	6.671475
28	H	7.284473	6.357047	5.711174	5.734892	7.551819
29	C	6.359070	6.023838	5.776825	5.900335	7.508035
30	H	6.048102	5.482002	5.512733	6.202791	7.579520
31	H	7.385716	7.080160	6.863788	6.874313	8.558066
32	H	5.810011	5.897932	5.665251	5.557275	7.090168

		16	17	18	19	20
16	C	0.000000				

17	C	1.326834	0.000000			
18	H	1.082587	2.120633	0.000000		
19	H	2.080487	1.081071	2.443977	0.000000	
20	H	2.126321	1.082568	3.098654	1.847083	0.000000
21	O	6.789546	7.993856	6.722883	8.837018	8.299793
22	H	6.772001	8.036348	6.551643	8.800524	8.461540
23	C	9.130064	10.447501	8.542049	10.970073	11.119341
24	C	9.680296	10.983275	9.217453	11.597514	11.554363
25	O	8.257451	9.561071	7.781367	10.161911	10.155988
26	H	9.133960	10.459208	8.542808	10.985558	11.132738
27	H	9.327315	10.624029	8.647472	11.055617	11.365704
28	H	10.208049	11.486500	9.735601	12.074695	12.062156
29	C	10.282543	11.580676	9.928881	12.284129	12.058424
30	H	10.264841	11.528947	10.010966	12.290886	11.925510
31	H	11.347914	12.651497	10.967913	13.340123	13.141748
32	H	9.889505	11.191574	9.551149	11.909524	11.660339

		21	22	23	24	25
21	O	0.000000				
22	H	0.970863	0.000000			
23	C	4.455065	3.572395	0.000000		
24	C	4.050230	3.370326	1.471624	0.000000	
25	O	3.149715	2.292498	1.424825	1.438895	0.000000
26	H	4.688141	3.815604	1.087933	2.220250	2.125986
27	H	5.235620	4.320257	1.087513	2.228138	2.127772
28	H	4.626697	4.016302	2.186907	1.090162	2.109079
29	C	4.079711	3.640070	2.611503	1.501994	2.510436
30	H	3.691083	3.494164	3.445642	2.150995	2.924946
31	H	5.158275	4.734167	3.168663	2.147149	3.418679
32	H	3.904571	3.457897	2.740153	2.148649	2.701095

		26	27	28	29	30
26	H	0.000000				
27	H	1.835643	0.000000			
28	H	3.122691	2.506579	0.000000		
29	C	2.840995	3.552662	2.209661	0.000000	
30	H	3.783765	4.356241	2.577614	1.093399	0.000000
31	H	3.336225	3.967272	2.564681	1.094556	1.769169
32	H	2.562535	3.799506	3.100648	1.091806	1.767466

		31	32
31	H	0.000000	
32	H	1.773495	0.000000

Stoichiometry C10H17BrN2O2

Framework group C1[X(C10H17BrN2O2)]

Deg. of freedom 90

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.041377	2.098868	-0.238996
2	6	0	-4.119578	1.318221	0.026975
3	7	0	-3.665942	0.003281	0.032434
4	6	0	-2.341883	-0.001487	-0.228831
5	7	0	-1.950160	1.261504	-0.403864
6	6	0	-0.552699	1.674721	-0.653406
7	6	0	0.243830	1.835264	0.658501
8	1	0	-2.958153	3.168023	-0.331530
9	1	0	-5.144938	1.582083	0.210575
10	1	0	-0.085715	0.886662	-1.243289
11	1	0	-0.582784	2.603865	-1.224155
12	1	0	-0.062175	2.748524	1.180062
13	1	0	0.037198	0.972616	1.299319
14	35	0	0.436854	-1.664910	-0.203887
15	1	0	-1.637256	-0.865228	-0.258350
16	6	0	-4.404235	-1.187925	0.264492
17	6	0	-5.713395	-1.240401	0.473860
18	1	0	-3.773055	-2.067414	0.254285
19	1	0	-6.181804	-2.199375	0.646123
20	1	0	-6.353677	-0.367530	0.483282
21	8	0	1.614661	1.951972	0.373465
22	1	0	1.983463	1.060921	0.261266
23	6	0	4.719123	-1.210311	-0.084666
24	6	0	5.192843	0.058052	0.491982
25	8	0	3.802039	-0.308973	0.529069
26	1	0	4.616631	-1.304418	-1.163664
27	1	0	4.871900	-2.146400	0.447389
28	1	0	5.662108	-0.000678	1.474222
29	6	0	5.567423	1.245490	-0.348057
30	1	0	5.291926	2.179303	0.149554
31	1	0	6.647061	1.265118	-0.527082
32	1	0	5.058165	1.215349	-1.313349

Rotational constants (GHZ): 0.8153943 0.1767760 0.1491180

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.

475 basis functions, 751 primitive gaussians, 492 cartesian basis functions
71 alpha electrons 71 beta electrons
nuclear repulsion energy 1288.8381685768 Hartrees.
NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 475 RedAO= T EigKep= 4.26D-06 NBF= 475
NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999987 0.003947 -0.000107 0.003301 Ang= 0.59 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3225.51128845 A.U. after 12 cycles
NFock= 12 Conv=0.39D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Atomic Forces (Hartrees/Bohr)
Number Number X Y Z

1	6	-0.000300927	0.000144348	0.000618804
2	6	0.000281183	0.000043301	-0.000442950
3	7	0.000340836	0.000245618	0.000015679
4	6	0.000335671	0.001591438	0.000534006
5	7	-0.000297390	-0.000772116	-0.000721683

6	6	0.000722613	0.000275968	-0.000575478
7	6	-0.001506974	-0.000480665	-0.000302837
8	1	-0.000032611	-0.000010304	0.000101947
9	1	-0.000002437	-0.000015517	-0.000042977
10	1	-0.000071867	0.000322084	0.000002266
11	1	0.000198184	0.000090606	0.000071296
12	1	-0.000039573	0.000064404	0.000054226
13	1	0.000183064	0.000310062	0.000307701
14	35	-0.000942211	0.002881323	0.000926856
15	1	-0.000637116	-0.003213859	-0.000027717
16	6	-0.000100813	0.000178086	-0.000050358
17	6	0.000081745	-0.000118386	-0.000003836
18	1	0.000027525	0.000003035	-0.000004081
19	1	0.000001717	0.000018535	0.000017761
20	1	0.000003712	0.000017101	-0.000005045
21	8	0.000740280	-0.000624440	0.000452327
22	1	0.001746271	0.002133832	-0.000471858
23	6	0.000662275	0.001596883	0.002201857
24	6	-0.001190475	0.003855551	-0.001547135
25	8	-0.001081671	-0.006064354	-0.001939258
26	1	0.000152946	-0.000160438	-0.000262451
27	1	-0.000201694	-0.000386253	-0.000122969
28	1	0.000812006	-0.000994267	0.000554462
29	6	0.000587537	-0.001690761	0.001061860
30	1	-0.000323378	0.000069610	-0.000550599
31	1	0.000218705	0.000365491	-0.000171788
32	1	-0.000367133	0.000324085	0.000321970

Cartesian Forces: Max 0.006064354 RMS 0.001092739

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.003079836 RMS 0.000553865
Search for a local minimum.
Step number 7 out of a maximum of 177
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 5 6 7
DE= -1.37D-03 DEPred=-9.14D-04 R= 1.50D+00
TightC=F SS= 1.41D+00 RLast= 3.54D-01 DXNew= 2.4000D+00 1.0609D+00
Trust test= 1.50D+00 RLast= 3.54D-01 DXMaxT set to 1.43D+00

ITU= 1 1 0 1 0 1 0

Eigenvalues ---	0.00159	0.00237	0.00265	0.00389	0.00570
Eigenvalues ---	0.00990	0.01265	0.01271	0.01402	0.01518
Eigenvalues ---	0.01690	0.01860	0.01950	0.02075	0.02149
Eigenvalues ---	0.02243	0.02313	0.02333	0.02390	0.02428
Eigenvalues ---	0.03062	0.03063	0.03122	0.03705	0.04085
Eigenvalues ---	0.04486	0.05069	0.05285	0.05468	0.05501
Eigenvalues ---	0.05882	0.06359	0.09286	0.09759	0.10656
Eigenvalues ---	0.10794	0.11007	0.11462	0.12969	0.13338
Eigenvalues ---	0.13855	0.14735	0.15980	0.15999	0.16000
Eigenvalues ---	0.16000	0.16000	0.16001	0.16007	0.16329
Eigenvalues ---	0.16938	0.18912	0.20765	0.21797	0.22006
Eigenvalues ---	0.22757	0.23555	0.23953	0.25001	0.27254
Eigenvalues ---	0.27664	0.28773	0.31697	0.32827	0.33054
Eigenvalues ---	0.33213	0.34068	0.34265	0.34419	0.34761
Eigenvalues ---	0.34938	0.35685	0.35689	0.35858	0.36434
Eigenvalues ---	0.36657	0.36801	0.37229	0.37541	0.37765
Eigenvalues ---	0.38904	0.42178	0.42479	0.45524	0.46991
Eigenvalues ---	0.49144	0.51761	0.54688	0.56138	0.60360

En-DIIS/RFO-DIIS IScMMF= 0 using points: 7 6

RFO step: Lambda=-3.60079291D-04.

DidBck=F Rises=F RFO-DIIS coefs: 3.17212 -2.17212

Iteration 1 RMS(Cart)= 0.16388656 RMS(Int)= 0.07238988

Iteration 2 RMS(Cart)= 0.09651667 RMS(Int)= 0.04699628

Iteration 3 RMS(Cart)= 0.04748891 RMS(Int)= 0.02913347

Iteration 4 RMS(Cart)= 0.02773632 RMS(Int)= 0.01354263

Iteration 5 RMS(Cart)= 0.02216161 RMS(Int)= 0.00417268

Iteration 6 RMS(Cart)= 0.00021185 RMS(Int)= 0.00417230

Iteration 7 RMS(Cart)= 0.00000095 RMS(Int)= 0.00417230

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56521	-0.00010	0.00215	-0.00067	0.00062	2.56583
R2	2.61788	-0.00006	-0.00074	0.00048	0.00016	2.61804
R3	2.03405	0.00001	0.00005	-0.00010	-0.00005	2.03400
R4	2.62861	0.00000	-0.00073	-0.00023	-0.00179	2.62682
R5	2.03064	0.00001	-0.00037	0.00036	-0.00001	2.03063
R6	2.55037	-0.00043	-0.00059	-0.00011	-0.00039	2.54998
R7	2.68441	0.00007	0.00008	-0.00030	-0.00022	2.68419
R8	2.52066	0.00000	-0.00317	-0.00006	0.00025	2.52091
R9	2.10721	-0.00176	-0.01035	-0.00498	-0.01384	2.09337
R10	2.79393	0.00010	0.00170	0.00234	0.00532	2.79925
R11	2.91614	-0.00066	-0.00392	-0.01055	-0.01598	2.90016
R12	2.05891	0.00021	0.00378	0.00078	0.00457	2.06348
R13	2.06142	-0.00003	-0.00163	-0.00008	-0.00171	2.05971

R14	2.06984	-0.00007	-0.00013	0.00086	0.00073	2.07057
R15	2.06794	0.00002	0.00116	-0.00128	-0.00012	2.06781
R16	2.65508	0.00075	0.01215	0.00888	0.02251	2.67759
R17	4.20199	0.00074	0.09901	0.03649	0.13622	4.33822
R18	6.99461	0.00155	0.39805	0.65354	1.05022	8.04483
R19	2.50735	-0.00008	0.00009	-0.00019	-0.00010	2.50725
R20	2.04579	0.00001	0.00036	0.00001	0.00037	2.04617
R21	2.04293	0.00001	-0.00005	0.00005	0.00000	2.04293
R22	2.04576	-0.00001	0.00022	-0.00013	0.00009	2.04585
R23	1.83466	0.00045	0.00275	-0.00154	-0.00010	1.83456
R24	4.33219	-0.00244	-0.25372	-0.30064	-0.55494	3.77725
R25	2.78097	-0.00015	-0.01422	0.00125	-0.01303	2.76793
R26	2.69253	0.00166	0.02131	0.00893	0.03013	2.72266
R27	2.05589	-0.00028	-0.01432	0.00221	-0.01211	2.04379
R28	2.05510	-0.00029	-0.01292	0.00161	-0.01132	2.04379
R29	2.71912	-0.00020	-0.00392	-0.00958	-0.01333	2.70579
R30	2.06011	-0.00033	0.00069	0.00021	0.00090	2.06101
R31	2.83836	0.00110	0.02455	0.00320	0.02775	2.86611
R32	2.06623	0.00026	-0.00548	0.00014	-0.00534	2.06089
R33	2.06841	0.00022	-0.00261	-0.00125	-0.00387	2.06455
R34	2.06321	0.00043	-0.00337	0.00057	-0.00281	2.06041
A1	1.87692	-0.00011	-0.00179	0.00113	0.00027	1.87719
A2	2.27770	0.00004	0.00249	-0.00051	0.00141	2.27911
A3	2.12853	0.00007	-0.00077	-0.00030	-0.00171	2.12682
A4	1.86019	0.00008	0.00239	-0.00106	0.00112	1.86131
A5	2.27861	-0.00005	-0.00015	0.00040	0.00032	2.27893
A6	2.14438	-0.00003	-0.00225	0.00072	-0.00147	2.14291
A7	1.89920	-0.00005	-0.00416	0.00146	-0.00182	1.89738
A8	2.24447	0.00002	0.00155	-0.00145	-0.00036	2.24410
A9	2.13952	0.00003	0.00262	-0.00001	0.00217	2.14169
A10	1.88617	0.00011	0.00430	-0.00068	0.00267	1.88884
A11	2.24953	-0.00051	-0.00189	-0.00494	-0.01337	2.23616
A12	2.14645	0.00040	-0.00198	0.00418	0.00928	2.15573
A13	1.90222	-0.00002	-0.00090	0.00004	-0.00246	1.89976
A14	2.20891	0.00059	0.01563	0.00155	0.01274	2.22165
A15	2.17046	-0.00056	-0.01564	0.00016	-0.00950	2.16096
A16	1.95354	-0.00031	0.00000	-0.00023	0.01932	1.97286
A17	1.86957	0.00002	-0.00479	-0.00200	-0.01058	1.85899
A18	1.87580	0.00019	0.00812	0.00691	0.00674	1.88254
A19	1.89051	0.00018	-0.01028	-0.00030	-0.01865	1.87186
A20	1.95027	-0.00005	0.00569	-0.00712	-0.00354	1.94672
A21	1.92264	-0.00002	0.00103	0.00301	0.00659	1.92922
A22	1.92555	0.00008	0.01322	0.00061	0.02306	1.94860
A23	1.89480	-0.00005	-0.00929	-0.00501	-0.01646	1.87834

A24	1.91748	-0.00041	-0.00500	-0.00774	-0.02863	1.88886
A25	1.90253	0.00014	0.00342	0.00607	0.00832	1.91085
A26	1.87541	0.00015	0.00927	0.00868	0.02107	1.89648
A27	1.94821	0.00009	-0.01091	-0.00237	-0.00710	1.94110
A28	2.37626	-0.00308	-0.10516	-0.13798	-0.24844	2.12782
A29	2.62064	0.00213	0.01468	0.00522	0.01926	2.63989
A30	2.17943	-0.00012	0.00034	-0.00124	-0.00090	2.17853
A31	1.95702	0.00004	-0.00008	0.00052	0.00044	1.95746
A32	2.14673	0.00008	-0.00026	0.00072	0.00046	2.14719
A33	2.08029	-0.00002	-0.00100	0.00009	-0.00092	2.07938
A34	2.15682	0.00001	0.00160	-0.00041	0.00119	2.15801
A35	2.04607	0.00000	-0.00059	0.00032	-0.00027	2.04580
A36	1.89424	-0.00034	-0.02148	0.01283	-0.01080	1.88345
A37	2.56124	0.00001	-0.01896	-0.01147	-0.01462	2.54662
A38	2.08691	0.00013	0.01330	-0.00247	0.01078	2.09769
A39	2.10011	-0.00015	0.01572	0.00194	0.01625	2.11637
A40	2.00566	-0.00018	-0.01858	0.00106	-0.01718	1.98848
A41	2.00887	0.00023	-0.01934	-0.00326	-0.02315	1.98573
A42	2.00865	0.00012	-0.00218	0.00343	-0.00060	2.00805
A43	2.03218	0.00117	0.02445	0.00567	0.03207	2.06424
A44	2.14422	-0.00084	-0.00877	0.00221	-0.00887	2.13535
A45	1.95962	0.00085	0.02385	-0.00285	0.02053	1.98015
A46	2.04555	-0.00089	-0.00289	-0.00558	-0.00837	2.03718
A47	2.02545	-0.00045	-0.02448	-0.00370	-0.02816	1.99729
A48	1.01756	0.00129	0.01242	0.00220	0.00632	1.02388
A49	1.84226	-0.00169	-0.04461	-0.04737	-0.08648	1.75578
A50	2.56492	-0.00052	-0.01083	-0.00995	-0.02486	2.54005
A51	2.22853	0.00049	0.02083	0.01911	0.04283	2.27137
A52	1.93673	-0.00067	-0.03451	0.00040	-0.03456	1.90217
A53	1.93012	-0.00036	0.00180	-0.00585	-0.00412	1.92600
A54	1.93513	-0.00034	-0.02855	0.00481	-0.02418	1.91095
A55	1.88352	0.00052	0.02354	0.00043	0.02390	1.90742
A56	1.88433	0.00052	0.02585	-0.00071	0.02431	1.90864
A57	1.89227	0.00039	0.01538	0.00096	0.01628	1.90856
A58	3.24609	0.00178	0.03325	0.02131	0.04915	3.29524
A59	3.42798	0.00112	0.05875	0.06577	0.12552	3.55351
D1	0.00883	-0.00030	0.02408	-0.05286	-0.02777	-0.01894
D2	-3.13579	-0.00017	0.01349	-0.03067	-0.01598	3.13141
D3	-3.14154	-0.00004	0.00584	-0.01045	-0.00617	3.13547
D4	-0.00297	0.00009	-0.00475	0.01174	0.00561	0.00264
D5	-0.01213	0.00039	-0.03185	0.07051	0.03609	0.02396
D6	-3.09476	0.00033	-0.01317	0.03818	0.01963	-3.07512
D7	3.13733	0.00015	-0.01551	0.03250	0.01676	-3.12910
D8	0.05470	0.00010	0.00318	0.00018	0.00031	0.05501

D9	-0.00264	0.00011	-0.00843	0.01789	0.01029	0.00764
D10	3.13891	0.00012	-0.00750	0.01520	0.00699	-3.13729
D11	-3.14150	-0.00001	0.00115	-0.00218	-0.00037	3.14132
D12	0.00006	0.00000	0.00208	-0.00488	-0.00367	-0.00361
D13	-0.00486	0.00012	-0.01127	0.02574	0.01206	0.00720
D14	3.08830	0.00010	-0.00157	-0.00777	-0.01359	3.07472
D15	3.13676	0.00012	-0.01213	0.02824	0.01513	-3.13129
D16	-0.05325	0.00010	-0.00242	-0.00527	-0.01052	-0.06377
D17	0.04779	-0.00001	-0.00243	0.00034	-0.00122	0.04657
D18	-3.09189	0.00000	-0.00127	-0.00206	-0.00247	-3.09435
D19	-3.09385	0.00000	-0.00139	-0.00268	-0.00494	-3.09878
D20	0.04966	0.00000	-0.00023	-0.00509	-0.00618	0.04348
D21	0.01043	-0.00031	0.02647	-0.05910	-0.02956	-0.01913
D22	3.09466	-0.00021	0.00939	-0.02759	-0.01290	3.08176
D23	-3.08623	-0.00026	0.01747	-0.02771	-0.00461	-3.09084
D24	-0.00200	-0.00016	0.00039	0.00380	0.01206	0.01005
D25	-2.81663	0.00001	-0.00335	0.07515	0.08662	-2.73001
D26	0.27008	-0.00003	0.00782	0.03699	0.05709	0.32717
D27	1.59772	-0.00014	-0.02700	-0.01541	-0.03556	1.56216
D28	-2.61571	-0.00009	-0.04256	-0.01716	-0.05410	-2.66982
D29	-0.54994	-0.00001	-0.03964	-0.01108	-0.04848	-0.59842
D30	-1.47633	-0.00023	-0.00619	-0.05245	-0.05469	-1.53101
D31	0.59343	-0.00018	-0.02176	-0.05420	-0.07323	0.52020
D32	2.65920	-0.00010	-0.01883	-0.04812	-0.06761	2.59159
D33	-1.28992	0.00001	0.14751	0.10582	0.25351	-1.03641
D34	0.79385	0.00020	0.15386	0.11052	0.26709	1.06094
D35	2.92876	0.00003	0.13118	0.09954	0.23160	-3.12283
D36	2.93597	0.00006	0.15992	0.10859	0.26715	-3.08006
D37	-1.26344	0.00025	0.16627	0.11329	0.28073	-0.98271
D38	0.87146	0.00008	0.14359	0.10232	0.24524	1.11670
D39	0.81498	0.00000	0.16192	0.10954	0.27348	1.08845
D40	2.89875	0.00019	0.16827	0.11424	0.28706	-3.09738
D41	-1.24953	0.00002	0.14559	0.10326	0.25157	-0.99796
D42	-1.45204	-0.00001	-0.02475	-0.04309	-0.05531	-1.50735
D43	2.73590	0.00004	-0.04338	-0.04460	-0.07900	2.65690
D44	0.65086	-0.00028	-0.04709	-0.05614	-0.09847	0.55238
D45	0.16741	-0.00005	-0.15269	-0.14677	-0.28815	-0.12074
D46	-0.19043	0.00019	0.16079	0.11769	0.27109	0.08066
D47	-2.77876	0.00022	0.14831	0.09699	0.23729	-2.54147
D48	-3.13629	-0.00001	0.00242	-0.00499	-0.00258	-3.13886
D49	0.00524	0.00000	0.00014	-0.00179	-0.00164	0.00360
D50	0.00319	-0.00002	0.00113	-0.00234	-0.00120	0.00199
D51	-3.13847	-0.00001	-0.00114	0.00087	-0.00027	-3.13874
D52	-2.56153	-0.00009	-0.07482	-0.07767	-0.15936	-2.72088

D53	2.90163	0.00058	0.00382	0.06040	0.06635	2.96797
D54	-2.19135	-0.00008	-0.05852	-0.02862	-0.08422	-2.27557
D55	-0.52636	-0.00054	-0.05493	-0.00537	-0.05917	-0.58553
D56	-2.71746	0.00028	-0.00920	-0.00464	-0.01422	-2.73168
D57	-0.01553	-0.00010	-0.03739	0.00520	-0.03331	-0.04884
D58	-0.03434	0.00056	0.05390	0.00339	0.05774	0.02341
D59	2.66759	0.00018	0.02571	0.01322	0.03866	2.70624
D60	1.06057	0.00021	-0.04387	-0.02834	-0.07327	0.98730
D61	0.09920	0.00013	-0.00129	0.03963	0.04120	0.14040
D62	-1.33422	-0.00003	0.00619	-0.03129	-0.02711	-1.36133
D63	-2.29559	-0.00012	0.04877	0.03668	0.08735	-2.20824
D64	1.91506	-0.00032	-0.00298	0.00048	-0.00055	1.91452
D65	-0.49501	0.00041	0.01118	0.01662	0.03018	-0.46483
D66	2.52325	0.00007	-0.02838	-0.00974	-0.03829	2.48496
D67	-1.67029	0.00005	-0.02017	-0.01278	-0.03332	-1.70361
D68	0.42929	0.00009	-0.01846	-0.01229	-0.03133	0.39796
D69	1.32636	-0.00017	-0.03987	-0.01422	-0.05366	1.27269
D70	-2.86718	-0.00019	-0.03166	-0.01726	-0.04870	-2.91588
D71	-0.76760	-0.00016	-0.02995	-0.01677	-0.04671	-0.81431
D72	-1.05646	0.00007	-0.04546	0.00222	-0.04287	-1.09933
D73	1.03319	0.00005	-0.03725	-0.00082	-0.03790	0.99528
D74	3.13277	0.00008	-0.03554	-0.00033	-0.03592	3.09685

Item	Value	Threshold	Converged?
Maximum Force	0.003080	0.000450	NO
RMS Force	0.000554	0.000300	NO
Maximum Displacement	0.911781	0.001800	NO
RMS Displacement	0.311593	0.001200	NO

Predicted change in Energy=-2.492353D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.548777	-1.910225	0.221704
2	6	0	-2.787111	-1.369276	0.089556
3	7	0	-2.622249	0.010896	0.103253
4	6	0	-1.307981	0.288632	0.231396
5	7	0	-0.641454	-0.865466	0.289505
6	6	0	0.835129	-0.962118	0.357367
7	6	0	1.499988	-0.980139	-1.025725
8	1	0	-1.234762	-2.938934	0.262636
9	1	0	-3.748880	-1.839408	-0.003499

10	1	0	1.181677	-0.063297	0.871537
11	1	0	1.085726	-1.852801	0.933457
12	1	0	1.152277	-1.825171	-1.630351
13	1	0	1.244615	-0.042265	-1.528258
14	35	0	1.030713	2.606168	-0.109493
15	1	0	-0.814209	1.280188	0.219458
16	6	0	-3.614102	1.022466	0.000662
17	6	0	-4.919319	0.798314	-0.080008
18	1	0	-3.184528	2.016372	-0.005607
19	1	0	-5.594067	1.639380	-0.157728
20	1	0	-5.359696	-0.190657	-0.072070
21	8	0	2.900002	-1.099223	-0.842858
22	1	0	3.262368	-0.206698	-0.722187
23	6	0	5.718345	1.918160	-0.199680
24	6	0	6.263977	0.643858	-0.672824
25	8	0	4.880845	0.956841	-0.870706
26	1	0	5.480184	2.052792	0.846670
27	1	0	5.865021	2.833113	-0.757393
28	1	0	6.844891	0.641524	-1.595876
29	6	0	6.575571	-0.504611	0.267519
30	1	0	6.318151	-1.444259	-0.222533
31	1	0	7.637978	-0.509647	0.522162
32	1	0	5.986141	-0.398893	1.178670

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357778	0.000000			
3	N	2.203878	1.390051	0.000000		
4	C	2.212024	2.226344	1.349392	0.000000	
5	N	1.385407	2.213064	2.173994	1.334008	0.000000
6	C	2.569108	3.654877	3.600665	2.484585	1.481298
7	C	3.422880	4.446853	4.387434	3.327886	2.515701
8	H	1.076347	2.214401	3.263743	3.228548	2.156851
9	H	2.212732	1.074561	2.168944	3.246801	3.269635
10	H	3.359882	4.250689	3.881445	2.594616	2.075101
11	H	2.729560	3.993099	4.232220	3.287622	2.091090
12	H	3.276131	4.322580	4.541318	3.739937	2.797203
13	H	3.788757	4.542367	4.197295	3.117951	2.745756
14	Br	5.211647	5.515393	4.486071	3.310085	3.873962
15	H	3.273886	3.305885	2.212151	1.107762	2.153737
16	C	3.593759	2.532241	1.420412	2.431037	3.533320
17	C	4.334486	3.045243	2.435188	3.660397	4.604870
18	H	4.259755	3.410221	2.085652	2.561773	3.854777

19	H	5.395186	4.122155	3.398790	4.510706	5.568002
20	H	4.191219	2.834335	2.750450	4.091235	4.779949
21	O	4.645712	5.769365	5.711632	4.559307	3.725425
22	H	5.190380	6.213430	5.946210	4.694972	4.086235
23	C	8.224668	9.123250	8.561246	7.225680	6.959520
24	C	8.268171	9.303555	8.942480	7.634026	7.133661
25	O	7.124146	8.070345	7.624947	6.321605	5.929812
26	H	8.093354	8.979530	8.388768	7.040597	6.804492
27	H	8.855636	9.655921	8.985510	7.674897	7.557096
28	H	8.959279	9.982959	9.639060	8.362582	7.865815
29	C	8.245173	9.404208	9.213719	7.923442	7.226074
30	H	7.893226	9.110918	9.063904	7.833700	7.002377
31	H	9.297761	10.469413	10.281961	8.986211	8.290340
32	H	7.744346	8.893693	8.684977	7.387438	6.703232

		6	7	8	9	10
6	C	0.000000				
7	C	1.534701	0.000000			
8	H	2.863778	3.602168	0.000000		
9	H	4.681132	5.416078	2.756913	0.000000	
10	H	1.091946	2.131086	3.805158	5.313252	0.000000
11	H	1.089952	2.184387	2.648462	4.924579	1.793144
12	H	2.190083	1.095698	3.243736	5.164125	3.060148
13	H	2.137613	1.094240	4.212517	5.521739	2.400712
14	Br	3.604008	3.731125	6.001584	6.528314	2.848026
15	H	2.786983	3.466276	4.240250	4.288809	2.492734
16	C	4.884820	5.587290	4.628453	2.865049	4.993676
17	C	6.033580	6.727910	5.259314	2.886756	6.234578
18	H	5.016054	5.653707	5.331848	3.896863	4.915094
19	H	6.954687	7.611892	6.335708	3.940872	7.061813
20	H	6.257429	6.970509	4.967910	2.306038	6.610308
21	O	2.392287	1.416919	4.658640	6.742404	2.639116
22	H	2.761808	1.948417	5.353426	7.234628	2.624842
23	C	5.696675	5.184306	8.494163	10.187549	5.065080
24	C	5.754376	5.045543	8.363168	10.337887	5.358628
25	O	4.643100	3.899502	7.339085	9.112804	4.214253
26	H	5.559284	5.342892	8.387427	10.052245	4.791202
27	H	6.398929	5.802276	9.206732	10.715778	5.742501
28	H	6.519514	5.614522	9.030755	10.996302	6.217467
29	C	5.759345	5.259292	8.180908	10.413905	5.445520
30	H	5.534643	4.906650	7.714657	10.077163	5.430231
31	H	6.819872	6.347618	9.202952	11.476285	6.481136
32	H	5.246398	5.032174	7.709239	9.911773	4.825954

		11	12	13	14	15
11	H	0.000000				

12	H	2.564820	0.000000			
13	H	3.059955	1.788212	0.000000		
14	Br	4.579648	4.686635	3.012116	0.000000	
15	H	3.732984	4.114865	3.007017	2.295685	0.000000
16	C	5.587991	5.786847	5.203688	4.908620	2.820229
17	C	6.641994	6.793416	6.387337	6.218688	4.144129
18	H	5.838442	6.017069	5.116029	4.257570	2.492194
19	H	7.616144	7.725599	7.174527	6.695126	4.808152
20	H	6.731810	6.892435	6.764571	6.975740	4.786420
21	O	2.648541	2.049802	2.080202	4.214497	4.537122
22	H	3.191956	2.810106	2.179017	3.642512	4.440271
23	C	6.079910	6.075222	5.061882	4.738711	6.577002
24	C	5.968897	5.756947	5.137756	5.617389	7.162529
25	O	5.054900	4.713689	3.827892	4.257140	5.807465
26	H	5.879834	6.317041	5.288629	4.584568	6.372574
27	H	6.903508	6.683683	5.496380	4.882808	6.926611
28	H	6.766621	6.204162	5.642272	6.314573	7.897161
29	C	5.692054	5.895583	5.644260	6.369029	7.602412
30	H	5.374150	5.367802	5.423216	6.661511	7.647779
31	H	6.701137	6.959040	6.730362	7.332342	8.644919
32	H	5.117426	5.769845	5.471446	5.936836	7.069949

		16	17	18	19	20
16	C	0.000000				
17	C	1.326779	0.000000			
18	H	1.082785	2.121014	0.000000		
19	H	2.079887	1.081072	2.443592	0.000000	
20	H	2.126983	1.082617	3.099476	1.846971	0.000000
21	O	6.902654	8.082348	6.886902	8.950896	8.345190
22	H	7.022762	8.268158	6.856967	9.064384	8.646554
23	C	9.377472	10.697115	8.905530	11.315924	11.277694
24	C	9.908248	11.200062	9.570957	11.910902	11.669066
25	O	8.539772	9.833287	8.180540	10.521310	10.335533
26	H	9.191482	10.515803	8.706603	11.127388	11.107661
27	H	9.680231	10.995510	9.117378	11.536693	11.645047
28	H	10.587001	11.862507	10.247361	12.561515	12.327467
29	C	10.306920	11.573715	10.084120	12.364369	11.944223
30	H	10.236415	11.459937	10.115529	12.305038	11.745904
31	H	11.367878	12.639584	11.125913	13.422652	13.015160
32	H	9.776126	11.042945	9.557049	11.833923	11.416467

		21	22	23	24	25
21	O	0.000000				
22	H	0.970810	0.000000			
23	C	4.178677	3.289356	0.000000		
24	C	3.792569	3.120183	1.464728	0.000000	

25	O	2.855156	1.998837	1.440770	1.431842	0.000000
26	H	4.409881	3.533457	1.081525	2.215466	2.123605
27	H	4.925639	4.001937	1.081525	2.226917	2.121754
28	H	4.377144	3.783819	2.201879	1.090638	2.117257
29	C	3.885397	3.470675	2.612075	1.516679	2.510676
30	H	3.491074	3.334519	3.415575	2.136803	2.872500
31	H	4.965814	4.559183	3.178096	2.155561	3.419423
32	H	3.755169	3.327031	2.709299	2.143024	2.694371

		26	27	28	29	30
26	H	0.000000				
27	H	1.824834	0.000000			
28	H	3.133710	2.542885	0.000000		
29	C	2.841760	3.563107	2.204178	0.000000	
30	H	3.751633	4.334433	2.552257	1.090575	0.000000
31	H	3.365631	3.994331	2.537768	1.092510	1.780454
32	H	2.525268	3.769466	3.085129	1.090321	1.779435

		31	32
31	H	0.000000	
32	H	1.780964	0.000000

Stoichiometry C10H17BrN2O2
Framework group C1[X(C10H17BrN2O2)]
Deg. of freedom 90
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.734125	2.260813	-0.238237
2	6	0	-3.922010	1.631541	-0.047166
3	7	0	-3.658567	0.266946	-0.073981
4	6	0	-2.335589	0.085187	-0.267765
5	7	0	-1.758029	1.284555	-0.354474
6	6	0	-0.297478	1.487960	-0.494696
7	6	0	0.431886	1.554051	0.853995
8	1	0	-2.497796	3.309575	-0.290868
9	1	0	-4.909503	2.030736	0.094894
10	1	0	0.087373	0.616639	-1.028582
11	1	0	-0.140787	2.394488	-1.079204
12	1	0	0.054240	2.371635	1.478088
13	1	0	0.270216	0.600114	1.365100
14	35	0	0.178690	-2.056792	-0.050994

15	1	0	-1.771362	-0.867980	-0.283781
16	6	0	-4.568318	-0.813846	0.073712
17	6	0	-5.880747	-0.684873	0.219441
18	1	0	-4.068151	-1.774010	0.055190
19	1	0	-6.488183	-1.572628	0.327278
20	1	0	-6.391400	0.269585	0.236810
21	8	0	1.808853	1.774286	0.602765
22	1	0	2.228458	0.910373	0.461140
23	6	0	4.802946	-1.030897	-0.189511
24	6	0	5.277637	0.279574	0.260778
25	8	0	3.932261	-0.132827	0.525468
26	1	0	4.523723	-1.182386	-1.223330
27	1	0	5.042847	-1.932841	0.356970
28	1	0	5.901774	0.323957	1.154073
29	6	0	5.458427	1.447647	-0.689609
30	1	0	5.158213	2.366147	-0.184057
31	1	0	6.503794	1.529670	-0.996298
32	1	0	4.833877	1.299534	-1.570972

Rotational constants (GHZ): 0.7190534 0.1760934 0.1452256

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.

475 basis functions, 751 primitive gaussians, 492 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1272.9300909081 Hartrees.

NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 475 RedAO= T EigKep= 4.30D-06 NBF= 475

NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999796 0.006119 -0.001166 0.019238 Ang= 2.32 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3225.51362922 A.U. after 13 cycles

NFock= 13 Conv=0.89D-08 -V/T= 2.0018

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.001024362	-0.000326498	-0.003006882
2	6	0.000201979	-0.000424641	0.001665935
3	7	0.001026177	0.000347263	-0.000137895
4	6	-0.000124679	0.000524183	-0.002608836
5	7	-0.000175715	0.002232005	0.001814418
6	6	-0.000791884	0.001170162	0.002264628
7	6	0.002352681	0.001142297	0.000037634
8	1	-0.000117591	-0.000122216	-0.000293353
9	1	0.000022596	-0.000145661	0.000381067
10	1	-0.000219121	-0.001143197	0.001476139
11	1	0.000028610	-0.000499534	-0.000147474
12	1	0.001087546	-0.000554936	0.001266924
13	1	-0.000131270	-0.000699702	-0.001668873
14	35	-0.002200585	-0.000249927	0.001094146
15	1	0.001418574	-0.001009367	-0.000052851
16	6	-0.000213830	0.000486926	0.000202217
17	6	0.000096608	0.000044376	0.000084089
18	1	-0.000019696	-0.000084535	-0.000089204
19	1	-0.000017453	0.000003416	-0.000110805
20	1	0.000019603	0.000042768	0.000007213
21	8	-0.007431144	-0.000204420	-0.000893811
22	1	0.005433620	-0.000259475	-0.001215132
23	6	-0.006277176	0.000682333	-0.002511659
24	6	0.006309950	-0.006555887	0.002867968
25	8	-0.000637060	-0.000684218	-0.000537375
26	1	0.000914756	-0.000218037	0.003809710

27	1	0.002224515	0.002240802	-0.001778182
28	1	-0.001145104	0.001890259	0.000016796
29	6	-0.003803715	0.007762670	-0.005197612
30	1	0.000451775	-0.002556312	0.001441271
31	1	0.000625387	-0.000590072	0.000283325
32	1	0.000067285	-0.002240825	0.001536461

Cartesian Forces: Max 0.007762670 RMS 0.002144294

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.005162545 RMS 0.001107249
Search for a local minimum.
Step number 8 out of a maximum of 177
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 7 8
DE= -2.34D-03 DEPred=-2.49D-03 R= 9.39D-01
TightC=F SS= 1.41D+00 RLast= 1.58D+00 DXNew= 2.4000D+00 4.7431D+00
Trust test= 9.39D-01 RLast= 1.58D+00 DXMaxT set to 2.40D+00
ITU= 1 1 1 0 1 0 1 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00151	0.00237	0.00254	0.00378	0.00612
Eigenvalues ---	0.00967	0.01246	0.01290	0.01402	0.01561
Eigenvalues ---	0.01653	0.01859	0.01950	0.02134	0.02147
Eigenvalues ---	0.02201	0.02262	0.02314	0.02391	0.02579
Eigenvalues ---	0.03062	0.03064	0.03142	0.03661	0.04136
Eigenvalues ---	0.04461	0.05194	0.05360	0.05629	0.05768
Eigenvalues ---	0.05927	0.06508	0.09410	0.09992	0.10552
Eigenvalues ---	0.10890	0.11072	0.11397	0.12928	0.13110
Eigenvalues ---	0.13695	0.14968	0.15994	0.15999	0.15999
Eigenvalues ---	0.16000	0.16000	0.16002	0.16015	0.16556
Eigenvalues ---	0.17196	0.18889	0.21461	0.22004	0.22063
Eigenvalues ---	0.22764	0.23549	0.23869	0.25006	0.27355
Eigenvalues ---	0.28243	0.28819	0.31849	0.32865	0.33054
Eigenvalues ---	0.33212	0.34075	0.34251	0.34421	0.34761
Eigenvalues ---	0.34938	0.35685	0.35689	0.35858	0.36435
Eigenvalues ---	0.36658	0.36958	0.37231	0.37740	0.37769
Eigenvalues ---	0.38905	0.42178	0.42509	0.45536	0.47462
Eigenvalues ---	0.49148	0.51795	0.54725	0.56094	0.60360

RFO step: Lambda=-1.24872417D-03 EMin= 1.51371594D-03

Quartic linear search produced a step of -0.14212.

Iteration 1 RMS(Cart)= 0.03894131 RMS(Int)= 0.00071509

Iteration 2 RMS(Cart)= 0.00099570 RMS(Int)= 0.00055331

Iteration 3 RMS(Cart)= 0.00000066 RMS(Int)= 0.00055331

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56583	-0.00031	-0.00009	0.00002	0.00003	2.56586
R2	2.61804	-0.00032	-0.00002	-0.00013	-0.00027	2.61777
R3	2.03400	0.00007	0.00001	0.00009	0.00010	2.03410
R4	2.62682	0.00060	0.00026	0.00041	0.00085	2.62767
R5	2.03063	0.00001	0.00000	0.00006	0.00006	2.03069
R6	2.54998	-0.00099	0.00006	-0.00084	-0.00078	2.54920
R7	2.68419	0.00043	0.00003	0.00050	0.00053	2.68472
R8	2.52091	-0.00125	-0.00004	-0.00180	-0.00231	2.51860
R9	2.09337	-0.00201	0.00197	-0.00340	-0.00163	2.09173
R10	2.79925	-0.00121	-0.00076	-0.00018	-0.00107	2.79817
R11	2.90016	0.00158	0.00227	0.00395	0.00653	2.90669
R12	2.06348	-0.00032	-0.00065	0.00010	-0.00055	2.06293
R13	2.05971	0.00034	0.00024	0.00026	0.00051	2.06022
R14	2.07057	-0.00062	-0.00010	-0.00101	-0.00112	2.06945
R15	2.06781	0.00020	0.00002	0.00058	0.00060	2.06841
R16	2.67759	-0.00381	-0.00320	0.00008	-0.00328	2.67431
R17	4.33822	-0.00213	-0.01936	-0.01022	-0.02972	4.30850
R18	8.04483	0.00076	-0.14926	0.26415	0.11499	8.15982
R19	2.50725	-0.00011	0.00001	-0.00003	-0.00002	2.50723
R20	2.04617	-0.00009	-0.00005	-0.00008	-0.00013	2.04603
R21	2.04293	0.00002	0.00000	0.00002	0.00002	2.04295
R22	2.04585	-0.00005	-0.00001	-0.00003	-0.00004	2.04581
R23	1.83456	0.00158	0.00001	0.00269	0.00289	1.83745
R24	3.77725	-0.00107	0.07887	-0.11038	-0.03138	3.74587
R25	2.76793	0.00210	0.00185	0.00318	0.00500	2.77294
R26	2.72266	-0.00020	-0.00428	0.00101	-0.00327	2.71939
R27	2.04379	0.00346	0.00172	0.00379	0.00551	2.04929
R28	2.04379	0.00311	0.00161	0.00323	0.00484	2.04862
R29	2.70579	0.00086	0.00189	0.00172	0.00364	2.70943
R30	2.06101	-0.00063	-0.00013	-0.00081	-0.00094	2.06007
R31	2.86611	-0.00356	-0.00394	-0.00327	-0.00722	2.85889
R32	2.06089	0.00145	0.00076	0.00186	0.00262	2.06351
R33	2.06455	0.00068	0.00055	0.00112	0.00166	2.06621
R34	2.06041	0.00103	0.00040	0.00129	0.00169	2.06210
A1	1.87719	-0.00036	-0.00004	0.00046	-0.00010	1.87709
A2	2.27911	0.00001	-0.00020	-0.00046	-0.00058	2.27853
A3	2.12682	0.00036	0.00024	0.00030	0.00062	2.12744
A4	1.86131	-0.00010	-0.00016	-0.00027	-0.00062	1.86070

A5	2.27893	-0.00011	-0.00005	-0.00034	-0.00035	2.27858
A6	2.14291	0.00022	0.00021	0.00072	0.00097	2.14387
A7	1.89738	-0.00022	0.00026	-0.00031	-0.00030	1.89708
A8	2.24410	0.00052	0.00005	0.00117	0.00133	2.24544
A9	2.14169	-0.00030	-0.00031	-0.00084	-0.00103	2.14066
A10	1.88884	0.00027	-0.00038	0.00112	0.00066	1.88950
A11	2.23616	0.00010	0.00190	-0.00129	0.00155	2.23771
A12	2.15573	-0.00034	-0.00132	0.00166	-0.00076	2.15497
A13	1.89976	0.00045	0.00035	0.00007	0.00034	1.90010
A14	2.22165	-0.00135	-0.00181	-0.00357	-0.00467	2.21698
A15	2.16096	0.00089	0.00135	0.00272	0.00322	2.16417
A16	1.97286	-0.00233	-0.00275	-0.00722	-0.01252	1.96033
A17	1.85899	0.00022	0.00150	0.00371	0.00565	1.86464
A18	1.88254	0.00091	-0.00096	0.00001	0.00008	1.88262
A19	1.87186	0.00208	0.00265	0.01416	0.01794	1.88980
A20	1.94672	-0.00014	0.00050	-0.00807	-0.00742	1.93930
A21	1.92922	-0.00076	-0.00094	-0.00207	-0.00330	1.92593
A22	1.94860	-0.00100	-0.00328	-0.00846	-0.01295	1.93565
A23	1.87834	0.00150	0.00234	0.01088	0.01347	1.89181
A24	1.88886	0.00081	0.00407	0.00748	0.01350	1.90236
A25	1.91085	-0.00012	-0.00118	-0.00215	-0.00313	1.90772
A26	1.89648	-0.00093	-0.00299	-0.00956	-0.01288	1.88360
A27	1.94110	-0.00024	0.00101	0.00205	0.00201	1.94311
A28	2.12782	-0.00046	0.03531	-0.05099	-0.01547	2.11235
A29	2.63989	0.00036	-0.00274	0.00673	0.00384	2.64374
A30	2.17853	0.00010	0.00013	0.00048	0.00060	2.17914
A31	1.95746	-0.00006	-0.00006	-0.00039	-0.00045	1.95701
A32	2.14719	-0.00004	-0.00007	-0.00009	-0.00016	2.14704
A33	2.07938	0.00002	0.00013	-0.00008	0.00005	2.07942
A34	2.15801	-0.00001	-0.00017	0.00023	0.00006	2.15807
A35	2.04580	-0.00001	0.00004	-0.00014	-0.00010	2.04569
A36	1.88345	0.00205	0.00153	0.01074	0.01215	1.89559
A37	2.54662	0.00516	0.00208	0.01083	0.01125	2.55787
A38	2.09769	-0.00057	-0.00153	-0.00437	-0.00595	2.09174
A39	2.11637	-0.00048	-0.00231	-0.00345	-0.00566	2.11071
A40	1.98848	0.00048	0.00244	0.00340	0.00577	1.99425
A41	1.98573	0.00043	0.00329	0.00301	0.00635	1.99207
A42	2.00805	0.00049	0.00009	0.00367	0.00379	2.01184
A43	2.06424	-0.00143	-0.00456	-0.00403	-0.00882	2.05543
A44	2.13535	0.00046	0.00126	0.00108	0.00259	2.13794
A45	1.98015	-0.00068	-0.00292	-0.00124	-0.00412	1.97603
A46	2.03718	0.00014	0.00119	-0.00075	0.00043	2.03761
A47	1.99729	0.00119	0.00400	0.00327	0.00727	2.00457
A48	1.02388	0.00152	-0.00090	0.00050	0.00051	1.02439

A49	1.75578	-0.00185	0.01229	-0.02319	-0.01141	1.74437
A50	2.54005	-0.00014	0.00353	-0.00526	-0.00128	2.53877
A51	2.27137	-0.00062	-0.00609	0.00795	0.00153	2.27289
A52	1.90217	0.00311	0.00491	0.00739	0.01230	1.91447
A53	1.92600	-0.00040	0.00059	-0.00149	-0.00089	1.92511
A54	1.91095	0.00303	0.00344	0.00884	0.01226	1.92321
A55	1.90742	-0.00169	-0.00340	-0.00546	-0.00884	1.89858
A56	1.90864	-0.00274	-0.00345	-0.00569	-0.00917	1.89946
A57	1.90856	-0.00135	-0.00231	-0.00364	-0.00595	1.90260
A58	3.29524	0.00090	-0.00699	0.00845	0.00204	3.29729
A59	3.55351	0.00061	-0.01784	0.03681	0.01870	3.57220
D1	-0.01894	0.00111	0.00395	0.03651	0.04029	0.02135
D2	3.13141	0.00072	0.00227	0.02097	0.02307	-3.12870
D3	3.13547	0.00011	0.00088	0.00886	0.00994	-3.13777
D4	0.00264	-0.00028	-0.00080	-0.00668	-0.00728	-0.00464
D5	0.02396	-0.00138	-0.00513	-0.04336	-0.04812	-0.02416
D6	-3.07512	-0.00110	-0.00279	-0.02345	-0.02554	-3.10066
D7	-3.12910	-0.00049	-0.00238	-0.01865	-0.02097	3.13312
D8	0.05501	-0.00021	-0.00004	0.00126	0.00161	0.05661
D9	0.00764	-0.00045	-0.00146	-0.01751	-0.01909	-0.01145
D10	-3.13729	-0.00038	-0.00099	-0.01205	-0.01294	3.13296
D11	3.14132	-0.00011	0.00005	-0.00349	-0.00353	3.13779
D12	-0.00361	-0.00003	0.00052	0.00198	0.00262	-0.00099
D13	0.00720	-0.00040	-0.00171	-0.00930	-0.01068	-0.00347
D14	3.07472	0.00015	0.00193	0.01334	0.01585	3.09057
D15	-3.13129	-0.00047	-0.00215	-0.01439	-0.01639	3.13551
D16	-0.06377	0.00007	0.00149	0.00826	0.01014	-0.05363
D17	0.04657	-0.00004	0.00017	-0.00247	-0.00242	0.04415
D18	-3.09435	0.00004	0.00035	-0.00068	-0.00045	-3.09480
D19	-3.09878	0.00005	0.00070	0.00369	0.00451	-3.09428
D20	0.04348	0.00013	0.00088	0.00548	0.00648	0.04996
D21	-0.01913	0.00109	0.00420	0.03230	0.03606	0.01693
D22	3.08176	0.00075	0.00183	0.01305	0.01409	3.09585
D23	-3.09084	0.00055	0.00065	0.01109	0.01096	-3.07987
D24	0.01005	0.00022	-0.00171	-0.00816	-0.01101	-0.00096
D25	-2.73001	0.00055	-0.01231	0.02152	0.00710	-2.72290
D26	0.32717	0.00120	-0.00811	0.04728	0.03738	0.36455
D27	1.56216	-0.00105	0.00505	-0.05559	-0.05152	1.51063
D28	-2.66982	0.00033	0.00769	-0.03998	-0.03308	-2.70290
D29	-0.59842	0.00002	0.00689	-0.04044	-0.03390	-0.63232
D30	-1.53101	-0.00071	0.00777	-0.03283	-0.02564	-1.55665
D31	0.52020	0.00067	0.01041	-0.01721	-0.00720	0.51300
D32	2.59159	0.00036	0.00961	-0.01767	-0.00802	2.58358
D33	-1.03641	-0.00042	-0.03603	0.01218	-0.02396	-1.06037

D34	1.06094	-0.00020	-0.03796	0.01147	-0.02700	1.03394
D35	-3.12283	0.00082	-0.03292	0.02427	-0.00886	-3.13169
D36	-3.08006	-0.00069	-0.03797	0.00272	-0.03509	-3.11515
D37	-0.98271	-0.00047	-0.03990	0.00201	-0.03813	-1.02084
D38	1.11670	0.00055	-0.03485	0.01481	-0.01999	1.09671
D39	1.08845	-0.00102	-0.03887	0.00094	-0.03816	1.05030
D40	-3.09738	-0.00081	-0.04080	0.00023	-0.04120	-3.13857
D41	-0.99796	0.00021	-0.03575	0.01303	-0.02306	-1.02102
D42	-1.50735	-0.00076	0.00786	-0.02731	-0.02123	-1.52858
D43	2.65690	0.00052	0.01123	-0.01587	-0.00591	2.65099
D44	0.55238	0.00143	0.01400	-0.00826	0.00502	0.55740
D45	-0.12074	0.00096	0.04095	-0.02348	0.01576	-0.10498
D46	0.08066	-0.00054	-0.03853	-0.01025	-0.04801	0.03265
D47	-2.54147	-0.00097	-0.03372	-0.02363	-0.05634	-2.59781
D48	-3.13886	0.00014	0.00037	0.00271	0.00308	-3.13578
D49	0.00360	0.00005	0.00023	0.00104	0.00127	0.00487
D50	0.00199	0.00005	0.00017	0.00073	0.00090	0.00289
D51	-3.13874	-0.00004	0.00004	-0.00094	-0.00091	-3.13964
D52	-2.72088	-0.00079	0.02265	-0.02318	-0.00009	-2.72097
D53	2.96797	0.00065	-0.00943	0.05146	0.04149	3.00946
D54	-2.27557	-0.00039	0.01197	0.00598	0.01747	-2.25810
D55	-0.58553	0.00004	0.00841	0.01464	0.02279	-0.56274
D56	-2.73168	0.00042	0.00202	0.00652	0.00857	-2.72311
D57	-0.04884	0.00125	0.00473	0.00809	0.01291	-0.03593
D58	0.02341	-0.00120	-0.00821	-0.00530	-0.01351	0.00990
D59	2.70624	-0.00036	-0.00549	-0.00373	-0.00916	2.69708
D60	0.98730	0.00078	0.01041	-0.01388	-0.00328	0.98402
D61	0.14040	0.00083	-0.00585	0.02091	0.01477	0.15517
D62	-1.36133	-0.00091	0.00385	-0.02622	-0.02218	-1.38352
D63	-2.20824	-0.00086	-0.01241	0.00857	-0.00413	-2.21236
D64	1.91452	0.00134	0.00008	0.00952	0.00937	1.92389
D65	-0.46483	0.00007	-0.00429	0.00660	0.00205	-0.46278
D66	2.48496	0.00002	0.00544	0.00359	0.00908	2.49404
D67	-1.70361	-0.00035	0.00474	0.00060	0.00537	-1.69824
D68	0.39796	-0.00033	0.00445	0.00079	0.00528	0.40323
D69	1.27269	0.00069	0.00763	0.00438	0.01199	1.28469
D70	-2.91588	0.00032	0.00692	0.00139	0.00828	-2.90760
D71	-0.81431	0.00034	0.00664	0.00158	0.00819	-0.80612
D72	-1.09933	0.00021	0.00609	0.00337	0.00946	-1.08986
D73	0.99528	-0.00016	0.00539	0.00038	0.00575	1.00104
D74	3.09685	-0.00015	0.00510	0.00057	0.00566	3.10251

Item	Value	Threshold	Converged?
Maximum Force	0.005163	0.000450	NO
RMS Force	0.001107	0.000300	NO

Maximum Displacement 0.192839 0.001800 NO
RMS Displacement 0.039225 0.001200 NO
Predicted change in Energy=-7.355796D-04
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.549179	-1.904923	0.164146
2	6	0	-2.790342	-1.366314	0.050034
3	7	0	-2.629650	0.014315	0.089194
4	6	0	-1.318251	0.292914	0.238718
5	7	0	-0.650829	-0.859128	0.299218
6	6	0	0.822768	-0.957691	0.405789
7	6	0	1.507016	-0.992171	-0.971358
8	1	0	-1.230856	-2.933117	0.175305
9	1	0	-3.749390	-1.838401	-0.060017
10	1	0	1.161970	-0.064798	0.934363
11	1	0	1.057270	-1.852136	0.983332
12	1	0	1.175385	-1.860208	-1.550831
13	1	0	1.245263	-0.076034	-1.510091
14	35	0	0.997447	2.624231	-0.007447
15	1	0	-0.827516	1.284768	0.263776
16	6	0	-3.622682	1.026216	-0.001964
17	6	0	-4.926892	0.802269	-0.097892
18	1	0	-3.194344	2.020489	0.012778
19	1	0	-5.601843	1.643880	-0.167712
20	1	0	-5.366219	-0.187079	-0.111804
21	8	0	2.906150	-1.099679	-0.788027
22	1	0	3.276917	-0.205331	-0.697946
23	6	0	5.721074	1.918465	-0.234145
24	6	0	6.267552	0.638435	-0.698986
25	8	0	4.879301	0.947070	-0.881172
26	1	0	5.506457	2.063128	0.818956
27	1	0	5.868715	2.827840	-0.805528
28	1	0	6.833203	0.636134	-1.630890
29	6	0	6.594310	-0.496919	0.245970
30	1	0	6.347576	-1.450509	-0.225382
31	1	0	7.659657	-0.491067	0.491948
32	1	0	6.016429	-0.399035	1.166418

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357795	0.000000			
3	N	2.203749	1.390500	0.000000		
4	C	2.211194	2.226139	1.348978	0.000000	
5	N	1.385267	2.212882	2.173187	1.332784	0.000000
6	C	2.565496	3.653505	3.600585	2.485133	1.480730
7	C	3.385677	4.432890	4.387458	3.331345	2.507660
8	H	1.076400	2.214173	3.263647	3.227838	2.157131
9	H	2.212602	1.074593	2.169940	3.246873	3.269420
10	H	3.365950	4.254028	3.885479	2.600649	2.078608
11	H	2.732659	3.988883	4.228061	3.286152	2.090857
12	H	3.219688	4.305077	4.547726	3.749219	2.785661
13	H	3.735881	4.514966	4.192949	3.125069	2.735325
14	Br	5.198844	5.502282	4.469545	3.295162	3.865830
15	H	3.271827	3.305542	2.211835	1.106897	2.151456
16	C	3.594244	2.533712	1.420693	2.430239	3.532300
17	C	4.336646	3.047865	2.435815	3.659923	4.604633
18	H	4.258913	3.411018	2.085535	2.560330	3.852753
19	H	5.397056	4.124708	3.399326	4.509928	5.567370
20	H	4.194870	2.837592	2.751322	4.091370	4.780741
21	O	4.626555	5.763980	5.714506	4.564985	3.727207
22	H	5.188739	6.222458	5.962832	4.716053	4.104750
23	C	8.223960	9.127691	8.571169	7.240036	6.971417
24	C	8.265285	9.307282	8.953823	7.651345	7.148643
25	O	7.109986	8.064882	7.628629	6.331802	5.936161
26	H	8.121342	9.010504	8.421782	7.074388	6.835340
27	H	8.852370	9.659306	8.996591	7.692124	7.570908
28	H	8.941110	9.972358	9.637994	8.370151	7.872221
29	C	8.264719	9.426873	9.239447	7.951887	7.254383
30	H	7.919404	9.142456	9.101387	7.875266	7.042913
31	H	9.322505	10.495896	10.309581	9.015630	8.320866
32	H	7.778860	8.929791	8.722726	7.425426	6.739143

		6	7	8	9	10
6	C	0.000000				
7	C	1.538154	0.000000			
8	H	2.858811	3.546555	0.000000		
9	H	4.679450	5.401523	2.756228	0.000000	
10	H	1.091653	2.147288	3.811697	5.315630	0.000000
11	H	1.090220	2.182344	2.656491	4.918613	1.791072
12	H	2.183401	1.095106	3.149710	5.145524	3.065920
13	H	2.150911	1.094557	4.139402	5.491376	2.445899
14	Br	3.609909	3.777187	5.990229	6.515391	2.853936
15	H	2.787872	3.487125	4.238049	4.289100	2.495811

16	C	4.885097	5.597089	4.629101	2.868006	4.995990
17	C	6.034048	6.736328	5.261979	2.891554	6.236313
18	H	5.016095	5.669870	5.331033	3.899283	4.916830
19	H	6.955048	7.624335	6.338145	3.945815	7.062812
20	H	6.258219	6.973404	4.972362	2.311641	6.612615
21	O	2.405378	1.415184	4.626481	6.735869	2.660784
22	H	2.794123	1.956124	5.340730	7.241744	2.675291
23	C	5.716222	5.174319	8.487333	10.189900	5.107267
24	C	5.780469	5.039421	8.351436	10.338381	5.406416
25	O	4.662601	3.891156	7.314780	9.104255	4.258943
26	H	5.588649	5.341872	8.412379	10.082917	4.839003
27	H	6.423326	5.800379	9.195355	10.716228	5.792066
28	H	6.543216	5.608443	9.001719	10.980995	6.263762
29	C	5.792111	5.254305	8.195930	10.434814	5.492807
30	H	5.582540	4.919104	7.732484	10.105768	5.491422
31	H	6.853337	6.344081	9.225242	11.501580	6.526666
32	H	5.278709	5.025605	7.741254	9.947218	4.871482

		11	12	13	14	15
11	H	0.000000				
12	H	2.536927	0.000000			
13	H	3.067090	1.786007	0.000000		
14	Br	4.585094	4.745934	3.100126	0.000000	
15	H	3.729658	4.146720	3.048737	2.279959	0.000000
16	C	5.581906	5.809637	5.214047	4.888689	2.819649
17	C	6.635142	6.814514	6.392277	6.198832	4.143487
18	H	5.832275	6.049729	5.140491	4.235095	2.491217
19	H	7.608602	7.753868	7.186302	6.673635	4.807217
20	H	6.725545	6.903821	6.758641	6.957773	4.786148
21	O	2.668757	2.038583	2.080330	4.256755	4.553257
22	H	3.235042	2.807573	2.191784	3.698539	4.471205
23	C	6.119702	6.056016	5.063492	4.781438	6.597995
24	C	6.014996	5.735767	5.137289	5.674118	7.189203
25	O	5.091154	4.695556	3.827338	4.317992	5.830327
26	H	5.928876	6.306079	5.306435	4.618327	6.405723
27	H	6.946380	6.675374	5.505016	4.940409	6.954422
28	H	6.810803	6.184581	5.634434	6.375276	7.918150
29	C	5.747967	5.869566	5.645636	6.413320	7.632708
30	H	5.441473	5.355019	5.438130	6.728661	7.694346
31	H	6.759104	6.934932	6.732375	7.371534	8.673971
32	H	5.170907	5.740573	5.480151	5.975640	7.105599

		16	17	18	19	20
16	C	0.000000				
17	C	1.326769	0.000000			
18	H	1.082714	2.120855	0.000000		

19	H	2.079918	1.081084	2.443452	0.000000	
20	H	2.126986	1.082594	3.099341	1.846903	0.000000
21	O	6.911077	8.090132	6.898752	8.960907	8.349983
22	H	7.043122	8.287207	6.880162	9.084773	8.663007
23	C	9.389132	10.707177	8.919421	11.326441	11.286113
24	C	9.922345	11.211767	9.588752	11.923745	11.677794
25	O	8.547689	9.838491	8.193603	10.528482	10.336774
26	H	9.224439	10.549177	8.738174	11.159910	11.142029
27	H	9.694234	11.006762	9.135671	11.549124	11.653099
28	H	10.589197	11.860755	10.255232	12.561322	12.321169
29	C	10.332877	11.599320	10.109870	12.389524	11.969890
30	H	10.275706	11.498038	10.156417	12.343710	11.782281
31	H	11.394616	12.666564	11.151093	13.448440	13.043404
32	H	9.813711	11.081420	9.592879	11.871716	11.456153

		21	22	23	24	25
21	O	0.000000				
22	H	0.972338	0.000000			
23	C	4.164106	3.271013	0.000000		
24	C	3.785233	3.107385	1.467376	0.000000	
25	O	2.844500	1.982230	1.439040	1.433767	0.000000
26	H	4.398561	3.523882	1.084439	2.216566	2.128226
27	H	4.919604	3.991130	1.084085	2.227985	2.126490
28	H	4.375524	3.771687	2.198204	1.090142	2.115772
29	C	3.877498	3.461373	2.612878	1.512859	2.509345
30	H	3.504720	3.347049	3.426743	2.143453	2.886915
31	H	4.960300	4.550375	3.176658	2.152221	3.418198
32	H	3.739598	3.319383	2.723897	2.149218	2.701423

		26	27	28	29	30
26	H	0.000000				
27	H	1.831656	0.000000			
28	H	3.130225	2.532792	0.000000		
29	C	2.839996	3.561764	2.205331	0.000000	
30	H	3.760820	4.343978	2.562296	1.091963	0.000000
31	H	3.356652	3.988240	2.541662	1.093391	1.776696
32	H	2.538316	3.784589	3.092511	1.091216	1.775489

		31	32
31	H	0.000000	
32	H	1.778645	0.000000

Stoichiometry C10H17BrN2O2

Framework group C1[X(C10H17BrN2O2)]

Deg. of freedom 90

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.714454	2.265271	-0.211088
2	6	0	-3.908319	1.645931	-0.024776
3	7	0	-3.654521	0.278950	-0.045817
4	6	0	-2.335816	0.087190	-0.255551
5	7	0	-1.753496	1.280440	-0.371189
6	6	0	-0.297198	1.476893	-0.553290
7	6	0	0.449241	1.588690	0.786952
8	1	0	-2.469004	3.312278	-0.257625
9	1	0	-4.891255	2.053834	0.124231
10	1	0	0.076879	0.597647	-1.081209
11	1	0	-0.153576	2.372141	-1.158669
12	1	0	0.086907	2.444798	1.365788
13	1	0	0.278079	0.669082	1.355353
14	35	0	0.144965	-2.074654	-0.081648
15	1	0	-1.779391	-0.869189	-0.286396
16	6	0	-4.569494	-0.796048	0.114095
17	6	0	-5.879860	-0.659505	0.270984
18	1	0	-4.074572	-1.758866	0.096723
19	1	0	-6.490722	-1.543429	0.390433
20	1	0	-6.385432	0.297633	0.288171
21	8	0	1.826989	1.787274	0.531762
22	1	0	2.253961	0.918514	0.440152
23	6	0	4.813815	-1.043425	-0.105253
24	6	0	5.292335	0.280955	0.307335
25	8	0	3.939301	-0.117519	0.564642
26	1	0	4.558724	-1.225855	-1.143355
27	1	0	5.051699	-1.927634	0.475115
28	1	0	5.901158	0.342631	1.209522
29	6	0	5.493318	1.414585	-0.674108
30	1	0	5.204390	2.359402	-0.209109
31	1	0	6.543275	1.475931	-0.972991
32	1	0	4.879484	1.256993	-1.562436

Rotational constants (GHZ): 0.7131404 0.1756928 0.1446394

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.

475 basis functions, 751 primitive gaussians, 492 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1271.2037364075 Hartrees.
NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 475 RedAO= T EigKep= 4.06D-06 NBF= 475
NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999994 0.002800 -0.000025 0.002078 Ang= 0.40 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3225.51456300 A.U. after 12 cycles
NFock= 12 Conv=0.30D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000026500	-0.000625754	0.001955698
2	6	0.000630476	-0.000299756	-0.001550218
3	7	0.000549286	0.000225804	0.000588304
4	6	-0.000842111	0.000855719	0.001009602
5	7	0.000984677	0.001097859	-0.002151765
6	6	0.000180513	0.000675576	-0.000302922
7	6	0.003054735	0.000867039	0.000228270

8	1	-0.000173797	-0.000076400	0.000243927
9	1	0.000059809	-0.000062154	-0.000214353
10	1	-0.000363212	-0.000600014	0.000332772
11	1	-0.000177103	-0.000344231	0.000061068
12	1	0.000033469	-0.000484545	0.000532686
13	1	-0.000477361	-0.000373786	-0.000291571
14	35	-0.001773259	-0.000153350	0.000858383
15	1	0.001572462	-0.000255675	-0.000350304
16	6	-0.000130868	0.000317742	-0.000025599
17	6	0.000119679	-0.000027906	-0.000017602
18	1	0.000024656	-0.000038431	-0.000058505
19	1	-0.000010251	0.000010718	0.000024721
20	1	0.000026382	0.000000760	-0.000000084
21	8	-0.005976580	0.000840791	0.000179728
22	1	0.003951614	-0.001417540	-0.000943654
23	6	-0.004223914	0.000341613	-0.000963706
24	6	0.004170389	-0.004052568	0.002332999
25	8	-0.000585673	-0.000162726	-0.000698149
26	1	0.000579283	-0.000134585	0.001647359
27	1	0.001228687	0.000869669	-0.000870786
28	1	-0.000821678	0.001046259	-0.000017278
29	6	-0.002236133	0.004585569	-0.003161275
30	1	0.000279714	-0.001241259	0.000758581
31	1	0.000371692	-0.000288600	0.000147019
32	1	0.000000917	-0.001095840	0.000716655

Cartesian Forces: Max 0.005976580 RMS 0.001437530

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.003881390 RMS 0.000712341
Search for a local minimum.
Step number 9 out of a maximum of 177
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Update second derivatives using D2CorX and points 8 9
DE= -9.34D-04 DEPred=-7.36D-04 R= 1.27D+00
TightC=F SS= 1.41D+00 RLast= 2.31D-01 DXNew= 4.0363D+00 6.9248D-01
Trust test= 1.27D+00 RLast= 2.31D-01 DXMaxT set to 2.40D+00
ITU= 1 1 1 1 0 1 0 1 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00148	0.00237	0.00250	0.00370	0.00556
Eigenvalues ---	0.00938	0.01246	0.01287	0.01401	0.01558
Eigenvalues ---	0.01659	0.01860	0.01941	0.02109	0.02142
Eigenvalues ---	0.02188	0.02275	0.02314	0.02390	0.03058
Eigenvalues ---	0.03062	0.03129	0.03603	0.03661	0.03874
Eigenvalues ---	0.04531	0.05163	0.05303	0.05575	0.05645
Eigenvalues ---	0.05891	0.06056	0.09274	0.09914	0.10412
Eigenvalues ---	0.10984	0.11110	0.11500	0.12936	0.13023
Eigenvalues ---	0.13687	0.15007	0.15552	0.15996	0.15999
Eigenvalues ---	0.16000	0.16000	0.16000	0.16007	0.16139
Eigenvalues ---	0.16664	0.18889	0.19450	0.21906	0.22010
Eigenvalues ---	0.22749	0.23554	0.23728	0.24992	0.26999
Eigenvalues ---	0.27655	0.28910	0.31842	0.32863	0.33054
Eigenvalues ---	0.33168	0.34076	0.34288	0.34457	0.34762
Eigenvalues ---	0.34940	0.35682	0.35688	0.35858	0.35929
Eigenvalues ---	0.36436	0.36658	0.37227	0.37292	0.37765
Eigenvalues ---	0.38887	0.42178	0.42410	0.45025	0.46179
Eigenvalues ---	0.49162	0.51899	0.54535	0.56144	0.60358

RFO step: Lambda=-9.27634981D-04 EMin= 1.47804193D-03

Quartic linear search produced a step of 0.43781.

Iteration 1 RMS(Cart)= 0.04418583 RMS(Int)= 0.00390334

Iteration 2 RMS(Cart)= 0.00614016 RMS(Int)= 0.00018470

Iteration 3 RMS(Cart)= 0.00001199 RMS(Int)= 0.00018464

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00018464

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56586	-0.00035	0.00001	-0.00019	-0.00015	2.56571
R2	2.61777	0.00012	-0.00012	0.00043	0.00026	2.61804
R3	2.03410	0.00003	0.00004	0.00007	0.00011	2.03422
R4	2.62767	0.00047	0.00037	0.00121	0.00165	2.62932
R5	2.03069	0.00000	0.00003	-0.00005	-0.00003	2.03066
R6	2.54920	-0.00070	-0.00034	-0.00117	-0.00150	2.54770
R7	2.68472	0.00016	0.00023	0.00039	0.00062	2.68534
R8	2.51860	-0.00017	-0.00101	-0.00167	-0.00274	2.51586
R9	2.09173	-0.00109	-0.00071	-0.00200	-0.00269	2.08905
R10	2.79817	-0.00105	-0.00047	-0.00325	-0.00374	2.79444
R11	2.90669	-0.00039	0.00286	0.00023	0.00325	2.90994
R12	2.06293	-0.00044	-0.00024	-0.00119	-0.00143	2.06150
R13	2.06022	0.00028	0.00022	0.00070	0.00092	2.06114
R14	2.06945	0.00009	-0.00049	0.00043	-0.00006	2.06939
R15	2.06841	-0.00005	0.00026	0.00023	0.00049	2.06891
R16	2.67431	-0.00335	-0.00144	-0.00653	-0.00800	2.66631
R17	4.30850	-0.00193	-0.01301	-0.04540	-0.05841	4.25009
R18	8.15982	0.00045	0.05035	0.20383	0.25413	8.41395

R19	2.50723	-0.00013	-0.00001	-0.00014	-0.00015	2.50708
R20	2.04603	-0.00003	-0.00006	-0.00003	-0.00009	2.04594
R21	2.04295	0.00001	0.00001	0.00001	0.00002	2.04297
R22	2.04581	-0.00001	-0.00002	0.00006	0.00004	2.04585
R23	1.83745	0.00023	0.00126	0.00145	0.00269	1.84014
R24	3.74587	-0.00073	-0.01374	-0.07536	-0.08909	3.65678
R25	2.77294	0.00111	0.00219	0.00271	0.00492	2.77786
R26	2.71939	-0.00057	-0.00143	-0.00324	-0.00471	2.71468
R27	2.04929	0.00147	0.00241	0.00245	0.00486	2.05415
R28	2.04862	0.00136	0.00212	0.00226	0.00438	2.05301
R29	2.70943	0.00069	0.00159	0.00542	0.00703	2.71646
R30	2.06007	-0.00041	-0.00041	-0.00103	-0.00144	2.05863
R31	2.85889	-0.00278	-0.00316	-0.00923	-0.01239	2.84650
R32	2.06351	0.00069	0.00115	0.00150	0.00265	2.06616
R33	2.06621	0.00039	0.00073	0.00136	0.00209	2.06830
R34	2.06210	0.00050	0.00074	0.00084	0.00158	2.06368
A1	1.87709	-0.00033	-0.00004	-0.00127	-0.00159	1.87549
A2	2.27853	0.00001	-0.00025	-0.00013	-0.00036	2.27817
A3	2.12744	0.00033	0.00027	0.00178	0.00207	2.12951
A4	1.86070	0.00013	-0.00027	0.00083	0.00043	1.86113
A5	2.27858	-0.00014	-0.00015	-0.00082	-0.00097	2.27762
A6	2.14387	0.00002	0.00042	0.00013	0.00056	2.14444
A7	1.89708	-0.00004	-0.00013	-0.00043	-0.00067	1.89642
A8	2.24544	0.00022	0.00058	0.00143	0.00205	2.24749
A9	2.14066	-0.00018	-0.00045	-0.00098	-0.00139	2.13927
A10	1.88950	0.00000	0.00029	0.00023	0.00041	1.88991
A11	2.23771	0.00020	0.00068	0.00205	0.00298	2.24069
A12	2.15497	-0.00020	-0.00033	-0.00266	-0.00327	2.15170
A13	1.90010	0.00027	0.00015	0.00161	0.00167	1.90177
A14	2.21698	-0.00095	-0.00204	-0.00333	-0.00513	2.21185
A15	2.16417	0.00071	0.00141	0.00229	0.00344	2.16761
A16	1.96033	-0.00108	-0.00548	-0.00934	-0.01544	1.94489
A17	1.86464	0.00013	0.00247	0.00167	0.00429	1.86893
A18	1.88262	0.00019	0.00004	-0.00115	-0.00100	1.88163
A19	1.88980	0.00090	0.00786	0.01214	0.02031	1.91011
A20	1.93930	0.00010	-0.00325	-0.00274	-0.00609	1.93321
A21	1.92593	-0.00026	-0.00144	-0.00048	-0.00198	1.92395
A22	1.93565	-0.00064	-0.00567	-0.01051	-0.01632	1.91933
A23	1.89181	0.00030	0.00590	0.00483	0.01057	1.90238
A24	1.90236	-0.00014	0.00591	0.00614	0.01227	1.91463
A25	1.90772	0.00008	-0.00137	-0.00225	-0.00351	1.90421
A26	1.88360	-0.00010	-0.00564	-0.00542	-0.01100	1.87260
A27	1.94311	0.00050	0.00088	0.00708	0.00740	1.95051
A28	2.11235	-0.00090	-0.00677	-0.03401	-0.04132	2.07103

A29	2.64374	0.00039	0.00168	0.00590	0.00737	2.65111
A30	2.17914	-0.00009	0.00026	0.00000	0.00026	2.17940
A31	1.95701	0.00001	-0.00020	-0.00036	-0.00056	1.95645
A32	2.14704	0.00008	-0.00007	0.00036	0.00029	2.14733
A33	2.07942	0.00002	0.00002	-0.00003	-0.00001	2.07941
A34	2.15807	-0.00004	0.00002	0.00009	0.00012	2.15819
A35	2.04569	0.00002	-0.00005	-0.00006	-0.00011	2.04559
A36	1.89559	0.00152	0.00532	0.00737	0.01195	1.90754
A37	2.55787	0.00388	0.00492	0.02227	0.02773	2.58560
A38	2.09174	-0.00032	-0.00260	-0.00452	-0.00721	2.08454
A39	2.11071	-0.00035	-0.00248	-0.00517	-0.00777	2.10294
A40	1.99425	0.00031	0.00253	0.00343	0.00595	2.00020
A41	1.99207	0.00006	0.00278	0.00416	0.00691	1.99898
A42	2.01184	0.00031	0.00166	0.00357	0.00495	2.01680
A43	2.05543	-0.00073	-0.00386	-0.00663	-0.01041	2.04501
A44	2.13794	0.00019	0.00113	0.00044	0.00148	2.13942
A45	1.97603	-0.00047	-0.00180	-0.00396	-0.00581	1.97022
A46	2.03761	0.00024	0.00019	0.00152	0.00171	2.03933
A47	2.00457	0.00070	0.00318	0.00663	0.00982	2.01438
A48	1.02439	0.00158	0.00023	0.00439	0.00438	1.02878
A49	1.74437	-0.00187	-0.00500	-0.02594	-0.03052	1.71385
A50	2.53877	-0.00020	-0.00056	-0.00527	-0.00602	2.53275
A51	2.27289	-0.00041	0.00067	0.00425	0.00503	2.27792
A52	1.91447	0.00157	0.00539	0.00813	0.01343	1.92790
A53	1.92511	-0.00020	-0.00039	0.00000	-0.00039	1.92472
A54	1.92321	0.00140	0.00537	0.00747	0.01276	1.93597
A55	1.89858	-0.00085	-0.00387	-0.00603	-0.00989	1.88868
A56	1.89946	-0.00137	-0.00402	-0.00610	-0.01028	1.88918
A57	1.90260	-0.00061	-0.00261	-0.00380	-0.00641	1.89619
A58	3.29729	0.00117	0.00089	0.00864	0.00941	3.30670
A59	3.57220	0.00077	0.00819	0.04174	0.04980	3.62200
D1	0.02135	-0.00085	0.01764	-0.03554	-0.01794	0.00341
D2	-3.12870	-0.00043	0.01010	-0.01756	-0.00750	-3.13621
D3	-3.13777	-0.00025	0.00435	-0.00990	-0.00549	3.13992
D4	-0.00464	0.00017	-0.00319	0.00808	0.00495	0.00031
D5	-0.02416	0.00089	-0.02107	0.03622	0.01526	-0.00890
D6	-3.10066	0.00055	-0.01118	0.02636	0.01538	-3.08528
D7	3.13312	0.00035	-0.00918	0.01329	0.00412	3.13724
D8	0.05661	0.00001	0.00070	0.00344	0.00425	0.06086
D9	-0.01145	0.00052	-0.00836	0.02297	0.01458	0.00313
D10	3.13296	0.00033	-0.00566	0.01407	0.00842	3.14138
D11	3.13779	0.00014	-0.00154	0.00672	0.00514	-3.14025
D12	-0.00099	-0.00005	0.00115	-0.00219	-0.00102	-0.00200
D13	-0.00347	0.00002	-0.00467	-0.00068	-0.00524	-0.00872

D14	3.09057	-0.00019	0.00694	-0.00961	-0.00252	3.08805
D15	3.13551	0.00020	-0.00717	0.00759	0.00046	3.13597
D16	-0.05363	-0.00001	0.00444	-0.00134	0.00318	-0.05045
D17	0.04415	0.00013	-0.00106	0.00706	0.00597	0.05012
D18	-3.09480	0.00014	-0.00020	0.00784	0.00761	-3.08719
D19	-3.09428	-0.00009	0.00197	-0.00296	-0.00095	-3.09523
D20	0.04996	-0.00007	0.00284	-0.00218	0.00068	0.05064
D21	0.01693	-0.00056	0.01579	-0.02171	-0.00606	0.01087
D22	3.09585	-0.00030	0.00617	-0.01248	-0.00657	3.08928
D23	-3.07987	-0.00037	0.00480	-0.01345	-0.00881	-3.08868
D24	-0.00096	-0.00011	-0.00482	-0.00422	-0.00932	-0.01027
D25	-2.72290	0.00048	0.00311	0.02367	0.02611	-2.69680
D26	0.36455	0.00025	0.01637	0.01360	0.02932	0.39387
D27	1.51063	-0.00022	-0.02256	-0.02083	-0.04359	1.46705
D28	-2.70290	0.00035	-0.01448	-0.01025	-0.02494	-2.72784
D29	-0.63232	0.00022	-0.01484	-0.01052	-0.02550	-0.65782
D30	-1.55665	-0.00058	-0.01123	-0.03201	-0.04331	-1.59997
D31	0.51300	-0.00001	-0.00315	-0.02143	-0.02467	0.48833
D32	2.58358	-0.00014	-0.00351	-0.02170	-0.02523	2.55835
D33	-1.06037	-0.00001	-0.01049	0.01968	0.00904	-1.05134
D34	1.03394	-0.00011	-0.01182	0.01362	0.00148	1.03542
D35	-3.13169	0.00059	-0.00388	0.02883	0.02476	-3.10694
D36	-3.11515	-0.00011	-0.01536	0.01538	0.00009	-3.11506
D37	-1.02084	-0.00021	-0.01669	0.00932	-0.00747	-1.02830
D38	1.09671	0.00049	-0.00875	0.02453	0.01581	1.11252
D39	1.05030	-0.00045	-0.01671	0.00975	-0.00695	1.04334
D40	-3.13857	-0.00055	-0.01804	0.00370	-0.01451	3.13010
D41	-1.02102	0.00015	-0.01010	0.01890	0.00877	-1.01225
D42	-1.52858	-0.00043	-0.00929	-0.01612	-0.02576	-1.55434
D43	2.65099	0.00048	-0.00259	-0.00381	-0.00664	2.64435
D44	0.55740	0.00016	0.00220	-0.00183	0.00029	0.55769
D45	-0.10498	0.00061	0.00690	0.01118	0.01723	-0.08775
D46	0.03265	-0.00001	-0.02102	-0.01665	-0.03750	-0.00485
D47	-2.59781	-0.00033	-0.02466	-0.03034	-0.05518	-2.65299
D48	-3.13578	-0.00002	0.00135	-0.00006	0.00129	-3.13449
D49	0.00487	0.00001	0.00056	0.00036	0.00092	0.00579
D50	0.00289	-0.00003	0.00040	-0.00092	-0.00052	0.00237
D51	-3.13964	-0.00001	-0.00040	-0.00050	-0.00089	-3.14054
D52	-2.72097	-0.00028	-0.00004	-0.01498	-0.01520	-2.73617
D53	3.00946	0.00053	0.01816	0.03820	0.05609	3.06555
D54	-2.25810	-0.00031	0.00765	-0.00618	0.00143	-2.25667
D55	-0.56274	-0.00024	0.00998	-0.00354	0.00629	-0.55645
D56	-2.72311	0.00015	0.00375	0.00472	0.00842	-2.71469
D57	-0.03593	0.00071	0.00565	0.00741	0.01296	-0.02297

D58	0.00990	-0.00079	-0.00591	-0.01181	-0.01764	-0.00774
D59	2.69708	-0.00023	-0.00401	-0.00912	-0.01309	2.68399
D60	0.98402	0.00045	-0.00144	-0.01833	-0.01972	0.96430
D61	0.15517	0.00033	0.00647	0.01375	0.02034	0.17551
D62	-1.38352	-0.00043	-0.00971	-0.03225	-0.04206	-1.42557
D63	-2.21236	-0.00055	-0.00181	-0.00016	-0.00199	-2.21435
D64	1.92389	0.00082	0.00410	0.01254	0.01671	1.94060
D65	-0.46278	-0.00003	0.00090	0.00479	0.00579	-0.45699
D66	2.49404	-0.00010	0.00398	0.00828	0.01228	2.50633
D67	-1.69824	-0.00028	0.00235	0.00596	0.00829	-1.68995
D68	0.40323	-0.00027	0.00231	0.00605	0.00830	0.41153
D69	1.28469	0.00048	0.00525	0.01112	0.01643	1.30112
D70	-2.90760	0.00030	0.00363	0.00880	0.01244	-2.89516
D71	-0.80612	0.00031	0.00359	0.00889	0.01245	-0.79367
D72	-1.08986	0.00011	0.00414	0.00778	0.01197	-1.07789
D73	1.00104	-0.00007	0.00252	0.00546	0.00798	1.00902
D74	3.10251	-0.00006	0.00248	0.00555	0.00799	3.11050

Item	Value	Threshold	Converged?
Maximum Force	0.003881	0.000450	NO
RMS Force	0.000712	0.000300	NO
Maximum Displacement	0.270471	0.001800	NO
RMS Displacement	0.047912	0.001200	NO

Predicted change in Energy=-5.966857D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.521260	-1.889042	0.139845
2	6	0	-2.766008	-1.365570	-0.001489
3	7	0	-2.629535	0.016200	0.088007
4	6	0	-1.327057	0.309717	0.275107
5	7	0	-0.643524	-0.831971	0.317392
6	6	0	0.827224	-0.915789	0.446165
7	6	0	1.510833	-0.966691	-0.932709
8	1	0	-1.187995	-2.912596	0.133640
9	1	0	-3.713489	-1.849410	-0.152803
10	1	0	1.153533	-0.022417	0.980455
11	1	0	1.060886	-1.809036	1.026820
12	1	0	1.168517	-1.846521	-1.487603
13	1	0	1.248117	-0.064341	-1.494289
14	35	0	0.921623	2.674160	0.135680

15	1	0	-0.850555	1.304936	0.342644
16	6	0	-3.634763	1.017023	0.003358
17	6	0	-4.933089	0.778703	-0.129554
18	1	0	-3.220393	2.015886	0.055679
19	1	0	-5.617839	1.612989	-0.191603
20	1	0	-5.358308	-0.215532	-0.181957
21	8	0	2.906450	-1.091974	-0.767346
22	1	0	3.304312	-0.205182	-0.708058
23	6	0	5.709842	1.892483	-0.281318
24	6	0	6.265383	0.605338	-0.723433
25	8	0	4.873048	0.909392	-0.911377
26	1	0	5.505027	2.051573	0.774302
27	1	0	5.869118	2.792474	-0.868618
28	1	0	6.827637	0.600384	-1.656491
29	6	0	6.594982	-0.508229	0.235880
30	1	0	6.370452	-1.479166	-0.213911
31	1	0	7.659252	-0.487039	0.490445
32	1	0	6.014044	-0.415134	1.155894

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357717	0.000000			
3	N	2.204747	1.391374	0.000000		
4	C	2.211459	2.225684	1.348187	0.000000	
5	N	1.385405	2.211640	2.171693	1.331336	0.000000
6	C	2.560553	3.648837	3.598064	2.484362	1.478752
7	C	3.345847	4.395184	4.376138	3.337912	2.494425
8	H	1.076460	2.213973	3.264654	3.228413	2.158522
9	H	2.212031	1.074578	2.171047	3.246536	3.268173
10	H	3.368299	4.258060	3.887102	2.600222	2.079529
11	H	2.731411	3.987380	4.222802	3.279704	2.088769
12	H	3.144089	4.233242	4.514142	3.739572	2.751511
13	H	3.697212	4.476030	4.188834	3.146776	2.729422
14	Br	5.175955	5.471458	4.435961	3.265975	3.843911
15	H	3.269935	3.304390	2.211437	1.105476	2.147061
16	C	3.595934	2.536042	1.421020	2.428917	3.530568
17	C	4.339356	3.051319	2.436207	3.658848	4.603738
18	H	4.259413	3.412327	2.085402	2.558102	3.849550
19	H	5.399633	4.128063	3.399688	4.508564	5.566033
20	H	4.198467	2.841685	2.751868	4.090938	4.781060
21	O	4.589437	5.730459	5.710237	4.579740	3.721097
22	H	5.180780	6.220493	5.991100	4.762491	4.126720
23	C	8.171056	9.084781	8.555820	7.234135	6.938757

24	C	8.221862	9.272093	8.951262	7.663526	7.133174
25	O	7.058576	8.022377	7.621373	6.341030	5.913948
26	H	8.080823	8.982691	8.413373	7.068283	6.806487
27	H	8.806321	9.623235	8.991659	7.697865	7.547034
28	H	8.895401	9.931869	9.634451	8.385379	7.859141
29	C	8.233423	9.403165	9.240595	7.964250	7.246200
30	H	7.910264	9.139635	9.128365	7.917758	7.063781
31	H	9.293565	10.473770	10.308945	9.024131	8.311739
32	H	7.745036	8.906861	8.719971	7.429197	6.723098

		6	7	8	9	10
6	C	0.000000				
7	C	1.539872	0.000000			
8	H	2.854123	3.493898	0.000000		
9	H	4.674237	5.355463	2.755093	0.000000	
10	H	1.090897	2.163218	3.814837	5.320722	0.000000
11	H	1.090709	2.179851	2.659526	4.918109	1.789620
12	H	2.173063	1.095075	3.052555	5.061194	3.069021
13	H	2.160434	1.094818	4.086239	5.440918	2.476905
14	Br	3.604587	3.839846	5.971795	6.483068	2.835305
15	H	2.785190	3.516101	4.236169	4.288562	2.486974
16	C	4.882743	5.593613	4.630935	2.871763	4.996292
17	C	6.031912	6.724253	5.265044	2.897402	6.238660
18	H	5.013024	5.679540	5.331666	3.902194	4.913362
19	H	6.952720	7.617214	6.341153	3.951742	7.063976
20	H	6.256652	6.950752	4.976471	2.318584	6.617595
21	O	2.413882	1.410953	4.570658	6.691410	2.696567
22	H	2.823678	1.961360	5.312191	7.229200	2.740498
23	C	5.679400	5.121608	8.416718	10.139894	5.100869
24	C	5.766746	5.012068	8.286331	10.292197	5.424788
25	O	4.641433	3.850277	7.241264	9.050694	4.275756
26	H	5.549302	5.289366	8.357629	10.052773	4.824877
27	H	6.395355	5.755874	9.129907	10.671731	5.794776
28	H	6.536428	5.589990	8.932858	10.926020	6.287831
29	C	5.785962	5.236828	8.146543	10.402616	5.513598
30	H	5.610746	4.939150	7.701016	10.090921	5.546609
31	H	6.845611	6.329178	9.180655	11.472100	6.540670
32	H	5.259037	4.994537	7.691014	9.919413	4.879505

		11	12	13	14	15
11	H	0.000000				
12	H	2.517005	0.000000			
13	H	3.071645	1.783970	0.000000		
14	Br	4.573026	4.809632	3.203558	0.000000	
15	H	3.717327	4.166310	3.107034	2.249049	0.000000
16	C	5.575231	5.787431	5.220614	4.850183	2.819544

17	C	6.630334	6.779800	6.385963	6.159607	4.143306
18	H	5.822585	6.046689	5.166946	4.194762	2.490770
19	H	7.602643	7.726736	7.186917	6.633081	4.807007
20	H	6.723573	6.853049	6.737204	6.920169	4.786112
21	O	2.671949	2.026949	2.081957	4.351867	4.592639
22	H	3.258083	2.804159	2.205887	3.831411	4.543936
23	C	6.084838	6.004907	5.020702	4.869491	6.616143
24	C	5.998281	5.707331	5.120123	5.794296	7.229283
25	O	5.067449	4.653026	3.798430	4.452471	5.872704
26	H	5.892237	6.254332	5.267341	4.669373	6.413830
27	H	6.919948	6.633180	5.468685	5.049784	6.988128
28	H	6.801535	6.167780	5.621318	6.511023	7.965397
29	C	5.739678	5.848756	5.637330	6.505738	7.663875
30	H	5.462575	5.368182	5.466207	6.860180	7.759118
31	H	6.750838	6.920297	6.724619	7.450817	8.697691
32	H	5.147174	5.702288	5.464485	6.042956	7.123393

		16	17	18	19	20
16	C	0.000000				
17	C	1.326692	0.000000			
18	H	1.082667	2.120910	0.000000		
19	H	2.079850	1.081095	2.443608	0.000000	
20	H	2.127002	1.082617	3.099415	1.846873	0.000000
21	O	6.915874	8.084836	6.919130	8.961685	8.331689
22	H	7.081714	8.316098	6.934567	9.120157	8.678587
23	C	9.389841	10.702127	8.937444	11.331484	11.267543
24	C	9.935322	11.215549	9.621675	11.937721	11.665214
25	O	8.557522	9.838123	8.225772	10.539063	10.318825
26	H	9.230407	10.554214	8.755036	11.173338	11.138502
27	H	9.707540	11.013136	9.169331	11.567183	11.643655
28	H	10.601439	11.860776	10.290679	12.572236	12.301919
29	C	10.345441	11.605436	10.136332	12.403036	11.964171
30	H	10.314190	11.527148	10.211385	12.380672	11.796677
31	H	11.404133	12.670973	11.172303	13.459438	13.037741
32	H	9.822367	11.086810	9.612241	11.884012	11.452514

		21	22	23	24	25
21	O	0.000000				
22	H	0.973760	0.000000			
23	C	4.123374	3.220074	0.000000		
24	C	3.763673	3.070036	1.469978	0.000000	
25	O	2.809577	1.935083	1.436547	1.437487	0.000000
26	H	4.360180	3.483314	1.087010	2.216516	2.132015
27	H	4.886368	3.948411	1.086404	2.227480	2.130723
28	H	4.362380	3.736613	2.193191	1.089381	2.114497
29	C	3.866845	3.436766	2.610438	1.506303	2.508167

30	H	3.529238	3.356848	3.436418	2.148444	2.904115
31	H	4.953495	4.525633	3.171427	2.147012	3.417317
32	H	3.716734	3.295610	2.735546	2.153231	2.707370

		26	27	28	29	30
26	H	0.000000				
27	H	1.838663	0.000000			
28	H	3.124740	2.518880	0.000000		
29	C	2.833811	3.555479	2.205498	0.000000	
30	H	3.767179	4.350504	2.571883	1.093364	0.000000
31	H	3.341528	3.975782	2.546254	1.094497	1.772410
32	H	2.547421	3.795840	3.098825	1.092054	1.770751

		31	32
31	H	0.000000	
32	H	1.776148	0.000000

Stoichiometry C10H17BrN2O2
Framework group C1[X(C10H17BrN2O2)]
Deg. of freedom 90
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.647320	2.281297	-0.229861
2	6	0	-3.849362	1.694725	0.003423
3	7	0	-3.633569	0.320423	-0.022035
4	6	0	-2.326472	0.093473	-0.262034
5	7	0	-1.716675	1.269016	-0.398784
6	6	0	-0.261928	1.431170	-0.608841
7	6	0	0.484619	1.596721	0.727746
8	1	0	-2.377119	3.321333	-0.293767
9	1	0	-4.815917	2.130109	0.179293
10	1	0	0.091386	0.530563	-1.112957
11	1	0	-0.112091	2.303586	-1.246090
12	1	0	0.117190	2.484019	1.253947
13	1	0	0.305428	0.712501	1.347966
14	35	0	0.066189	-2.124979	-0.119772
15	1	0	-1.794157	-0.874522	-0.303325
16	6	0	-4.570557	-0.731125	0.166642
17	6	0	-5.872830	-0.561902	0.355217
18	1	0	-4.099208	-1.705539	0.143980
19	1	0	-6.501587	-1.430018	0.495952

20	1	0	-6.354707	0.407272	0.378769
21	8	0	1.860132	1.793843	0.483017
22	1	0	2.307854	0.929803	0.448518
23	6	0	4.812651	-1.044392	0.004197
24	6	0	5.309931	0.295052	0.349796
25	8	0	3.949694	-0.078854	0.626054
26	1	0	4.565988	-1.272330	-1.029628
27	1	0	5.055281	-1.900297	0.627759
28	1	0	5.916263	0.383481	1.250514
29	6	0	5.523276	1.372070	-0.681447
30	1	0	5.262528	2.351323	-0.270937
31	1	0	6.572977	1.399046	-0.990192
32	1	0	4.904331	1.195402	-1.563647

Rotational constants (GHZ): 0.6970476 0.1759359 0.1443321

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.

475 basis functions, 751 primitive gaussians, 492 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1269.7675591719 Hartrees.

NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 475 RedAO= T EigKep= 4.10D-06 NBF= 475

NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999976 0.004511 -0.000108 0.005259 Ang= 0.79 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3225.51530539 A.U. after 12 cycles
NFock= 12 Conv=0.63D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000466567	-0.000111005	0.000035186
2	6	0.000089292	-0.000134742	0.000186620
3	7	-0.000039740	-0.000214975	-0.000616212
4	6	-0.001408142	0.000289959	0.001396474
5	7	0.001008347	-0.000357947	-0.000168732
6	6	0.000579271	-0.000188485	-0.001134384
7	6	0.002161265	-0.000696258	0.000260190
8	1	-0.000078580	0.000028294	0.000055315
9	1	-0.000052666	0.000009054	-0.000028582
10	1	0.000011011	0.000149406	-0.000470648
11	1	-0.000047434	-0.000167546	0.000018133
12	1	-0.000830454	-0.000191705	-0.000293426
13	1	-0.000447672	0.000070556	0.000634681
14	35	-0.000857724	0.000553541	0.000578597
15	1	0.001697146	0.001113703	-0.000527417
16	6	0.000042185	-0.000029254	-0.000219103
17	6	-0.000001936	-0.000066559	-0.000013122
18	1	0.000046286	-0.000008258	0.000001729
19	1	-0.000011787	0.000011033	0.000043078
20	1	0.000067114	-0.000013040	0.000018524
21	8	-0.003338871	0.002182263	0.000990463
22	1	0.002830316	-0.002634327	-0.000536412
23	6	-0.001537034	0.000208264	0.000540030
24	6	0.001338062	-0.000324827	0.001141701
25	8	-0.000100569	0.000243978	-0.001098637
26	1	0.000060537	0.000064720	-0.000281043
27	1	0.000082075	-0.000229105	0.000072562
28	1	-0.000453469	0.000064543	-0.000129067
29	6	-0.000278024	0.000215540	-0.000369712
30	1	0.000064530	-0.000003635	-0.000005712
31	1	-0.000012216	0.000089580	-0.000046922

```
      32        1             -0.000114550       0.000077236      -0.000034151
 ---------------------------------------------------------------------
 Cartesian Forces:  Max         0.003338871 RMS         0.000792655

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 GSVD:  received Info=                 1 from GESDD.
 Internal  Forces:  Max         0.003004910 RMS         0.000479294
 Search for a local minimum.
 Step number   10 out of a maximum of   177
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swapping is turned off.
 Update second derivatives using D2CorX and points      8      9     10
 DE= -7.42D-04 DEPred=-5.97D-04 R= 1.24D+00
 TightC=F SS=  1.41D+00  RLast= 3.31D-01 DXNew= 4.0363D+00 9.9317D-01
 Trust test= 1.24D+00 RLast= 3.31D-01 DXMaxT set to 2.40D+00
 ITU=  1  1  1  1  1  0  1  0  1  0
      Eigenvalues ---      0.00122     0.00235     0.00241     0.00382     0.00522
      Eigenvalues ---      0.00935     0.01245     0.01291     0.01400     0.01551
      Eigenvalues ---      0.01659     0.01855     0.01974     0.02068     0.02126
      Eigenvalues ---      0.02168     0.02260     0.02316     0.02391     0.03059
      Eigenvalues ---      0.03062     0.03150     0.03336     0.03719     0.03922
      Eigenvalues ---      0.04607     0.05124     0.05304     0.05486     0.05562
      Eigenvalues ---      0.05864     0.06390     0.09184     0.09842     0.10258
      Eigenvalues ---      0.10985     0.11360     0.11751     0.12713     0.13127
      Eigenvalues ---      0.14049     0.14809     0.15353     0.15998     0.16000
      Eigenvalues ---      0.16000     0.16000     0.16001     0.16038     0.16069
      Eigenvalues ---      0.16715     0.18687     0.19163     0.21862     0.22019
      Eigenvalues ---      0.22753     0.23554     0.23758     0.25025     0.26699
      Eigenvalues ---      0.28027     0.28903     0.31917     0.32986     0.33055
      Eigenvalues ---      0.33289     0.34098     0.34287     0.34480     0.34761
      Eigenvalues ---      0.34937     0.35685     0.35690     0.35858     0.36433
      Eigenvalues ---      0.36655     0.37023     0.37231     0.37582     0.37853
      Eigenvalues ---      0.39034     0.42191     0.42657     0.45069     0.46030
      Eigenvalues ---      0.49235     0.51956     0.54610     0.56278     0.60357
 En-DIIS/RFO-DIIS IScMMF=              0 using points:      10       9
 RFO step:  Lambda=-1.20489337D-04.
 DidBck=F Rises=F RFO-DIIS coefs:       1.53640     -0.53640
 Iteration  1 RMS(Cart)=  0.07674415 RMS(Int)=  0.02348056
 Iteration  2 RMS(Cart)=  0.02488012 RMS(Int)=  0.00752897
 Iteration  3 RMS(Cart)=  0.01191198 RMS(Int)=  0.00029862
```

Iteration 4 RMS(Cart)= 0.00004009 RMS(Int)= 0.00029815

Iteration 5 RMS(Cart)= 0.00000001 RMS(Int)= 0.00029815

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56571	-0.00023	-0.00008	-0.00088	-0.00107	2.56464
R2	2.61804	0.00040	0.00014	0.00118	0.00134	2.61938
R3	2.03422	-0.00005	0.00006	-0.00014	-0.00008	2.03413
R4	2.62932	-0.00002	0.00089	-0.00039	0.00040	2.62972
R5	2.03066	0.00005	-0.00001	0.00020	0.00018	2.03084
R6	2.54770	0.00020	-0.00080	0.00043	-0.00031	2.54739
R7	2.68534	-0.00018	0.00033	-0.00033	0.00000	2.68534
R8	2.51586	0.00107	-0.00147	0.00188	0.00065	2.51651
R9	2.08905	0.00106	-0.00144	0.00277	0.00160	2.09064
R10	2.79444	0.00006	-0.00200	0.00039	-0.00175	2.79268
R11	2.90994	-0.00122	0.00174	-0.00547	-0.00371	2.90623
R12	2.06150	-0.00010	-0.00077	0.00023	-0.00054	2.06096
R13	2.06114	0.00014	0.00050	0.00049	0.00099	2.06213
R14	2.06939	0.00056	-0.00003	0.00182	0.00179	2.07118
R15	2.06891	-0.00016	0.00026	-0.00025	0.00002	2.06892
R16	2.66631	-0.00134	-0.00429	-0.00152	-0.00592	2.66039
R17	4.25009	-0.00096	-0.03133	-0.02094	-0.05203	4.19805
R18	8.41395	0.00029	0.13631	0.37466	0.51098	8.92493
R19	2.50708	-0.00004	-0.00008	-0.00009	-0.00016	2.50692
R20	2.04594	0.00001	-0.00005	0.00002	-0.00002	2.04592
R21	2.04297	0.00001	0.00001	0.00005	0.00006	2.04303
R22	2.04585	-0.00001	0.00002	-0.00003	-0.00001	2.04584
R23	1.84014	-0.00047	0.00144	-0.00016	0.00102	1.84116
R24	3.65678	0.00004	-0.04779	-0.14421	-0.19224	3.46454
R25	2.77786	0.00041	0.00264	0.00005	0.00283	2.78069
R26	2.71468	-0.00055	-0.00253	0.00157	-0.00101	2.71367
R27	2.05415	-0.00028	0.00261	-0.00045	0.00216	2.05631
R28	2.05301	-0.00021	0.00235	-0.00040	0.00195	2.05496
R29	2.71646	0.00007	0.00377	0.00176	0.00545	2.72191
R30	2.05863	-0.00012	-0.00077	-0.00067	-0.00144	2.05719
R31	2.84650	-0.00066	-0.00665	-0.00239	-0.00904	2.83746
R32	2.06616	-0.00001	0.00142	0.00017	0.00159	2.06775
R33	2.06830	-0.00002	0.00112	-0.00005	0.00107	2.06937
R34	2.06368	0.00004	0.00085	0.00021	0.00106	2.06474
A1	1.87549	0.00018	-0.00085	0.00116	0.00029	1.87578
A2	2.27817	-0.00014	-0.00019	-0.00108	-0.00131	2.27686
A3	2.12951	-0.00003	0.00111	-0.00016	0.00092	2.13043
A4	1.86113	0.00011	0.00023	-0.00068	-0.00058	1.86055
A5	2.27762	-0.00002	-0.00052	0.00044	-0.00007	2.27755
A6	2.14444	-0.00008	0.00030	0.00028	0.00059	2.14502

A7	1.89642	0.00025	-0.00036	0.00132	0.00103	1.89744
A8	2.24749	-0.00028	0.00110	-0.00098	0.00007	2.24756
A9	2.13927	0.00003	-0.00074	-0.00031	-0.00110	2.13817
A10	1.88991	-0.00030	0.00022	-0.00078	-0.00076	1.88914
A11	2.24069	0.00027	0.00160	-0.00482	-0.00385	2.23684
A12	2.15170	0.00002	-0.00175	0.00532	0.00437	2.15606
A13	1.90177	-0.00023	0.00090	-0.00108	-0.00025	1.90152
A14	2.21185	-0.00021	-0.00275	-0.00413	-0.00725	2.20461
A15	2.16761	0.00044	0.00185	0.00438	0.00658	2.17419
A16	1.94489	0.00006	-0.00828	-0.00101	-0.00904	1.93585
A17	1.86893	0.00005	0.00230	0.00053	0.00290	1.87182
A18	1.88163	-0.00003	-0.00053	0.00129	0.00041	1.88203
A19	1.91011	-0.00023	0.01090	0.00165	0.01235	1.92246
A20	1.93321	-0.00003	-0.00327	-0.00489	-0.00815	1.92506
A21	1.92395	0.00019	-0.00106	0.00265	0.00165	1.92560
A22	1.91933	-0.00025	-0.00875	-0.00179	-0.01004	1.90929
A23	1.90238	-0.00049	0.00567	-0.00618	-0.00084	1.90154
A24	1.91463	-0.00054	0.00658	-0.00351	0.00249	1.91712
A25	1.90421	0.00009	-0.00188	-0.00090	-0.00283	1.90137
A26	1.87260	0.00071	-0.00590	0.00910	0.00330	1.87590
A27	1.95051	0.00049	0.00397	0.00343	0.00753	1.95804
A28	2.07103	-0.00114	-0.02216	-0.07683	-0.09837	1.97267
A29	2.65111	0.00076	0.00395	0.01430	0.01908	2.67019
A30	2.17940	-0.00022	0.00014	-0.00098	-0.00084	2.17856
A31	1.95645	0.00006	-0.00030	0.00001	-0.00029	1.95615
A32	2.14733	0.00015	0.00016	0.00098	0.00114	2.14847
A33	2.07941	0.00005	-0.00001	0.00027	0.00027	2.07968
A34	2.15819	-0.00010	0.00006	-0.00052	-0.00046	2.15773
A35	2.04559	0.00005	-0.00006	0.00025	0.00019	2.04578
A36	1.90754	0.00108	0.00641	0.00968	0.01541	1.92295
A37	2.58560	0.00300	0.01487	0.02892	0.04510	2.63069
A38	2.08454	0.00001	-0.00386	-0.00114	-0.00506	2.07948
A39	2.10294	-0.00003	-0.00417	-0.00052	-0.00473	2.09821
A40	2.00020	0.00016	0.00319	0.00033	0.00367	2.00387
A41	1.99898	-0.00014	0.00371	-0.00139	0.00218	2.00116
A42	2.01680	-0.00001	0.00266	0.00157	0.00404	2.02084
A43	2.04501	-0.00005	-0.00559	0.00088	-0.00432	2.04069
A44	2.13942	0.00003	0.00079	0.00067	0.00104	2.14046
A45	1.97022	-0.00021	-0.00312	-0.00496	-0.00812	1.96210
A46	2.03933	0.00019	0.00092	-0.00172	-0.00072	2.03860
A47	2.01438	0.00013	0.00527	0.00175	0.00700	2.02138
A48	1.02878	0.00199	0.00235	0.01050	0.01233	1.04111
A49	1.71385	-0.00212	-0.01637	-0.04669	-0.06213	1.65173
A50	2.53275	-0.00021	-0.00323	-0.01141	-0.01538	2.51737

A51	2.27792	-0.00040	0.00270	0.00861	0.01156	2.28948
A52	1.92790	0.00008	0.00721	0.00163	0.00878	1.93668
A53	1.92472	-0.00013	-0.00021	-0.00205	-0.00225	1.92248
A54	1.93597	-0.00017	0.00684	0.00115	0.00794	1.94391
A55	1.88868	0.00003	-0.00531	-0.00054	-0.00583	1.88285
A56	1.88918	0.00006	-0.00551	-0.00029	-0.00591	1.88327
A57	1.89619	0.00013	-0.00344	0.00006	-0.00337	1.89281
A58	3.30670	0.00159	0.00505	0.01911	0.02389	3.33058
A59	3.62200	0.00081	0.02671	0.07246	0.09916	3.72116
D1	0.00341	-0.00004	-0.00962	0.03065	0.02106	0.02447
D2	-3.13621	-0.00014	-0.00403	0.01059	0.00658	-3.12962
D3	3.13992	0.00011	-0.00294	0.01301	0.01005	-3.13321
D4	0.00031	0.00002	0.00265	-0.00704	-0.00442	-0.00411
D5	-0.00890	0.00027	0.00819	-0.02272	-0.01459	-0.02349
D6	-3.08528	0.00026	0.00825	-0.00919	-0.00105	-3.08633
D7	3.13724	0.00013	0.00221	-0.00691	-0.00470	3.13255
D8	0.06086	0.00013	0.00228	0.00663	0.00884	0.06970
D9	0.00313	-0.00019	0.00782	-0.02827	-0.02046	-0.01732
D10	3.14138	-0.00009	0.00452	-0.01874	-0.01427	3.12711
D11	-3.14025	-0.00010	0.00276	-0.01011	-0.00735	3.13559
D12	-0.00200	0.00000	-0.00055	-0.00059	-0.00116	-0.00316
D13	-0.00872	0.00036	-0.00281	0.01442	0.01159	0.00288
D14	3.08805	0.00014	-0.00135	0.00749	0.00596	3.09400
D15	3.13597	0.00027	0.00025	0.00561	0.00587	-3.14134
D16	-0.05045	0.00004	0.00171	-0.00132	0.00024	-0.05021
D17	0.05012	-0.00001	0.00320	-0.00104	0.00219	0.05232
D18	-3.08719	-0.00005	0.00408	-0.00231	0.00180	-3.08539
D19	-3.09523	0.00011	-0.00051	0.00968	0.00914	-3.08609
D20	0.05064	0.00007	0.00037	0.00841	0.00875	0.05939
D21	0.01087	-0.00039	-0.00325	0.00491	0.00170	0.01257
D22	3.08928	-0.00042	-0.00352	-0.00859	-0.01218	3.07710
D23	-3.08868	-0.00019	-0.00472	0.01171	0.00726	-3.08142
D24	-0.01027	-0.00022	-0.00500	-0.00179	-0.00662	-0.01689
D25	-2.69680	-0.00012	0.01400	0.03148	0.04549	-2.65130
D26	0.39387	-0.00038	0.01573	0.02341	0.03891	0.43278
D27	1.46705	-0.00007	-0.02338	-0.04285	-0.06594	1.40111
D28	-2.72784	-0.00028	-0.01338	-0.04108	-0.05432	-2.78216
D29	-0.65782	-0.00005	-0.01368	-0.03701	-0.05061	-0.70843
D30	-1.59997	-0.00004	-0.02323	-0.02711	-0.05004	-1.65000
D31	0.48833	-0.00026	-0.01323	-0.02534	-0.03841	0.44992
D32	2.55835	-0.00003	-0.01353	-0.02127	-0.03471	2.52364
D33	-1.05134	0.00023	0.00485	0.06746	0.07228	-0.97906
D34	1.03542	-0.00011	0.00079	0.06151	0.06236	1.09778
D35	-3.10694	-0.00016	0.01328	0.05954	0.07276	-3.03418

D36	-3.11506	0.00028	0.00005	0.06637	0.06645	-3.04862
D37	-1.02830	-0.00006	-0.00401	0.06041	0.05652	-0.97178
D38	1.11252	-0.00011	0.00848	0.05844	0.06693	1.17945
D39	1.04334	0.00022	-0.00373	0.06513	0.06152	1.10487
D40	3.13010	-0.00012	-0.00778	0.05917	0.05159	-3.10149
D41	-1.01225	-0.00017	0.00470	0.05720	0.06200	-0.95025
D42	-1.55434	-0.00019	-0.01382	-0.01777	-0.03078	-1.58512
D43	2.64435	0.00000	-0.00356	-0.01901	-0.02205	2.62230
D44	0.55769	-0.00085	0.00015	-0.02569	-0.02513	0.53256
D45	-0.08775	0.00005	0.00924	-0.04971	-0.04145	-0.12920
D46	-0.00485	0.00047	-0.02012	0.04306	0.02273	0.01789
D47	-2.65299	0.00027	-0.02960	0.02102	-0.01030	-2.66329
D48	-3.13449	-0.00006	0.00069	-0.00132	-0.00063	-3.13512
D49	0.00579	-0.00001	0.00049	-0.00023	0.00026	0.00605
D50	0.00237	-0.00002	-0.00028	0.00008	-0.00020	0.00217
D51	-3.14054	0.00003	-0.00048	0.00117	0.00069	-3.13985
D52	-2.73617	0.00002	-0.00815	-0.03720	-0.04557	-2.78174
D53	3.06555	0.00025	0.03009	0.03020	0.06029	3.12584
D54	-2.25667	-0.00028	0.00077	-0.04226	-0.04085	-2.29752
D55	-0.55645	-0.00055	0.00338	-0.04225	-0.03888	-0.59532
D56	-2.71469	-0.00015	0.00452	-0.00528	-0.00085	-2.71554
D57	-0.02297	0.00015	0.00695	0.00349	0.01029	-0.01268
D58	-0.00774	-0.00023	-0.00946	-0.00512	-0.01455	-0.02229
D59	2.68399	0.00007	-0.00702	0.00365	-0.00341	2.68057
D60	0.96430	0.00020	-0.01058	-0.03834	-0.04902	0.91528
D61	0.17551	-0.00033	0.01091	0.01303	0.02421	0.19972
D62	-1.42557	0.00019	-0.02256	-0.03962	-0.06239	-1.48796
D63	-2.21435	-0.00034	-0.00107	0.01176	0.01083	-2.20352
D64	1.94060	0.00019	0.00896	0.01063	0.02001	1.96061
D65	-0.45699	0.00001	0.00311	0.01578	0.01929	-0.43770
D66	2.50633	-0.00015	0.00659	0.00863	0.01517	2.52150
D67	-1.68995	-0.00014	0.00445	0.00769	0.01206	-1.67789
D68	0.41153	-0.00017	0.00445	0.00717	0.01152	0.42305
D69	1.30112	0.00015	0.00881	0.00891	0.01781	1.31892
D70	-2.89516	0.00016	0.00667	0.00797	0.01469	-2.88046
D71	-0.79367	0.00013	0.00668	0.00745	0.01415	-0.77952
D72	-1.07789	0.00010	0.00642	0.01705	0.02353	-1.05436
D73	1.00902	0.00011	0.00428	0.01612	0.02042	1.02944
D74	3.11050	0.00008	0.00429	0.01559	0.01988	3.13038

Item	Value	Threshold	Converged?
Maximum Force	0.003005	0.000450	NO
RMS Force	0.000479	0.000300	NO
Maximum Displacement	0.284650	0.001800	NO
RMS Displacement	0.090048	0.001200	NO

Predicted change in Energy=-4.265237D-04
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.445086	-1.852503	0.090688
2	6	0	-2.708698	-1.369684	-0.018979
3	7	0	-2.617821	0.013533	0.103350
4	6	0	-1.327025	0.346108	0.304364
5	7	0	-0.604338	-0.772405	0.309429
6	6	0	0.868285	-0.818799	0.424293
7	6	0	1.525582	-0.882755	-0.964606
8	1	0	-1.077171	-2.863080	0.045466
9	1	0	-3.639805	-1.881538	-0.180131
10	1	0	1.180587	0.086364	0.946390
11	1	0	1.130254	-1.702708	1.008129
12	1	0	1.131136	-1.744846	-1.514586
13	1	0	1.282517	0.031663	-1.515429
14	35	0	0.770993	2.821706	0.214355
15	1	0	-0.888903	1.357261	0.402166
16	6	0	-3.655630	0.982367	0.043267
17	6	0	-4.945490	0.703386	-0.092056
18	1	0	-3.273889	1.992776	0.117335
19	1	0	-5.658429	1.515071	-0.133500
20	1	0	-5.336685	-0.303415	-0.165325
21	8	0	2.914481	-1.067777	-0.827932
22	1	0	3.366620	-0.205424	-0.793623
23	6	0	5.685567	1.824280	-0.348010
24	6	0	6.261636	0.518856	-0.707530
25	8	0	4.878018	0.816227	-0.975559
26	1	0	5.437712	2.025793	0.692200
27	1	0	5.881690	2.697761	-0.965330
28	1	0	6.860891	0.477726	-1.615436
29	6	0	6.539699	-0.551127	0.308532
30	1	0	6.354090	-1.545317	-0.109104
31	1	0	7.587645	-0.509059	0.623494
32	1	0	5.908033	-0.434829	1.192432

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				

2	C	1.357150	0.000000			
3	N	2.203987	1.391587	0.000000		
4	C	2.212123	2.226547	1.348023	0.000000	
5	N	1.386116	2.211996	2.171239	1.331681	0.000000
6	C	2.555685	3.646200	3.598432	2.488128	1.477824
7	C	3.298322	4.365826	4.371687	3.355258	2.484332
8	H	1.076417	2.212750	3.263718	3.229295	2.159669
9	H	2.211555	1.074674	2.171660	3.247474	3.268624
10	H	3.374254	4.263631	3.891519	2.601497	2.080664
11	H	2.737977	3.987908	4.220447	3.275844	2.088649
12	H	3.037336	4.137862	4.445705	3.704487	2.698989
13	H	3.683682	4.486973	4.222962	3.196909	2.745333
14	Br	5.174411	5.452563	4.402523	3.246285	3.849442
15	H	3.272452	3.305336	2.209989	1.106321	2.150594
16	C	3.595168	2.536276	1.421019	2.428043	3.529936
17	C	4.338063	3.050606	2.435595	3.657606	4.602689
18	H	4.258098	3.412354	2.085192	2.556712	3.848328
19	H	5.398433	4.127450	3.399414	4.507689	5.565301
20	H	4.196398	2.839835	2.750430	4.088992	4.779169
21	O	4.523879	5.689085	5.713395	4.612108	3.709841
22	H	5.162111	6.234185	6.055248	4.851811	4.160132
23	C	8.034763	8.987400	8.510510	7.196321	6.836513
24	C	8.102719	9.192800	8.930712	7.657777	7.059969
25	O	6.945549	7.953082	7.615508	6.353092	5.850742
26	H	7.923125	8.854323	8.323914	6.980933	6.669542
27	H	8.689174	9.551673	8.977129	7.688171	7.465630
28	H	8.793753	9.876165	9.644464	8.411001	7.810095
29	C	8.093073	9.290325	9.177206	7.917727	7.147463
30	H	7.807780	9.064937	9.108805	7.921362	7.013721
31	H	9.147620	10.352203	10.232066	8.961278	8.202229
32	H	7.569149	8.751544	8.606818	7.331071	6.580626

		6	7	8	9	10
6	C	0.000000				
7	C	1.537910	0.000000			
8	H	2.847349	3.422902	0.000000		
9	H	4.670933	5.319229	2.753437	0.000000	
10	H	1.090614	2.170281	3.822088	5.327088	0.000000
11	H	1.091232	2.172623	2.673184	4.919086	1.790844
12	H	2.164695	1.096024	2.925889	4.955939	3.067928
13	H	2.158099	1.094827	4.047722	5.447257	2.464535
14	Br	3.647850	3.960098	5.980052	6.459973	2.861073
15	H	2.797041	3.565877	4.239571	4.289097	2.488805
16	C	4.884177	5.598164	4.629894	2.872648	5.000744
17	C	6.031885	6.719521	5.263315	2.897309	6.244029

18	H	5.015654	5.698614	5.330110	3.902908	4.915699
19	H	6.953854	7.619077	6.339414	3.951452	7.069619
20	H	6.254193	6.932907	4.973910	2.317346	6.622890
21	O	2.411841	1.407818	4.463095	6.636303	2.736175
22	H	2.846265	1.969120	5.245425	7.230195	2.809186
23	C	5.548741	5.001370	8.237767	10.036127	4.999067
24	C	5.670853	4.945786	8.115576	10.201891	5.360929
25	O	4.550918	3.758389	7.074184	8.970170	4.230554
26	H	5.389169	5.148729	8.170866	9.921165	4.684988
27	H	6.279449	5.638774	8.964955	10.594593	5.707403
28	H	6.461641	5.544367	8.771113	10.857756	6.243555
29	C	5.678907	5.183843	7.964361	10.277699	5.434459
30	H	5.559352	4.948268	7.548777	9.999801	5.526444
31	H	6.729444	6.277763	8.997475	11.339539	6.442762
32	H	5.112390	4.905031	7.483650	9.753877	4.762450

		11	12	13	14	15
11	H	0.000000				
12	H	2.523067	0.000000			
13	H	3.065872	1.782948	0.000000		
14	Br	4.607544	4.896155	3.322370	0.000000	
15	H	3.715857	4.168641	3.185819	2.221514	0.000000
16	C	5.571828	5.725182	5.264851	4.796606	2.814983
17	C	6.626791	6.703940	6.423805	6.104043	4.138563
18	H	5.817782	6.003102	5.222328	4.130086	2.484586
19	H	7.598924	7.657196	7.230972	6.570066	4.802106
20	H	6.719845	6.762465	6.763793	6.871264	4.781491
21	O	2.637750	2.027371	2.084401	4.561686	4.675434
22	H	3.238750	2.808380	2.218265	4.113005	4.688430
23	C	5.918584	5.902746	4.895222	5.046202	6.633591
24	C	5.848923	5.665485	5.067710	6.024960	7.284542
25	O	4.932118	4.570424	3.719493	4.722869	5.953841
26	H	5.705762	6.134674	5.110364	4.758159	6.368446
27	H	6.770141	6.527343	5.344444	5.246546	7.036187
28	H	6.669152	6.146552	5.597074	6.777111	8.056278
29	C	5.574735	5.831062	5.595037	6.683026	7.670388
30	H	5.344290	5.412434	5.494130	7.095525	7.819674
31	H	6.578042	6.912674	6.679971	7.597903	8.682396
32	H	4.946581	5.644718	5.380105	6.160425	7.073504

		16	17	18	19	20
16	C	0.000000				
17	C	1.326605	0.000000			
18	H	1.082654	2.121467	0.000000		
19	H	2.079958	1.081126	2.444822	0.000000	
20	H	2.126662	1.082612	3.099600	1.847004	0.000000

21	O	6.937466	8.090592	6.968245	8.980430	8.312944
22	H	7.170998	8.391025	7.053955	9.211264	8.726505
23	C	9.387219	10.693049	8.973115	11.350237	11.227222
24	C	9.956440	11.225530	9.683960	11.975387	11.640067
25	O	8.595857	9.863804	8.308566	10.593119	10.307776
26	H	9.175985	10.496413	8.730610	11.138535	11.056590
27	H	9.742706	11.043911	9.246286	11.630351	11.640404
28	H	10.658479	11.906395	10.392865	12.649332	12.308285
29	C	10.313423	11.560443	10.139749	12.379778	11.888415
30	H	10.325061	11.521174	10.259988	12.396257	11.756687
31	H	11.356594	12.611958	11.157432	13.421200	12.950013
32	H	9.736153	10.988376	9.558075	11.804375	11.327156

		21	22	23	24	25
21	O	0.000000				
22	H	0.974300	0.000000			
23	C	4.034011	3.113806	0.000000		
24	C	3.706123	2.985483	1.471476	0.000000	
25	O	2.725206	1.833356	1.436010	1.440370	0.000000
26	H	4.271730	3.387539	1.088153	2.215617	2.134884
27	H	4.796091	3.844937	1.087436	2.226758	2.132518
28	H	4.310789	3.654039	2.191110	1.088619	2.110879
29	C	3.834147	3.376786	2.608284	1.501520	2.505939
30	H	3.546219	3.344975	3.443571	2.151156	2.916577
31	H	4.925166	4.462898	3.163256	2.141619	3.414005
32	H	3.666586	3.233546	2.743360	2.155088	2.706706

		26	27	28	29	30
26	H	0.000000				
27	H	1.842842	0.000000			
28	H	3.122040	2.511977	0.000000		
29	C	2.828798	3.551193	2.205301	0.000000	
30	H	3.772886	4.354308	2.572662	1.094205	0.000000
31	H	3.324517	3.964636	2.552395	1.095062	1.769799
32	H	2.554622	3.803913	3.102389	1.092614	1.768091

		31	32
31	H	0.000000	
32	H	1.774907	0.000000

Stoichiometry C10H17BrN2O2
Framework group C1[X(C10H17BrN2O2)]
Deg. of freedom 90
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.496239	2.327293	-0.223265
2	6	0	-3.730211	1.805887	-0.005770
3	7	0	-3.586530	0.421908	-0.027487
4	6	0	-2.295214	0.124941	-0.275436
5	7	0	-1.622667	1.266815	-0.406504
6	6	0	-0.161663	1.361168	-0.607819
7	6	0	0.565626	1.559162	0.732709
8	1	0	-2.170288	3.351818	-0.275960
9	1	0	-4.672540	2.292279	0.168480
10	1	0	0.160949	0.430694	-1.076411
11	1	0	0.030395	2.206131	-1.271099
12	1	0	0.164409	2.445727	1.236988
13	1	0	0.391975	0.681955	1.364374
14	35	0	-0.090734	-2.252735	-0.116411
15	1	0	-1.819818	-0.873004	-0.320713
16	6	0	-4.576957	-0.578776	0.164821
17	6	0	-5.868546	-0.340307	0.351399
18	1	0	-4.156571	-1.576309	0.146310
19	1	0	-6.542635	-1.173300	0.494791
20	1	0	-6.298252	0.653202	0.369924
21	8	0	1.935968	1.786658	0.503882
22	1	0	2.422337	0.942459	0.509700
23	6	0	4.799372	-1.024410	0.089084
24	6	0	5.337101	0.326527	0.315050
25	8	0	3.983892	-0.002395	0.682887
26	1	0	4.505134	-1.316240	-0.917065
27	1	0	5.065667	-1.838589	0.758948
28	1	0	5.981738	0.461857	1.181780
29	6	0	5.514082	1.323622	-0.793572
30	1	0	5.308441	2.339517	-0.442922
31	1	0	6.544516	1.297704	-1.163292
32	1	0	4.841632	1.114033	-1.628850

Rotational constants (GHZ): 0.6572132 0.1770569 0.1436000
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 492 symmetry adapted cartesian basis functions of A symmetry.
There are 475 symmetry adapted basis functions of A symmetry.
475 basis functions, 751 primitive gaussians, 492 cartesian basis functions
71 alpha electrons 71 beta electrons
nuclear repulsion energy 1265.8619368898 Hartrees.
NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F

Big=F
 Integral buffers will be 131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis= 475 RedAO= T EigKep= 3.93D-06 NBF= 475
 NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475
 Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"
 B after Tr= 0.000000 0.000000 0.000000
 Rot= 0.999917 0.006770 -0.000556 0.010986 Ang= 1.48 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
 Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
 HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
 FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
 NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
 wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
 NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on energy=1.00D-06.
 No special actions if energy rises.
 EnCoef did 1 forward-backward iterations
 SCF Done: E(RB3LYP) = -3225.51571374 A.U. after 12 cycles
 NFock= 12 Conv=0.82D-08 -V/T= 2.0018
 Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****

 Center Atomic Forces (Hartrees/Bohr)
 Number Number X Y Z

1	6	-0.000597172	-0.000331017	0.002020748
2	6	0.000217530	0.000254604	-0.002012265
3	7	-0.000562885	-0.000310611	0.001124505
4	6	-0.001490994	-0.000541769	0.000957977
5	7	0.000353580	-0.000349468	-0.000862505
6	6	-0.000150689	-0.000764839	-0.000819396
7	6	0.001339102	-0.000736474	0.000196634
8	1	0.000005470	0.000002483	0.000344524

9	1	0.000043420	0.000085516	-0.000314549
10	1	-0.000012700	0.000439855	-0.000464120
11	1	-0.000129266	0.000193677	0.000177034
12	1	-0.000355114	0.000239035	-0.000593539
13	1	-0.000142439	0.000186543	0.000222345
14	35	-0.000027125	0.000660229	0.000457688
15	1	0.001942812	0.001200459	-0.000621442
16	6	0.000100455	-0.000142400	0.000141837
17	6	-0.000192808	-0.000023373	-0.000032742
18	1	0.000033226	0.000047522	-0.000024446
19	1	0.000006625	-0.000006307	-0.000007342
20	1	0.000069543	-0.000002489	0.000026225
21	8	-0.002664516	0.000676967	0.000821016
22	1	0.001748763	-0.002963945	-0.000303005
23	6	0.000284194	0.000081741	0.001265295
24	6	-0.000816170	0.001534325	-0.000185839
25	8	0.000831627	0.002084094	-0.001476822
26	1	-0.000236488	0.000181458	-0.001282069
27	1	-0.000549527	-0.000691628	0.000638673
28	1	0.000121616	-0.000297025	-0.000049038
29	6	0.001172972	-0.002460051	0.001805629
30	1	-0.000052584	0.000768289	-0.000528104
31	1	-0.000197331	0.000177249	-0.000087016
32	1	-0.000093127	0.000807351	-0.000535893

Cartesian Forces: Max 0.002963945 RMS 0.000877460

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.003249004 RMS 0.000579364
Search for a local minimum.
Step number 11 out of a maximum of 177
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 10 11
DE= -4.08D-04 DEPred=-4.27D-04 R= 9.57D-01
TightC=F SS= 1.41D+00 RLast= 6.41D-01 DXNew= 4.0363D+00 1.9228D+00
Trust test= 9.57D-01 RLast= 6.41D-01 DXMaxT set to 2.40D+00
ITU= 1 1 1 1 1 1 0 1 0 1 0
Eigenvalues --- 0.00137 0.00229 0.00242 0.00384 0.00479

Eigenvalues --- 0.00937 0.01230 0.01289 0.01398 0.01533
Eigenvalues --- 0.01742 0.01876 0.02007 0.02033 0.02152
Eigenvalues --- 0.02163 0.02314 0.02389 0.02471 0.03060
Eigenvalues --- 0.03064 0.03103 0.03212 0.03718 0.04202
Eigenvalues --- 0.04679 0.05128 0.05315 0.05419 0.05540
Eigenvalues --- 0.05882 0.06400 0.09056 0.09403 0.10158
Eigenvalues --- 0.10966 0.11501 0.11642 0.12029 0.12928
Eigenvalues --- 0.13972 0.14843 0.15496 0.15997 0.15999
Eigenvalues --- 0.16000 0.16000 0.16000 0.16029 0.16064
Eigenvalues --- 0.16838 0.18140 0.19224 0.21847 0.22015
Eigenvalues --- 0.22834 0.23548 0.23821 0.25021 0.26677
Eigenvalues --- 0.27909 0.29192 0.31901 0.32943 0.33054
Eigenvalues --- 0.33267 0.34094 0.34283 0.34484 0.34763
Eigenvalues --- 0.34942 0.35685 0.35690 0.35858 0.36435
Eigenvalues --- 0.36658 0.37017 0.37232 0.37662 0.37828
Eigenvalues --- 0.39097 0.42186 0.42569 0.45135 0.46087
Eigenvalues --- 0.49156 0.52331 0.54687 0.56191 0.60362
En-DIIS/RFO-DIIS IScMMF= 0 using points: 11 10 9
RFO step: Lambda=-1.52119081D-04.
DidBck=T Rises=F RFO-DIIS coefs: 0.77806 0.57184 -0.34989
Iteration 1 RMS(Cart)= 0.02979529 RMS(Int)= 0.00033019
Iteration 2 RMS(Cart)= 0.00062049 RMS(Int)= 0.00017120
Iteration 3 RMS(Cart)= 0.00000014 RMS(Int)= 0.00017120

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56464	0.00003	0.00019	-0.00077	-0.00057	2.56407
R2	2.61938	0.00022	-0.00021	0.00089	0.00066	2.62004
R3	2.03413	-0.00001	0.00006	-0.00009	-0.00003	2.03410
R4	2.62972	-0.00007	0.00049	-0.00023	0.00028	2.63000
R5	2.03084	-0.00003	-0.00005	0.00005	0.00000	2.03084
R6	2.54739	0.00046	-0.00045	0.00083	0.00038	2.54778
R7	2.68534	-0.00012	0.00022	-0.00028	-0.00007	2.68527
R8	2.51651	0.00060	-0.00110	0.00207	0.00097	2.51748
R9	2.09064	0.00174	-0.00129	0.00628	0.00502	2.09566
R10	2.79268	0.00044	-0.00092	-0.00024	-0.00116	2.79152
R11	2.90623	0.00025	0.00196	-0.00190	0.00026	2.90649
R12	2.06096	0.00014	-0.00038	0.00015	-0.00023	2.06073
R13	2.06213	-0.00009	0.00010	0.00030	0.00041	2.06254
R14	2.07118	0.00024	-0.00042	0.00138	0.00096	2.07215
R15	2.06892	0.00008	0.00017	0.00006	0.00022	2.06915
R16	2.66039	-0.00007	-0.00148	-0.00431	-0.00580	2.65459
R17	4.19805	-0.00030	-0.00889	-0.02914	-0.03804	4.16001
R18	8.92493	-0.00008	-0.02449	0.11823	0.09366	9.01859
R19	2.50692	0.00013	-0.00001	0.00009	0.00007	2.50699

R20	2.04592	0.00005	-0.00003	0.00007	0.00004	2.04596
R21	2.04303	-0.00001	-0.00001	0.00001	0.00000	2.04304
R22	2.04584	-0.00002	0.00002	-0.00010	-0.00008	2.04576
R23	1.84116	0.00105	0.00071	0.00113	0.00183	1.84299
R24	3.46454	0.00231	0.01149	0.02249	0.03400	3.49854
R25	2.78069	0.00003	0.00109	-0.00127	-0.00019	2.78050
R26	2.71367	-0.00039	-0.00142	-0.00030	-0.00174	2.71193
R27	2.05631	-0.00114	0.00122	-0.00075	0.00047	2.05678
R28	2.05496	-0.00102	0.00110	-0.00058	0.00052	2.05548
R29	2.72191	0.00015	0.00125	0.00324	0.00451	2.72642
R30	2.05719	0.00012	-0.00018	-0.00032	-0.00051	2.05668
R31	2.83746	0.00109	-0.00233	-0.00121	-0.00354	2.83392
R32	2.06775	-0.00049	0.00057	-0.00044	0.00013	2.06788
R33	2.06937	-0.00021	0.00049	-0.00039	0.00010	2.06947
R34	2.06474	-0.00029	0.00032	-0.00019	0.00013	2.06487
A1	1.87578	0.00008	-0.00062	0.00054	-0.00011	1.87567
A2	2.27686	0.00003	0.00016	-0.00041	-0.00023	2.27662
A3	2.13043	-0.00010	0.00052	-0.00010	0.00044	2.13087
A4	1.86055	0.00015	0.00028	-0.00007	0.00023	1.86077
A5	2.27755	-0.00002	-0.00032	0.00020	-0.00013	2.27742
A6	2.14502	-0.00011	0.00007	-0.00010	-0.00004	2.14499
A7	1.89744	0.00005	-0.00046	0.00111	0.00064	1.89809
A8	2.24756	-0.00024	0.00070	-0.00129	-0.00059	2.24697
A9	2.13817	0.00019	-0.00024	0.00019	-0.00005	2.13812
A10	1.88914	-0.00017	0.00031	-0.00131	-0.00101	1.88813
A11	2.23684	0.00044	0.00190	-0.00132	0.00068	2.23752
A12	2.15606	-0.00027	-0.00211	0.00251	0.00031	2.15637
A13	1.90152	-0.00007	0.00064	-0.00014	0.00054	1.90206
A14	2.20461	0.00025	-0.00019	-0.00262	-0.00275	2.20185
A15	2.17419	-0.00016	-0.00026	0.00254	0.00221	2.17640
A16	1.93585	0.00137	-0.00340	0.00262	-0.00135	1.93451
A17	1.87182	-0.00038	0.00086	-0.00197	-0.00099	1.87084
A18	1.88203	-0.00052	-0.00044	0.00023	-0.00005	1.88198
A19	1.92246	-0.00071	0.00437	-0.00247	0.00221	1.92467
A20	1.92506	-0.00006	-0.00032	0.00006	-0.00035	1.92471
A21	1.92560	0.00030	-0.00106	0.00157	0.00046	1.92605
A22	1.90929	0.00015	-0.00348	0.00120	-0.00252	1.90677
A23	1.90154	-0.00027	0.00388	-0.00522	-0.00133	1.90021
A24	1.91712	0.00011	0.00374	-0.00261	0.00140	1.91852
A25	1.90137	-0.00014	-0.00060	-0.00242	-0.00296	1.89841
A26	1.87590	0.00014	-0.00458	0.00728	0.00273	1.87864
A27	1.95804	0.00002	0.00092	0.00194	0.00255	1.96059
A28	1.97267	-0.00042	0.00738	-0.02064	-0.01360	1.95906
A29	2.67019	0.00151	-0.00166	0.01414	0.01260	2.68278

A30	2.17856	-0.00013	0.00028	-0.00104	-0.00076	2.17780
A31	1.95615	0.00005	-0.00013	0.00021	0.00008	1.95624
A32	2.14847	0.00008	-0.00015	0.00083	0.00067	2.14914
A33	2.07968	0.00005	-0.00006	0.00053	0.00047	2.08014
A34	2.15773	-0.00010	0.00014	-0.00093	-0.00079	2.15694
A35	2.04578	0.00004	-0.00008	0.00040	0.00032	2.04610
A36	1.92295	0.00086	0.00076	0.00646	0.00678	1.92973
A37	2.63069	0.00325	-0.00031	0.03299	0.03295	2.66364
A38	2.07948	0.00015	-0.00140	-0.00010	-0.00157	2.07790
A39	2.09821	0.00019	-0.00167	-0.00031	-0.00203	2.09618
A40	2.00387	0.00004	0.00127	0.00106	0.00234	2.00621
A41	2.00116	-0.00025	0.00193	0.00001	0.00191	2.00307
A42	2.02084	-0.00021	0.00084	-0.00074	-0.00006	2.02078
A43	2.04069	0.00033	-0.00268	-0.00073	-0.00333	2.03736
A44	2.14046	-0.00008	0.00029	0.00036	0.00054	2.14101
A45	1.96210	0.00002	-0.00023	-0.00430	-0.00457	1.95753
A46	2.03860	0.00028	0.00076	-0.00044	0.00034	2.03894
A47	2.02138	-0.00025	0.00188	0.00251	0.00440	2.02578
A48	1.04111	0.00203	-0.00120	0.01629	0.01499	1.05609
A49	1.65173	-0.00210	0.00311	-0.03436	-0.03090	1.62083
A50	2.51737	-0.00021	0.00131	-0.00644	-0.00534	2.51202
A51	2.28948	-0.00032	-0.00081	-0.00184	-0.00262	2.28686
A52	1.93668	-0.00087	0.00275	0.00073	0.00344	1.94012
A53	1.92248	0.00016	0.00036	-0.00083	-0.00046	1.92201
A54	1.94391	-0.00112	0.00270	-0.00175	0.00090	1.94481
A55	1.88285	0.00048	-0.00217	0.00028	-0.00188	1.88097
A56	1.88327	0.00098	-0.00228	0.00122	-0.00115	1.88212
A57	1.89281	0.00047	-0.00149	0.00045	-0.00104	1.89177
A58	3.33058	0.00171	-0.00201	0.01445	0.01237	3.34295
A59	3.72116	0.00090	-0.00459	0.05093	0.04610	3.76727
D1	0.02447	-0.00103	-0.01095	-0.00525	-0.01624	0.00823
D2	-3.12962	-0.00047	-0.00409	-0.00257	-0.00671	-3.13633
D3	-3.13321	-0.00034	-0.00415	-0.00286	-0.00695	-3.14016
D4	-0.00411	0.00022	0.00271	-0.00018	0.00258	-0.00153
D5	-0.02349	0.00095	0.00858	0.00415	0.01285	-0.01064
D6	-3.08633	0.00074	0.00562	0.00693	0.01278	-3.07355
D7	3.13255	0.00033	0.00249	0.00201	0.00451	3.13706
D8	0.06970	0.00012	-0.00048	0.00479	0.00444	0.07414
D9	-0.01732	0.00077	0.00964	0.00459	0.01420	-0.00313
D10	3.12711	0.00051	0.00611	0.00179	0.00793	3.13504
D11	3.13559	0.00026	0.00343	0.00216	0.00556	3.14115
D12	-0.00316	0.00001	-0.00010	-0.00064	-0.00070	-0.00387
D13	0.00288	-0.00018	-0.00441	-0.00206	-0.00634	-0.00346
D14	3.09400	-0.00027	-0.00221	-0.00470	-0.00675	3.08725

D15	-3.14134	0.00005	-0.00114	0.00053	-0.00055	3.14130
D16	-0.05021	-0.00004	0.00106	-0.00211	-0.00096	-0.05117
D17	0.05232	0.00015	0.00160	0.00544	0.00700	0.05932
D18	-3.08539	0.00017	0.00226	0.00574	0.00796	-3.07743
D19	-3.08609	-0.00013	-0.00236	0.00229	-0.00003	-3.08612
D20	0.05939	-0.00011	-0.00170	0.00259	0.00093	0.06032
D21	0.01257	-0.00047	-0.00250	-0.00127	-0.00391	0.00866
D22	3.07710	-0.00024	0.00040	-0.00427	-0.00411	3.07299
D23	-3.08142	-0.00041	-0.00469	0.00135	-0.00354	-3.08496
D24	-0.01689	-0.00018	-0.00179	-0.00165	-0.00374	-0.02063
D25	-2.65130	-0.00030	-0.00096	-0.00203	-0.00372	-2.65502
D26	0.43278	-0.00040	0.00162	-0.00516	-0.00422	0.42857
D27	1.40111	0.00026	-0.00061	-0.01748	-0.01837	1.38274
D28	-2.78216	-0.00004	0.00333	-0.02020	-0.01708	-2.79924
D29	-0.70843	-0.00016	0.00231	-0.01928	-0.01710	-0.72554
D30	-1.65000	0.00002	-0.00405	-0.01413	-0.01833	-1.66834
D31	0.44992	-0.00029	-0.00011	-0.01684	-0.01705	0.43288
D32	2.52364	-0.00041	-0.00112	-0.01593	-0.01707	2.50658
D33	-0.97906	0.00015	-0.01288	0.01758	0.00459	-0.97446
D34	1.09778	-0.00009	-0.01332	0.01226	-0.00125	1.09653
D35	-3.03418	-0.00017	-0.00749	0.00955	0.00195	-3.03223
D36	-3.04862	0.00021	-0.01472	0.01995	0.00526	-3.04336
D37	-0.97178	-0.00003	-0.01516	0.01463	-0.00058	-0.97237
D38	1.17945	-0.00011	-0.00932	0.01192	0.00262	1.18207
D39	1.10487	0.00034	-0.01609	0.01958	0.00345	1.10831
D40	-3.10149	0.00010	-0.01653	0.01426	-0.00240	-3.10388
D41	-0.95025	0.00002	-0.01069	0.01156	0.00080	-0.94945
D42	-1.58512	-0.00022	-0.00218	-0.00473	-0.00735	-1.59247
D43	2.62230	-0.00055	0.00257	-0.00898	-0.00671	2.61559
D44	0.53256	-0.00047	0.00568	-0.01188	-0.00636	0.52620
D45	-0.12920	-0.00021	0.01523	0.00738	0.02161	-0.10759
D46	0.01789	0.00030	-0.01817	-0.00456	-0.02262	-0.00473
D47	-2.66329	0.00023	-0.01702	-0.01811	-0.03531	-2.69860
D48	-3.13512	0.00002	0.00059	0.00060	0.00119	-3.13393
D49	0.00605	0.00002	0.00026	0.00098	0.00124	0.00729
D50	0.00217	0.00000	-0.00014	0.00027	0.00013	0.00230
D51	-3.13985	0.00001	-0.00047	0.00065	0.00018	-3.13966
D52	-2.78174	0.00028	0.00480	0.00057	0.00492	-2.77682
D53	3.12584	0.00029	0.00625	0.01218	0.01800	-3.13934
D54	-2.29752	-0.00002	0.00957	-0.02668	-0.01715	-2.31466
D55	-0.59532	-0.00061	0.01083	-0.03875	-0.02810	-0.62342
D56	-2.71554	-0.00018	0.00313	-0.00303	0.00008	-2.71546
D57	-0.01268	-0.00025	0.00225	0.00308	0.00527	-0.00742
D58	-0.02229	0.00012	-0.00294	-0.00607	-0.00896	-0.03125

D59	2.68057	0.00005	-0.00382	0.00004	-0.00378	2.67680
D60	0.91528	-0.00007	0.00398	-0.02927	-0.02530	0.88998
D61	0.19972	-0.00073	0.00175	-0.00605	-0.00422	0.19550
D62	-1.48796	0.00051	-0.00087	-0.02935	-0.03030	-1.51826
D63	-2.20352	-0.00015	-0.00310	-0.00613	-0.00923	-2.21275
D64	1.96061	-0.00004	0.00140	0.00867	0.01014	1.97075
D65	-0.43770	0.00003	-0.00225	0.01028	0.00813	-0.42957
D66	2.52150	-0.00015	0.00093	0.01060	0.01154	2.53304
D67	-1.67789	0.00000	0.00022	0.01088	0.01108	-1.66681
D68	0.42305	-0.00005	0.00035	0.00974	0.01005	0.43310
D69	1.31892	-0.00002	0.00180	0.01132	0.01315	1.33208
D70	-2.88046	0.00012	0.00109	0.01160	0.01270	-2.86777
D71	-0.77952	0.00008	0.00122	0.01046	0.01166	-0.76786
D72	-1.05436	-0.00008	-0.00104	0.01591	0.01491	-1.03945
D73	1.02944	0.00006	-0.00174	0.01618	0.01445	1.04389
D74	3.13038	0.00002	-0.00162	0.01505	0.01342	-3.13939

Item	Value	Threshold	Converged?
Maximum Force	0.003249	0.000450	NO
RMS Force	0.000579	0.000300	NO
Maximum Displacement	0.137841	0.001800	NO
RMS Displacement	0.029998	0.001200	NO

Predicted change in Energy=-2.698900D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.450945	-1.851244	0.075182
2	6	0	-2.709787	-1.359426	-0.045101
3	7	0	-2.614012	0.020688	0.106681
4	6	0	-1.322458	0.344944	0.317534
5	7	0	-0.605187	-0.777633	0.308298
6	6	0	0.866428	-0.836218	0.422595
7	6	0	1.520553	-0.913041	-0.967300
8	1	0	-1.088619	-2.863383	0.021012
9	1	0	-3.641788	-1.863704	-0.223987
10	1	0	1.185707	0.068474	0.941025
11	1	0	1.121081	-1.720241	1.009888
12	1	0	1.112302	-1.772722	-1.511971
13	1	0	1.282584	0.000664	-1.521754
14	35	0	0.758217	2.819495	0.287297
15	1	0	-0.878811	1.354829	0.432151

16	6	0	-3.647654	0.994546	0.057909
17	6	0	-4.937944	0.721980	-0.086462
18	1	0	-3.262107	2.002218	0.148117
19	1	0	-5.648331	1.536303	-0.119121
20	1	0	-5.331464	-0.282590	-0.175566
21	8	0	2.904841	-1.111629	-0.834536
22	1	0	3.372961	-0.256368	-0.811273
23	6	0	5.666334	1.825751	-0.378648
24	6	0	6.270279	0.524980	-0.707584
25	8	0	4.884027	0.796280	-1.001279
26	1	0	5.403371	2.040046	0.655541
27	1	0	5.861629	2.692270	-1.006443
28	1	0	6.879884	0.481986	-1.608162
29	6	0	6.550051	-0.522758	0.328233
30	1	0	6.400409	-1.528324	-0.076592
31	1	0	7.588972	-0.449914	0.666776
32	1	0	5.895945	-0.410644	1.196296

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.356848	0.000000			
3	N	2.204052	1.391735	0.000000		
4	C	2.213251	2.227344	1.348225	0.000000	
5	N	1.386466	2.211949	2.171024	1.332195	0.000000
6	C	2.553662	3.644421	3.598271	2.489459	1.477209
7	C	3.285848	4.352642	4.372632	3.363932	2.482792
8	H	1.076402	2.212339	3.263745	3.230475	2.160230
9	H	2.211210	1.074673	2.171773	3.248178	3.268612
10	H	3.374453	4.264530	3.890537	2.599244	2.079313
11	H	2.739737	3.989830	4.218713	3.273412	2.088239
12	H	3.015867	4.114716	4.440920	3.709401	2.693204
13	H	3.667689	4.468711	4.223228	3.207453	2.741991
14	Br	5.171188	5.440673	4.386099	3.233192	3.846900
15	H	3.276227	3.308689	2.212868	1.108976	2.153510
16	C	3.595045	2.536018	1.420984	2.428153	3.529862
17	C	4.336677	3.049367	2.435113	3.657472	4.601897
18	H	4.258497	3.412190	2.085235	2.556853	3.848695
19	H	5.397339	4.126228	3.399289	4.508123	5.565095
20	H	4.193087	2.837214	2.748852	4.087673	4.776703
21	O	4.510819	5.675268	5.711897	4.617243	3.706470
22	H	5.157470	6.229252	6.063269	4.866492	4.165431
23	C	8.023834	8.967497	8.488693	7.177790	6.825062
24	C	8.116432	9.199536	8.935768	7.663742	7.071128

25	O	6.949822	7.951564	7.619036	6.361088	5.858640
26	H	7.903202	8.824435	8.285981	6.944379	6.645499
27	H	8.676817	9.529407	8.956164	7.672937	7.455768
28	H	8.813643	9.889173	9.658547	8.426476	7.828521
29	C	8.114484	9.305052	9.182835	7.920191	7.159804
30	H	7.859458	9.111816	9.148377	7.956579	7.056207
31	H	9.166996	10.363322	10.229177	8.953623	8.208542
32	H	7.570272	8.746421	8.590266	7.310847	6.571753

		6	7	8	9	10
6	C	0.000000				
7	C	1.538048	0.000000			
8	H	2.844798	3.404170	0.000000		
9	H	4.668812	5.301513	2.752827	0.000000	
10	H	1.090494	2.171912	3.822927	5.328721	0.000000
11	H	1.091447	2.172653	2.677205	4.922190	1.791206
12	H	2.163340	1.096534	2.895450	4.926312	3.067993
13	H	2.157326	1.094946	4.025605	5.423053	2.465617
14	Br	3.659816	4.010860	5.981372	6.446224	2.859759
15	H	2.801185	3.585896	4.243391	4.292262	2.485135
16	C	4.884837	5.603598	4.629648	2.872123	4.999889
17	C	6.031406	6.720220	5.261528	2.895633	6.243548
18	H	5.017655	5.711106	5.330505	3.902303	4.914379
19	H	6.954452	7.623096	6.337811	3.949336	7.069831
20	H	6.251253	6.926359	4.969997	2.314578	6.621446
21	O	2.410676	1.404748	4.443909	6.617910	2.738738
22	H	2.853308	1.971542	5.234016	7.220466	2.821374
23	C	5.546816	5.003498	8.232685	10.013847	4.990549
24	C	5.686103	4.969432	8.134202	10.207289	5.364623
25	O	4.564381	3.773048	7.078893	8.964888	4.240262
26	H	5.376896	5.141071	8.160403	9.890790	4.664471
27	H	6.280478	5.643114	8.956947	10.568068	5.704488
28	H	6.482537	5.574874	8.794472	10.868476	6.252439
29	C	5.693042	5.208318	7.995136	10.294497	5.431506
30	H	5.599388	4.998493	7.607723	10.048877	5.547831
31	H	6.738060	6.301619	9.030085	11.354393	6.430066
32	H	5.106443	4.906894	7.495422	9.751766	4.741419

		11	12	13	14	15
11	H	0.000000				
12	H	2.522420	0.000000			
13	H	3.065422	1.781570	0.000000		
14	Br	4.611183	4.944815	3.390197	0.000000	
15	H	3.713409	4.186373	3.212963	2.201384	0.000000
16	C	5.569306	5.725337	5.271659	4.774386	2.817154
17	C	6.624063	6.697842	6.424587	6.081572	4.140775

18	H	5.814782	6.011782	5.239170	4.104914	2.485938
19	H	7.596360	7.654791	7.236238	6.546420	4.804701
20	H	6.716211	6.747488	6.755597	6.849919	4.782947
21	O	2.637064	2.027106	2.083551	4.617384	4.690835
22	H	3.245075	2.810851	2.222729	4.183858	4.713769
23	C	5.929706	5.913766	4.884148	5.051793	6.611965
24	C	5.874093	5.703613	5.080835	6.052884	7.286778
25	O	4.953527	4.592003	3.724822	4.772435	5.964646
26	H	5.709932	6.135844	5.087296	4.724468	6.323388
27	H	6.782966	6.538181	5.336473	5.266380	7.020814
28	H	6.698342	6.193380	5.618621	6.821401	8.069825
29	C	5.601101	5.875192	5.607374	6.687127	7.663166
30	H	5.393382	5.484899	5.533393	7.132340	7.845918
31	H	6.600384	6.960174	6.690533	7.582364	8.661149
32	H	4.954706	5.663321	5.370296	6.136474	7.042594

		16	17	18	19	20
16	C	0.000000				
17	C	1.326643	0.000000			
18	H	1.082676	2.121902	0.000000		
19	H	2.080276	1.081128	2.445927	0.000000	
20	H	2.126218	1.082571	3.099574	1.847150	0.000000
21	O	6.940290	8.088944	6.978030	8.982211	8.304112
22	H	7.183961	8.399622	7.074303	9.223689	8.727647
23	C	9.361189	10.665570	8.945707	11.321341	11.199906
24	C	9.958508	11.227148	9.684051	11.975906	11.641978
25	O	8.599464	9.864762	8.314740	10.595112	10.305437
26	H	9.130788	10.451347	8.680404	11.090265	11.014630
27	H	9.718105	11.016314	9.222350	11.601843	11.611437
28	H	10.670875	11.917811	10.404595	12.660371	12.318844
29	C	10.313510	11.562671	10.133429	12.379030	11.894616
30	H	10.360818	11.559507	10.289773	12.432453	11.798241
31	H	11.345438	12.604139	11.136781	13.408538	12.948947
32	H	9.713432	10.968201	9.528404	11.780969	11.311636

		21	22	23	24	25
21	O	0.000000				
22	H	0.975269	0.000000			
23	C	4.057324	3.127610	0.000000		
24	C	3.744433	3.002617	1.471379	0.000000	
25	O	2.754106	1.851349	1.435089	1.442759	0.000000
26	H	4.289060	3.398180	1.088402	2.214738	2.135819
27	H	4.820974	3.863421	1.087714	2.225637	2.133192
28	H	4.351904	3.671336	2.188633	1.088350	2.109628
29	C	3.871222	3.385756	2.606939	1.499648	2.506611
30	H	3.600987	3.364978	3.446727	2.152009	2.925448

31	H	4.963154	4.471783	3.157230	2.139682	3.413522
32	H	3.682711	3.227938	2.744929	2.154131	2.703697

		26	27	28	29	30
26	H	0.000000				
27	H	1.843255	0.000000			
28	H	3.119614	2.506844	0.000000		
29	C	2.826653	3.548477	2.206338	0.000000	
30	H	3.776688	4.355264	2.572343	1.094276	0.000000
31	H	3.313137	3.956855	2.558630	1.095114	1.768685
32	H	2.557523	3.805432	3.103209	1.092684	1.767467

		31	32
31	H	0.000000	
32	H	1.774338	0.000000

Stoichiometry C10H17BrN2O2
Framework group C1[X(C10H17BrN2O2)]
Deg. of freedom 90
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.492168	2.327239	-0.237072
2	6	0	-3.721453	1.805449	0.002992
3	7	0	-3.577833	0.421349	-0.020835
4	6	0	-2.287537	0.123784	-0.274411
5	7	0	-1.617254	1.266476	-0.414831
6	6	0	-0.157679	1.365505	-0.619722
7	6	0	0.567563	1.601522	0.715910
8	1	0	-2.169049	3.351971	-0.301567
9	1	0	-4.662123	2.291616	0.186575
10	1	0	0.169528	0.426118	-1.066559
11	1	0	0.028277	2.196017	-1.303043
12	1	0	0.154859	2.495578	1.198326
13	1	0	0.397673	0.738854	1.368480
14	35	0	-0.109026	-2.260776	-0.127819
15	1	0	-1.809942	-0.876169	-0.317128
16	6	0	-4.566662	-0.578916	0.181362
17	6	0	-5.857211	-0.339243	0.373767
18	1	0	-4.145791	-1.576323	0.166070
19	1	0	-6.530925	-1.171007	0.525807
20	1	0	-6.285970	0.654690	0.388725

21	8	0	1.933292	1.834890	0.484306
22	1	0	2.433971	0.998553	0.516087
23	6	0	4.783431	-1.033663	0.152666
24	6	0	5.350806	0.313645	0.319404
25	8	0	3.994859	0.023697	0.718019
26	1	0	4.473447	-1.357647	-0.839082
27	1	0	5.047872	-1.826893	0.848352
28	1	0	6.006336	0.466388	1.174656
29	6	0	5.530687	1.263814	-0.826792
30	1	0	5.362412	2.298361	-0.512409
31	1	0	6.551714	1.194822	-1.216690
32	1	0	4.835353	1.043950	-1.640505

Rotational constants (GHZ): 0.6507346 0.1770297 0.1434440

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.

475 basis functions, 751 primitive gaussians, 492 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1264.5351507745 Hartrees.

NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 475 RedAO= T EigKep= 3.95D-06 NBF= 475

NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999994 0.003281 -0.000051 0.001087 Ang= 0.40 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3225.51608300 A.U. after 11 cycles
NFock= 11 Conv=0.30D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000337256	0.000004727	0.000508753
2	6	-0.000154409	0.000227192	-0.000338640
3	7	-0.000294245	-0.000249007	-0.000012418
4	6	-0.001336704	-0.000619058	0.001065814
5	7	-0.000182101	-0.000594555	-0.000146912
6	6	-0.000306984	-0.000671286	-0.000460498
7	6	-0.000519031	-0.000132908	0.000222109
8	1	0.000065693	0.000025790	0.000130556
9	1	0.000009416	0.000067608	-0.000084058
10	1	0.000192066	0.000502849	-0.000379389
11	1	-0.000032530	0.000326855	0.000145372
12	1	0.000045066	0.000360901	-0.000588001
13	1	-0.000010043	0.000260791	0.000097931
14	35	0.000423529	0.001009135	0.000372816
15	1	0.001541668	0.000392484	-0.000603620
16	6	0.000113538	-0.000153835	-0.000068718
17	6	-0.000155267	0.000027822	-0.000001590
18	1	0.000015949	0.000043375	0.000021712
19	1	0.000015268	-0.000011286	0.000017148
20	1	0.000005523	-0.000006681	0.000019973
21	8	0.000389041	0.001067961	0.000759555
22	1	0.000739479	-0.003343980	-0.000273655
23	6	0.000900165	0.000349424	0.001790225
24	6	-0.002015653	0.002337508	-0.001332436
25	8	0.000504829	0.001092866	-0.001317295
26	1	-0.000471342	0.000190055	-0.001509312
27	1	-0.000804393	-0.000775456	0.000702528
28	1	0.000479234	-0.000595984	0.000077793
29	6	0.001569044	-0.003120826	0.002581991
30	1	-0.000144899	0.000855073	-0.000725889
31	1	-0.000162697	0.000170788	-0.000078761
32	1	-0.000081950	0.000961658	-0.000593082

Cartesian Forces: Max 0.003343980 RMS 0.000851659

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.002349768 RMS 0.000548663

Search for a local minimum.

Step number 12 out of a maximum of 177

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 11 12

DE= -3.69D-04 DEPred=-2.70D-04 R= 1.37D+00

TightC=F SS= 1.41D+00 RLast= 1.64D-01 DXNew= 4.0363D+00 4.9315D-01

Trust test= 1.37D+00 RLast= 1.64D-01 DXMaxT set to 2.40D+00

ITU= 1 1 1 1 1 1 1 0 1 0 1 0

Eigenvalues ---	0.00116	0.00220	0.00240	0.00384	0.00440
Eigenvalues ---	0.00933	0.01117	0.01314	0.01398	0.01603
Eigenvalues ---	0.01703	0.01873	0.02014	0.02067	0.02152
Eigenvalues ---	0.02157	0.02313	0.02386	0.02554	0.02906
Eigenvalues ---	0.03062	0.03066	0.03290	0.03781	0.04057
Eigenvalues ---	0.04664	0.05076	0.05242	0.05397	0.05526
Eigenvalues ---	0.05909	0.06483	0.07324	0.09220	0.09920
Eigenvalues ---	0.10785	0.11000	0.11847	0.11920	0.12890
Eigenvalues ---	0.13818	0.15144	0.15525	0.15997	0.16000
Eigenvalues ---	0.16000	0.16000	0.16002	0.16019	0.16106
Eigenvalues ---	0.16895	0.17310	0.19347	0.21834	0.22023
Eigenvalues ---	0.22775	0.23563	0.23694	0.25011	0.26695
Eigenvalues ---	0.27880	0.29227	0.31914	0.32889	0.33054
Eigenvalues ---	0.33177	0.34096	0.34308	0.34540	0.34769
Eigenvalues ---	0.34952	0.35684	0.35688	0.35859	0.36197
Eigenvalues ---	0.36441	0.36660	0.37228	0.37315	0.37782
Eigenvalues ---	0.38865	0.42188	0.42521	0.45338	0.46882
Eigenvalues ---	0.49292	0.53577	0.54564	0.56248	0.60357

En-DIIS/RFO-DIIS IScMMF= 0 using points: 12 11 10 9

RFO step: Lambda=-1.87006801D-04.

EnCoef did 100 forward-backward iterations

DidBck=T Rises=F En-DIIS coefs: 0.76382 0.00000 0.00339 0.23279

Iteration 1 RMS(Cart)= 0.11971240 RMS(Int)= 0.01212438

Iteration 2 RMS(Cart)= 0.01646707 RMS(Int)= 0.00035256

Iteration 3 RMS(Cart)= 0.00009575 RMS(Int)= 0.00035013

Iteration 4 RMS(Cart)= 0.00000002 RMS(Int)= 0.00035013

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56407	0.00019	0.00042	-0.00125	-0.00089	2.56318
R2	2.62004	0.00013	-0.00053	0.00209	0.00156	2.62160
R3	2.03410	-0.00001	0.00000	0.00003	0.00002	2.03413
R4	2.63000	-0.00020	-0.00055	0.00082	0.00023	2.63023
R5	2.03084	-0.00002	-0.00004	-0.00009	-0.00012	2.03071
R6	2.54778	0.00035	0.00033	0.00023	0.00060	2.54837
R7	2.68527	-0.00008	-0.00013	0.00030	0.00017	2.68544
R8	2.51748	0.00022	0.00025	0.00132	0.00185	2.51933
R9	2.09566	0.00134	-0.00094	0.01335	0.01249	2.10815
R10	2.79152	0.00075	0.00156	-0.00228	-0.00057	2.79095
R11	2.90649	0.00044	0.00006	0.00259	0.00301	2.90950
R12	2.06073	0.00029	0.00051	0.00103	0.00154	2.06228
R13	2.06254	-0.00019	-0.00054	0.00059	0.00005	2.06259
R14	2.07215	-0.00001	-0.00064	0.00168	0.00104	2.07319
R15	2.06915	0.00017	-0.00017	0.00215	0.00197	2.07112
R16	2.65459	0.00149	0.00463	-0.01272	-0.00793	2.64666
R17	4.16001	0.00022	0.03487	-0.10739	-0.07256	4.08745
R18	9.01859	-0.00023	-0.20197	0.56372	0.36146	9.38006
R19	2.50699	0.00013	0.00006	0.00034	0.00039	2.50738
R20	2.04596	0.00004	0.00002	0.00024	0.00026	2.04622
R21	2.04304	-0.00002	-0.00002	-0.00007	-0.00009	2.04295
R22	2.04576	0.00001	0.00001	-0.00017	-0.00016	2.04560
R23	1.84299	-0.00067	-0.00130	0.00203	0.00073	1.84372
R24	3.49854	0.00143	0.05811	-0.04026	0.01795	3.51649
R25	2.78050	0.00012	-0.00177	-0.00337	-0.00570	2.77480
R26	2.71193	-0.00026	0.00175	0.00207	0.00410	2.71602
R27	2.05678	-0.00128	-0.00175	-0.00062	-0.00237	2.05441
R28	2.05548	-0.00117	-0.00160	-0.00042	-0.00202	2.05346
R29	2.72642	-0.00027	-0.00399	0.01480	0.01110	2.73752
R30	2.05668	0.00023	0.00079	-0.00134	-0.00055	2.05614
R31	2.83392	0.00182	0.00585	-0.00214	0.00371	2.83764
R32	2.06788	-0.00050	-0.00102	-0.00052	-0.00155	2.06634
R33	2.06947	-0.00017	-0.00076	-0.00004	-0.00080	2.06866
R34	2.06487	-0.00032	-0.00065	-0.00007	-0.00072	2.06415
A1	1.87567	0.00011	0.00033	-0.00113	-0.00083	1.87484
A2	2.27662	0.00004	0.00045	-0.00007	0.00036	2.27699
A3	2.13087	-0.00015	-0.00080	0.00129	0.00047	2.13134
A4	1.86077	0.00002	-0.00002	0.00082	0.00071	1.86148
A5	2.27742	0.00004	0.00027	-0.00062	-0.00035	2.27707
A6	2.14499	-0.00006	-0.00026	-0.00016	-0.00042	2.14457
A7	1.89809	0.00002	-0.00024	0.00103	0.00081	1.89890

A8	2.24697	-0.00012	-0.00036	-0.00057	-0.00094	2.24603
A9	2.13812	0.00010	0.00060	-0.00049	0.00009	2.13821
A10	1.88813	0.00001	0.00032	-0.00186	-0.00165	1.88648
A11	2.23752	0.00033	0.00005	0.00182	0.00159	2.23911
A12	2.15637	-0.00034	-0.00034	-0.00030	-0.00027	2.15611
A13	1.90206	-0.00015	-0.00046	0.00144	0.00084	1.90290
A14	2.20185	0.00054	0.00356	-0.00462	-0.00137	2.20048
A15	2.17640	-0.00038	-0.00288	0.00320	0.00079	2.17719
A16	1.93451	0.00149	0.00605	0.00132	0.00796	1.94246
A17	1.87084	-0.00025	-0.00145	-0.00319	-0.00481	1.86603
A18	1.88198	-0.00056	0.00015	-0.00040	-0.00039	1.88160
A19	1.92467	-0.00082	-0.00817	0.00726	-0.00105	1.92362
A20	1.92471	-0.00011	0.00343	-0.00411	-0.00078	1.92393
A21	1.92605	0.00027	-0.00004	-0.00101	-0.00100	1.92505
A22	1.90677	0.00034	0.00677	-0.00481	0.00211	1.90889
A23	1.90021	-0.00016	-0.00195	0.00109	-0.00070	1.89951
A24	1.91852	0.00027	-0.00377	0.00427	0.00003	1.91855
A25	1.89841	-0.00016	0.00219	-0.01162	-0.00948	1.88893
A26	1.87864	-0.00023	0.00114	-0.00005	0.00114	1.87978
A27	1.96059	-0.00005	-0.00410	0.01053	0.00673	1.96731
A28	1.95906	-0.00061	0.03606	-0.11247	-0.07773	1.88134
A29	2.68278	0.00167	-0.00920	0.06292	0.05355	2.73634
A30	2.17780	0.00002	0.00032	-0.00164	-0.00132	2.17648
A31	1.95624	-0.00001	0.00018	-0.00028	-0.00010	1.95614
A32	2.14914	-0.00001	-0.00050	0.00191	0.00142	2.15056
A33	2.08014	0.00001	-0.00017	0.00108	0.00090	2.08105
A34	2.15694	-0.00001	0.00027	-0.00183	-0.00156	2.15538
A35	2.04610	0.00001	-0.00010	0.00075	0.00066	2.04676
A36	1.92973	0.00017	-0.00802	0.01526	0.00748	1.93721
A37	2.66364	0.00235	-0.02489	0.13975	0.11544	2.77908
A38	2.07790	0.00033	0.00324	0.00018	0.00306	2.08097
A39	2.09618	0.00024	0.00340	-0.00232	0.00153	2.09771
A40	2.00621	-0.00003	-0.00280	0.00165	-0.00101	2.00520
A41	2.00307	-0.00021	-0.00257	-0.00012	-0.00296	2.00011
A42	2.02078	-0.00027	-0.00209	-0.00130	-0.00322	2.01756
A43	2.03736	0.00067	0.00423	-0.00210	0.00266	2.04002
A44	2.14101	-0.00021	-0.00072	-0.00246	-0.00375	2.13725
A45	1.95753	0.00027	0.00435	-0.00721	-0.00300	1.95453
A46	2.03894	0.00018	-0.00031	-0.00034	-0.00053	2.03841
A47	2.02578	-0.00051	-0.00498	0.00710	0.00215	2.02793
A48	1.05609	0.00195	-0.00747	0.06972	0.06221	1.11831
A49	1.62083	-0.00218	0.02908	-0.16042	-0.13099	1.48983
A50	2.51202	-0.00040	0.00630	-0.03068	-0.02538	2.48664
A51	2.28686	-0.00031	-0.00328	-0.00215	-0.00588	2.28098

A52	1.94012	-0.00116	-0.00601	0.00337	-0.00260	1.93751
A53	1.92201	0.00025	0.00073	-0.00133	-0.00061	1.92140
A54	1.94481	-0.00127	-0.00506	-0.00335	-0.00837	1.93644
A55	1.88097	0.00059	0.00413	-0.00117	0.00295	1.88391
A56	1.88212	0.00120	0.00406	0.00296	0.00710	1.88922
A57	1.89177	0.00050	0.00254	-0.00042	0.00210	1.89387
A58	3.34295	0.00164	-0.01075	0.06757	0.05633	3.39928
A59	3.76727	0.00085	-0.04590	0.24184	0.19447	3.96174
D1	0.00823	-0.00024	0.00304	-0.02939	-0.02635	-0.01812
D2	-3.13633	-0.00015	0.00178	-0.01290	-0.01113	3.13572
D3	-3.14016	-0.00004	0.00055	-0.01421	-0.01364	3.12939
D4	-0.00153	0.00005	-0.00072	0.00228	0.00158	0.00005
D5	-0.01064	0.00032	-0.00314	0.02771	0.02460	0.01397
D6	-3.07355	0.00024	-0.00635	0.02720	0.02088	-3.05267
D7	3.13706	0.00014	-0.00092	0.01408	0.01319	-3.13294
D8	0.07414	0.00006	-0.00412	0.01357	0.00947	0.08361
D9	-0.00313	0.00009	-0.00192	0.02131	0.01937	0.01625
D10	3.13504	0.00011	-0.00046	0.01342	0.01295	-3.13520
D11	3.14115	0.00001	-0.00078	0.00637	0.00559	-3.13644
D12	-0.00387	0.00003	0.00068	-0.00152	-0.00084	-0.00470
D13	-0.00346	0.00010	-0.00002	-0.00427	-0.00423	-0.00770
D14	3.08725	-0.00001	0.00078	-0.01182	-0.01109	3.07616
D15	3.14130	0.00009	-0.00137	0.00303	0.00172	-3.14017
D16	-0.05117	-0.00002	-0.00057	-0.00452	-0.00514	-0.05631
D17	0.05932	0.00003	-0.00356	0.02155	0.01798	0.07730
D18	-3.07743	0.00000	-0.00408	0.02153	0.01745	-3.05998
D19	-3.08612	0.00005	-0.00193	0.01269	0.01077	-3.07535
D20	0.06032	0.00001	-0.00244	0.01267	0.01024	0.07055
D21	0.00866	-0.00026	0.00193	-0.01428	-0.01240	-0.00375
D22	3.07299	-0.00013	0.00538	-0.01422	-0.00887	3.06412
D23	-3.08496	-0.00018	0.00117	-0.00724	-0.00602	-3.09098
D24	-0.02063	-0.00005	0.00462	-0.00718	-0.00248	-0.02311
D25	-2.65502	-0.00028	-0.01594	0.01704	0.00085	-2.65417
D26	0.42857	-0.00039	-0.01502	0.00841	-0.00699	0.42157
D27	1.38274	0.00020	0.03006	-0.09388	-0.06387	1.31887
D28	-2.79924	-0.00009	0.02267	-0.08626	-0.06354	-2.86277
D29	-0.72554	-0.00020	0.02193	-0.08938	-0.06748	-0.79301
D30	-1.66834	0.00010	0.02623	-0.09431	-0.06813	-1.73646
D31	0.43288	-0.00020	0.01884	-0.08668	-0.06779	0.36508
D32	2.50658	-0.00031	0.01810	-0.08980	-0.07174	2.43484
D33	-0.97446	0.00014	-0.02026	0.06806	0.04790	-0.92656
D34	1.09653	0.00004	-0.01478	0.05187	0.03729	1.13381
D35	-3.03223	0.00005	-0.02341	0.06848	0.04524	-2.98699
D36	-3.04336	0.00003	-0.01696	0.06659	0.04955	-2.99381

D37	-0.97237	-0.00006	-0.01147	0.05040	0.03893	-0.93344
D38	1.18207	-0.00005	-0.02011	0.06701	0.04688	1.22895
D39	1.10831	0.00031	-0.01373	0.06576	0.05202	1.16033
D40	-3.10388	0.00022	-0.00824	0.04957	0.04140	-3.06248
D41	-0.94945	0.00023	-0.01687	0.06618	0.04935	-0.90010
D42	-1.59247	-0.00029	0.01500	-0.05708	-0.04193	-1.63441
D43	2.61559	-0.00071	0.00834	-0.05367	-0.04517	2.57042
D44	0.52620	-0.00033	0.00737	-0.04558	-0.03823	0.48797
D45	-0.10759	-0.00028	0.00067	0.03115	0.03083	-0.07676
D46	-0.00473	0.00017	0.00870	-0.05671	-0.04901	-0.05375
D47	-2.69860	0.00025	0.02362	-0.12752	-0.10478	-2.80339
D48	-3.13393	-0.00003	-0.00043	0.00127	0.00084	-3.13309
D49	0.00729	-0.00001	-0.00057	0.00290	0.00233	0.00962
D50	0.00230	0.00001	0.00014	0.00129	0.00143	0.00373
D51	-3.13966	0.00004	0.00000	0.00291	0.00291	-3.13675
D52	-2.77682	0.00021	0.01314	-0.01042	0.00136	-2.77547
D53	-3.13934	0.00026	-0.03155	0.10126	0.06828	-3.07106
D54	-2.31466	-0.00005	0.01337	-0.09513	-0.08118	-2.39584
D55	-0.62342	-0.00058	0.01435	-0.14058	-0.12619	-0.74961
D56	-2.71546	-0.00027	-0.00178	-0.00358	-0.00528	-2.72074
D57	-0.00742	-0.00052	-0.00669	0.00476	-0.00189	-0.00931
D58	-0.03125	0.00037	0.00966	-0.01230	-0.00273	-0.03398
D59	2.67680	0.00012	0.00475	-0.00396	0.00066	2.67746
D60	0.88998	-0.00018	0.02214	-0.14290	-0.12189	0.76809
D61	0.19550	-0.00077	-0.00946	-0.01785	-0.02663	0.16886
D62	-1.51826	0.00055	0.03168	-0.14261	-0.11192	-1.63018
D63	-2.21275	-0.00004	0.00008	-0.01756	-0.01666	-2.22941
D64	1.97075	-0.00017	-0.01101	0.04414	0.03362	2.00437
D65	-0.42957	0.00011	-0.00782	0.04171	0.03434	-0.39523
D66	2.53304	-0.00016	-0.00917	0.02365	0.01449	2.54752
D67	-1.66681	0.00001	-0.00740	0.02348	0.01611	-1.65070
D68	0.43310	-0.00003	-0.00703	0.01987	0.01290	0.44600
D69	1.33208	-0.00009	-0.01114	0.02622	0.01501	1.34709
D70	-2.86777	0.00008	-0.00937	0.02605	0.01663	-2.85114
D71	-0.76786	0.00005	-0.00900	0.02244	0.01342	-0.75444
D72	-1.03945	-0.00013	-0.01187	0.02985	0.01799	-1.02146
D73	1.04389	0.00003	-0.01009	0.02968	0.01961	1.06350
D74	-3.13939	0.00000	-0.00972	0.02607	0.01640	-3.12299

Item	Value	Threshold	Converged?
Maximum Force	0.002350	0.000450	NO
RMS Force	0.000549	0.000300	NO
Maximum Displacement	0.414959	0.001800	NO
RMS Displacement	0.117321	0.001200	NO

Predicted change in Energy=-6.027139D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.444732	-1.843033	-0.003346
2	6	0	-2.694804	-1.327785	-0.111062
3	7	0	-2.584553	0.039337	0.125760
4	6	0	-1.288889	0.338391	0.350229
5	7	0	-0.584079	-0.790582	0.272702
6	6	0	0.887574	-0.872234	0.366629
7	6	0	1.531717	-0.980208	-1.027614
8	1	0	-1.095927	-2.856479	-0.103009
9	1	0	-3.632037	-1.809643	-0.321273
10	1	0	1.224625	0.036377	0.868404
11	1	0	1.135602	-1.750020	0.966037
12	1	0	1.072121	-1.810898	-1.577453
13	1	0	1.336842	-0.053934	-1.580095
14	35	0	0.725161	2.844743	0.491495
15	1	0	-0.829754	1.341375	0.516819
16	6	0	-3.608570	1.024605	0.135423
17	6	0	-4.902878	0.770346	-0.008275
18	1	0	-3.211603	2.022887	0.270812
19	1	0	-5.606805	1.590741	0.005151
20	1	0	-5.304951	-0.226091	-0.139536
21	8	0	2.898755	-1.257472	-0.901631
22	1	0	3.424667	-0.435786	-0.913953
23	6	0	5.570187	1.799411	-0.500084
24	6	0	6.271421	0.521665	-0.678186
25	8	0	4.897803	0.684364	-1.108588
26	1	0	5.204347	2.071138	0.486940
27	1	0	5.768340	2.629818	-1.172359
28	1	0	6.956411	0.449582	-1.520487
29	6	0	6.516531	-0.428323	0.458602
30	1	0	6.473425	-1.466541	0.118167
31	1	0	7.509108	-0.254664	0.886363
32	1	0	5.771414	-0.295472	1.246176

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.356379	0.000000			

3	N	2.204355	1.391856	0.000000		
4	C	2.215382	2.228346	1.348542	0.000000	
5	N	1.387292	2.211565	2.170773	1.333172	0.000000
6	C	2.553230	3.642684	3.597867	2.490557	1.476906
7	C	3.263869	4.338705	4.394704	3.404846	2.490657
8	H	1.076415	2.212098	3.264061	3.232623	2.161267
9	H	2.210541	1.074608	2.171586	3.248893	3.268231
10	H	3.378994	4.264061	3.880898	2.584081	2.076086
11	H	2.757985	4.001304	4.212769	3.258656	2.087711
12	H	2.968736	4.071047	4.437969	3.729580	2.684607
13	H	3.663901	4.476039	4.277380	3.282459	2.768654
14	Br	5.189272	5.428555	4.354109	3.218408	3.870086
15	H	3.284696	3.316181	2.219808	1.115587	2.159905
16	C	3.595108	2.535638	1.421076	2.428569	3.530056
17	C	4.334576	3.047673	2.434537	3.657325	4.600812
18	H	4.259382	3.411732	2.085354	2.557472	3.849610
19	H	5.395714	4.124445	3.399324	4.509086	5.565074
20	H	4.187403	2.833268	2.746161	4.085005	4.772339
21	O	4.473889	5.649588	5.727470	4.652988	3.705021
22	H	5.149815	6.236042	6.116982	4.941165	4.195721
23	C	7.919800	8.845381	8.365962	7.064314	6.721626
24	C	8.098532	9.172528	8.905461	7.632137	7.044434
25	O	6.916433	7.917795	7.610869	6.365768	5.842471
26	H	7.731195	8.620143	8.057644	6.721846	6.460744
27	H	8.567462	9.402860	8.841183	7.574522	7.358027
28	H	8.839514	9.914205	9.690636	8.455585	7.849365
29	C	8.099167	9.272661	9.119168	7.843735	7.112275
30	H	7.928034	9.172143	9.182303	7.972775	7.091485
31	H	9.137054	10.308552	10.126546	8.834246	8.134093
32	H	7.485253	8.636238	8.437393	7.145095	6.448649

		6	7	8	9	10
6	C	0.000000				
7	C	1.539640	0.000000			
8	H	2.844655	3.358542	0.000000		
9	H	4.666779	5.277427	2.752336	0.000000	
10	H	1.091310	2.173163	3.833695	5.330130	0.000000
11	H	1.091474	2.173514	2.710504	4.938735	1.791276
12	H	2.166703	1.097086	2.822704	4.868993	3.068860
13	H	2.158979	1.095990	3.994297	5.418201	2.452732
14	Br	3.722618	4.193861	6.014459	6.427213	2.877228
15	H	2.805679	3.653979	4.251706	4.299314	2.459086
16	C	4.885362	5.638659	4.629582	2.870903	4.987347
17	C	6.030585	6.745925	5.258869	2.892982	6.233264
18	H	5.019379	5.762255	5.331420	3.900720	4.897291

19	H	6.955132	7.657341	6.335414	3.945741	7.059015
20	H	6.246685	6.935230	4.963482	2.310694	6.612126
21	O	2.408681	1.400550	4.376312	6.579738	2.758583
22	H	2.875277	1.972960	5.191643	7.213585	2.870526
23	C	5.460379	4.930903	8.140765	9.886261	4.885177
24	C	5.658657	4.984226	8.125300	10.180415	5.300716
25	O	4.547659	3.756047	7.033744	8.921777	4.221448
26	H	5.226131	5.009271	8.020156	9.684799	4.485973
27	H	6.201188	5.567963	8.852182	10.430735	5.615692
28	H	6.491470	5.631565	8.819265	10.892999	6.223416
29	C	5.647183	5.230849	8.010048	10.271790	5.328053
30	H	5.622870	5.096058	7.699087	10.120829	5.511035
31	H	6.670549	6.318142	9.044055	11.313772	6.291244
32	H	4.995813	4.859425	7.452478	9.652693	4.574508

		11	12	13	14	15
11	H	0.000000				
12	H	2.545010	0.000000			
13	H	3.065940	1.776797	0.000000		
14	Br	4.637401	5.106458	3.614964	0.000000	
15	H	3.690683	4.235555	3.322359	2.162988	0.000000
16	C	5.558384	5.734360	5.344469	4.713906	2.822698
17	C	6.615495	6.695204	6.487231	6.018946	4.146341
18	H	5.797962	6.038567	5.331735	4.027686	2.489615
19	H	7.585778	7.660537	7.309733	6.473240	4.810842
20	H	6.710095	6.726535	6.798402	6.796357	4.786977
21	O	2.615243	2.024749	2.085279	4.847007	4.761070
22	H	3.240584	2.804574	2.224537	4.474873	4.827577
23	C	5.866302	5.867508	4.745789	5.054723	6.496393
24	C	5.851551	5.769077	5.049239	6.125834	7.247526
25	O	4.938061	4.591515	3.667130	4.963713	5.989868
26	H	5.602273	6.033839	4.873003	4.545502	6.078143
27	H	6.724431	6.475997	5.196820	5.314909	6.931684
28	H	6.700959	6.303799	5.642396	6.972327	8.097547
29	C	5.564060	5.974834	5.579034	6.652369	7.556660
30	H	5.412170	5.671666	5.591424	7.195073	7.834521
31	H	6.547061	7.065908	6.649855	7.468881	8.498265
32	H	4.866717	5.687948	5.264178	5.991257	6.840076

		16	17	18	19	20
16	C	0.000000				
17	C	1.326850	0.000000			
18	H	1.082811	2.123008	0.000000		
19	H	2.080967	1.081083	2.448330	0.000000	
20	H	2.125454	1.082487	3.099742	1.847411	0.000000
21	O	6.973423	8.110217	7.033623	9.015493	8.303333

22	H	7.259500	8.463038	7.175571	9.301561	8.766409
23	C	9.233296	10.534986	8.818393	11.190350	11.068030
24	C	9.926183	11.197124	9.647901	11.945799	11.612996
25	O	8.603587	9.862628	8.334078	10.602298	10.289033
26	H	8.881796	10.202612	8.418863	10.832539	10.775671
27	H	9.602783	10.894385	9.115398	11.483036	11.482191
28	H	10.709412	11.959616	10.443780	12.706856	12.357369
29	C	10.233919	11.491635	10.033957	12.298679	11.838332
30	H	10.385216	11.594823	10.295590	12.461608	11.846319
31	H	11.216202	12.486329	10.977239	13.274382	12.855092
32	H	9.537319	10.800469	9.328489	11.600077	11.162924

		21	22	23	24	25
21	O	0.000000				
22	H	0.975655	0.000000			
23	C	4.079500	3.125804	0.000000		
24	C	3.819702	3.012691	1.468361	0.000000	
25	O	2.794593	1.860846	1.437257	1.448634	0.000000
26	H	4.280599	3.378525	1.087148	2.212924	2.136076
27	H	4.839301	3.867494	1.086644	2.222973	2.132298
28	H	4.445400	3.691203	2.187437	1.088062	2.112498
29	C	3.952977	3.382837	2.603353	1.501613	2.512854
30	H	3.723165	3.379741	3.444490	2.151266	2.934944
31	H	5.045582	4.467281	3.146566	2.140647	3.417677
32	H	3.713581	3.192658	2.734676	2.149625	2.695957

		26	27	28	29	30
26	H	0.000000				
27	H	1.839425	0.000000			
28	H	3.119124	2.507217	0.000000		
29	C	2.823108	3.545709	2.209300	0.000000	
30	H	3.776470	4.352328	2.567097	1.093458	0.000000
31	H	3.298608	3.948272	2.567950	1.094690	1.769579
32	H	2.549284	3.795609	3.100605	1.092301	1.771052

		31	32
31	H	0.000000	
32	H	1.775024	0.000000

Stoichiometry C10H17BrN2O2
Framework group C1[X(C10H17BrN2O2)]
Deg. of freedom 90
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-2.450737	2.341204	-0.259857
2	6	0	-3.675606	1.824273	0.008917
3	7	0	-3.537769	0.439436	-0.013240
4	6	0	-2.249367	0.135017	-0.269977
5	7	0	-1.576261	1.276078	-0.419159
6	6	0	-0.116138	1.371996	-0.619394
7	6	0	0.607098	1.716687	0.695372
8	1	0	-2.127934	3.364466	-0.345890
9	1	0	-4.612883	2.314193	0.199371
10	1	0	0.217924	0.401551	-0.990331
11	1	0	0.068234	2.146597	-1.365929
12	1	0	0.156063	2.615459	1.133977
13	1	0	0.474428	0.887778	1.400001
14	35	0	-0.171261	-2.319036	-0.138634
15	1	0	-1.770427	-0.871971	-0.303520
16	6	0	-4.529692	-0.555504	0.200390
17	6	0	-5.820223	-0.308279	0.384625
18	1	0	-4.111046	-1.554111	0.200832
19	1	0	-6.498090	-1.134512	0.547639
20	1	0	-6.244155	0.687736	0.380740
21	8	0	1.954894	1.998279	0.439066
22	1	0	2.505641	1.200408	0.548530
23	6	0	4.690167	-1.027328	0.359597
24	6	0	5.361176	0.276671	0.285973
25	8	0	4.021606	0.157068	0.824292
26	1	0	4.274140	-1.462167	-0.545790
27	1	0	4.953882	-1.734186	1.141647
28	1	0	6.093061	0.497801	1.060133
29	6	0	5.508080	1.035807	-1.001263
30	1	0	5.453593	2.114212	-0.828857
31	1	0	6.477995	0.816055	-1.458777
32	1	0	4.721369	0.762295	-1.707944

Rotational constants (GHZ): 0.6200152 0.1786223 0.1435865
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 492 symmetry adapted cartesian basis functions of A symmetry.
There are 475 symmetry adapted basis functions of A symmetry.
475 basis functions, 751 primitive gaussians, 492 cartesian basis functions
71 alpha electrons 71 beta electrons
nuclear repulsion energy 1260.3446923791 Hartrees.
NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 475 RedAO= T EigKep= 3.97D-06 NBF= 475
NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999905 0.012963 -0.000548 0.004609 Ang= 1.58 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3225.51702919 A.U. after 12 cycles
NFock= 12 Conv=0.38D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000423072	0.000556273	-0.001922678
2	6	-0.000776585	-0.000174252	0.002268941
3	7	0.000258148	0.000103222	-0.001247940
4	6	-0.000395642	-0.000315513	0.000183997
5	7	-0.000674291	-0.000500765	0.000645778
6	6	-0.000223289	0.000115039	0.000365569
7	6	-0.004329310	0.000492863	-0.000072333
8	1	0.000111088	0.000098292	-0.000352350
9	1	-0.000091485	-0.000023595	0.000246028
10	1	0.000196474	0.000054163	0.000112408

11	1	0.000400691	0.000253039	-0.000129368
12	1	0.000040476	0.000292115	-0.000229971
13	1	0.000580436	0.000046484	0.000220504
14	35	0.001294254	0.001371071	0.000281635
15	1	0.000158626	-0.001252503	-0.000636889
16	6	0.000013713	-0.000056854	-0.000214143
17	6	0.000124577	0.000048719	0.000082980
18	1	-0.000006216	0.000008928	0.000055995
19	1	0.000025301	0.000012854	0.000017653
20	1	-0.000110354	-0.000022755	-0.000019782
21	8	0.004342105	0.001134514	0.000614102
22	1	-0.000160349	-0.002784939	0.000101459
23	6	-0.000399308	0.001307480	0.001445266
24	6	-0.002740985	0.000836186	-0.001593818
25	8	0.001746820	-0.000290989	-0.000527628
26	1	-0.000523492	0.000138747	-0.000736998
27	1	-0.000413672	-0.000296951	0.000205653
28	1	0.000551032	-0.000478773	0.000184265
29	6	0.000651205	-0.001223401	0.001258133
30	1	-0.000130939	0.000203145	-0.000385184
31	1	-0.000029071	0.000042664	-0.000038178
32	1	0.000086972	0.000305492	-0.000183104

Cartesian Forces: Max 0.004342105 RMS 0.000973364

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.003949708 RMS 0.000573539
Search for a local minimum.
Step number 13 out of a maximum of 177
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 12 13
DE= -9.46D-04 DEPred=-6.03D-04 R= 1.57D+00
TightC=F SS= 1.41D+00 RLast= 5.93D-01 DXNew= 4.0363D+00 1.7798D+00
Trust test= 1.57D+00 RLast= 5.93D-01 DXMaxT set to 2.40D+00
ITU= 1 1 1 1 1 1 1 1 0 1 0 1 0
Eigenvalues --- 0.00081 0.00203 0.00238 0.00361 0.00405
Eigenvalues --- 0.00878 0.00984 0.01343 0.01397 0.01549
Eigenvalues --- 0.01721 0.01871 0.02031 0.02065 0.02149

Eigenvalues --- 0.02160 0.02314 0.02385 0.02558 0.02766
Eigenvalues --- 0.03062 0.03066 0.03330 0.03776 0.03952
Eigenvalues --- 0.04617 0.05217 0.05441 0.05514 0.05557
Eigenvalues --- 0.05957 0.06498 0.06620 0.09291 0.09887
Eigenvalues --- 0.10949 0.11144 0.11834 0.11990 0.12940
Eigenvalues --- 0.13868 0.15206 0.15503 0.15997 0.16000
Eigenvalues --- 0.16000 0.16001 0.16001 0.16048 0.16102
Eigenvalues --- 0.17016 0.17411 0.19387 0.21915 0.22033
Eigenvalues --- 0.22798 0.23565 0.23630 0.25029 0.26790
Eigenvalues --- 0.27888 0.29022 0.32035 0.32926 0.33054
Eigenvalues --- 0.33167 0.34101 0.34354 0.34532 0.34767
Eigenvalues --- 0.34948 0.35685 0.35690 0.35858 0.36318
Eigenvalues --- 0.36443 0.36660 0.37231 0.37298 0.37778
Eigenvalues --- 0.39649 0.42194 0.42498 0.45324 0.47064
Eigenvalues --- 0.49411 0.53993 0.54750 0.56305 0.60363
En-DIIS/RFO-DIIS IScMMF= 0 using points: 13 12 11 10 9
RFO step: Lambda=-1.83632478D-04.
EnCoef did 100 forward-backward iterations
DidBck=F Rises=F En-DIIS coefs: 0.79923 0.00000 0.00061 0.00211 0.19804
Iteration 1 RMS(Cart)= 0.18780421 RMS(Int)= 0.03257891
Iteration 2 RMS(Cart)= 0.08421674 RMS(Int)= 0.00980228
Iteration 3 RMS(Cart)= 0.01444398 RMS(Int)= 0.00161663
Iteration 4 RMS(Cart)= 0.00005616 RMS(Int)= 0.00161639
Iteration 5 RMS(Cart)= 0.00000006 RMS(Int)= 0.00161639

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56318	0.00038	0.00054	-0.00099	-0.00067	2.56252
R2	2.62160	-0.00006	-0.00077	0.00322	0.00253	2.62413
R3	2.03413	-0.00002	-0.00001	-0.00007	-0.00007	2.03406
R4	2.63023	-0.00022	-0.00051	0.00108	0.00037	2.63060
R5	2.03071	0.00004	-0.00001	0.00007	0.00006	2.03078
R6	2.54837	-0.00007	0.00016	-0.00044	-0.00019	2.54818
R7	2.68544	-0.00005	-0.00014	0.00041	0.00026	2.68571
R8	2.51933	-0.00043	-0.00015	0.00164	0.00269	2.52202
R9	2.10815	0.00007	-0.00330	0.02062	0.01793	2.12608
R10	2.79095	0.00053	0.00144	-0.00252	-0.00061	2.79034
R11	2.90950	-0.00018	-0.00056	0.00167	0.00224	2.91173
R12	2.06228	0.00016	0.00013	0.00224	0.00236	2.06464
R13	2.06259	-0.00018	-0.00047	0.00028	-0.00019	2.06239
R14	2.07319	-0.00012	-0.00075	0.00264	0.00189	2.07508
R15	2.07112	-0.00017	-0.00054	0.00230	0.00176	2.07288
R16	2.64666	0.00395	0.00553	-0.00803	-0.00195	2.64471
R17	4.08745	0.00108	0.04419	-0.12666	-0.08218	4.00528

R18	9.38006	-0.00062	-0.24398	0.80769	0.56266	9.94272
R19	2.50738	-0.00005	-0.00003	0.00026	0.00023	2.50761
R20	2.04622	0.00001	-0.00004	0.00051	0.00047	2.04669
R21	2.04295	-0.00001	0.00000	-0.00010	-0.00010	2.04285
R22	2.04560	0.00007	0.00004	-0.00002	0.00002	2.04562
R23	1.84372	-0.00193	-0.00125	0.00084	-0.00058	1.84314
R24	3.51649	0.00026	0.04569	-0.03308	0.01260	3.52909
R25	2.77480	0.00106	-0.00036	-0.00685	-0.00948	2.76532
R26	2.71602	-0.00024	0.00066	0.00937	0.01109	2.72711
R27	2.05441	-0.00046	-0.00101	-0.00313	-0.00414	2.05027
R28	2.05346	-0.00043	-0.00096	-0.00262	-0.00358	2.04988
R29	2.73752	-0.00190	-0.00562	0.01815	0.01377	2.75129
R30	2.05614	0.00024	0.00078	-0.00170	-0.00092	2.05522
R31	2.83764	0.00101	0.00423	0.00287	0.00710	2.84474
R32	2.06634	-0.00007	-0.00056	-0.00111	-0.00167	2.06467
R33	2.06866	-0.00003	-0.00049	-0.00041	-0.00089	2.06777
R34	2.06415	-0.00015	-0.00041	-0.00047	-0.00087	2.06328
A1	1.87484	0.00012	0.00045	-0.00193	-0.00117	1.87367
A2	2.27699	0.00002	0.00031	0.00033	0.00050	2.27749
A3	2.13134	-0.00013	-0.00078	0.00158	0.00067	2.13201
A4	1.86148	-0.00024	-0.00016	0.00062	0.00054	1.86202
A5	2.27707	0.00016	0.00030	-0.00042	-0.00014	2.27693
A6	2.14457	0.00008	-0.00014	-0.00028	-0.00044	2.14413
A7	1.89890	0.00004	-0.00037	0.00169	0.00167	1.90057
A8	2.24603	0.00014	-0.00011	0.00001	-0.00027	2.24577
A9	2.13821	-0.00018	0.00049	-0.00171	-0.00139	2.13682
A10	1.88648	0.00025	0.00061	-0.00237	-0.00211	1.88438
A11	2.23911	-0.00016	-0.00027	0.00166	-0.00003	2.23907
A12	2.15611	-0.00008	-0.00024	0.00037	0.00186	2.15797
A13	1.90290	-0.00015	-0.00056	0.00168	0.00088	1.90377
A14	2.20048	0.00057	0.00329	-0.00138	0.00060	2.20108
A15	2.17719	-0.00043	-0.00260	0.00024	-0.00083	2.17636
A16	1.94246	0.00037	0.00354	0.00657	0.01124	1.95370
A17	1.86603	0.00006	-0.00027	-0.00587	-0.00633	1.85970
A18	1.88160	0.00006	0.00020	0.00354	0.00328	1.88488
A19	1.92362	-0.00014	-0.00673	0.01085	0.00363	1.92725
A20	1.92393	-0.00030	0.00306	-0.01008	-0.00708	1.91685
A21	1.92505	-0.00003	0.00017	-0.00508	-0.00478	1.92027
A22	1.90889	0.00011	0.00532	-0.00283	0.00324	1.91213
A23	1.89951	0.00022	-0.00152	0.00066	-0.00121	1.89830
A24	1.91855	0.00006	-0.00322	0.00296	-0.00081	1.91774
A25	1.88893	-0.00001	0.00376	-0.01680	-0.01308	1.87586
A26	1.87978	-0.00002	0.00074	0.00785	0.00852	1.88829
A27	1.96731	-0.00035	-0.00483	0.00761	0.00327	1.97058

A28	1.88134	-0.00092	0.04621	-0.19035	-0.14859	1.73274
A29	2.73634	0.00146	-0.01856	0.12239	0.10382	2.84016
A30	2.17648	0.00021	0.00053	-0.00207	-0.00154	2.17494
A31	1.95614	-0.00010	0.00017	-0.00090	-0.00073	1.95541
A32	2.15056	-0.00011	-0.00071	0.00298	0.00227	2.15283
A33	2.08105	-0.00010	-0.00033	0.00079	0.00047	2.08152
A34	2.15538	0.00015	0.00054	-0.00178	-0.00124	2.15414
A35	2.04676	-0.00004	-0.00021	0.00098	0.00077	2.04753
A36	1.93721	-0.00044	-0.00831	0.01476	0.00591	1.94312
A37	2.77908	0.00134	-0.04431	0.25992	0.21949	2.99857
A38	2.08097	0.00043	0.00214	0.00615	0.00596	2.08693
A39	2.09771	0.00024	0.00259	0.00115	0.00593	2.10364
A40	2.00520	0.00007	-0.00218	-0.00245	-0.00369	2.00150
A41	2.00011	0.00018	-0.00159	-0.00544	-0.00850	1.99161
A42	2.01756	-0.00029	-0.00113	-0.00415	-0.00521	2.01236
A43	2.04002	0.00059	0.00306	0.00678	0.01307	2.05309
A44	2.13725	-0.00008	0.00014	-0.00532	-0.00872	2.12854
A45	1.95453	0.00037	0.00430	-0.00489	-0.00150	1.95303
A46	2.03841	0.00000	-0.00016	-0.00396	-0.00334	2.03507
A47	2.02793	-0.00055	-0.00466	0.00230	-0.00224	2.02569
A48	1.11831	0.00170	-0.01884	0.14056	0.12217	1.24047
A49	1.48983	-0.00243	0.05098	-0.30812	-0.25264	1.23720
A50	2.48664	-0.00079	0.01044	-0.06063	-0.05647	2.43017
A51	2.28098	-0.00067	-0.00160	-0.01386	-0.01737	2.26361
A52	1.93751	-0.00056	-0.00458	-0.00169	-0.00626	1.93125
A53	1.92140	0.00009	0.00074	-0.00321	-0.00250	1.91890
A54	1.93644	-0.00030	-0.00262	-0.00967	-0.01229	1.92415
A55	1.88391	0.00027	0.00291	0.00278	0.00569	1.88960
A56	1.88922	0.00042	0.00202	0.01027	0.01232	1.90154
A57	1.89387	0.00011	0.00173	0.00213	0.00382	1.89769
A58	3.39928	0.00104	-0.02044	0.12670	0.10480	3.50408
A59	3.96174	0.00053	-0.07801	0.46719	0.38202	4.34376
D1	-0.01812	0.00106	0.00789	-0.01539	-0.00749	-0.02561
D2	3.13572	0.00044	0.00375	-0.00801	-0.00432	3.13140
D3	3.12939	0.00037	0.00321	-0.01217	-0.00889	3.12050
D4	0.00005	-0.00025	-0.00093	-0.00479	-0.00572	-0.00567
D5	0.01397	-0.00093	-0.00762	0.01706	0.00950	0.02347
D6	-3.05267	-0.00082	-0.00959	0.00914	-0.00036	-3.05303
D7	-3.13294	-0.00031	-0.00343	0.01416	0.01076	-3.12218
D8	0.08361	-0.00020	-0.00540	0.00624	0.00090	0.08451
D9	0.01625	-0.00085	-0.00553	0.00873	0.00307	0.01932
D10	-3.13520	-0.00052	-0.00300	0.00846	0.00534	-3.12986
D11	-3.13644	-0.00028	-0.00179	0.00203	0.00021	-3.13624
D12	-0.00470	0.00005	0.00074	0.00176	0.00247	-0.00223

D13	-0.00770	0.00027	0.00084	0.00184	0.00284	-0.00486
D14	3.07616	0.00034	0.00289	-0.00473	-0.00216	3.07400
D15	-3.14017	-0.00004	-0.00150	0.00207	0.00073	-3.13944
D16	-0.05631	0.00003	0.00055	-0.00449	-0.00426	-0.06057
D17	0.07730	-0.00015	-0.00664	0.03094	0.02430	0.10160
D18	-3.05998	-0.00021	-0.00697	0.02878	0.02182	-3.03816
D19	-3.07535	0.00022	-0.00380	0.03065	0.02686	-3.04849
D20	0.07055	0.00016	-0.00413	0.02850	0.02437	0.09493
D21	-0.00375	0.00040	0.00414	-0.01157	-0.00757	-0.01132
D22	3.06412	0.00034	0.00634	-0.00387	0.00219	3.06631
D23	-3.09098	0.00034	0.00221	-0.00545	-0.00280	-3.09378
D24	-0.02311	0.00028	0.00442	0.00225	0.00697	-0.01615
D25	-2.65417	-0.00017	-0.01370	-0.00912	-0.02381	-2.67798
D26	0.42157	-0.00008	-0.01134	-0.01668	-0.02965	0.39193
D27	1.31887	-0.00009	0.03834	-0.14386	-0.10528	1.21359
D28	-2.86277	-0.00001	0.03200	-0.13050	-0.09831	-2.96108
D29	-0.79301	0.00002	0.03216	-0.13773	-0.10557	-0.89858
D30	-1.73646	0.00001	0.03595	-0.15302	-0.11670	-1.85316
D31	0.36508	0.00010	0.02961	-0.13965	-0.10973	0.25536
D32	2.43484	0.00013	0.02977	-0.14688	-0.11698	2.31786
D33	-0.92656	0.00012	-0.02680	0.11907	0.09255	-0.83401
D34	1.13381	0.00029	-0.02001	0.09757	0.07795	1.21177
D35	-2.98699	0.00004	-0.02894	0.10946	0.08069	-2.90629
D36	-2.99381	-0.00010	-0.02432	0.11526	0.09094	-2.90287
D37	-0.93344	0.00007	-0.01753	0.09376	0.07634	-0.85710
D38	1.22895	-0.00018	-0.02646	0.10565	0.07908	1.30803
D39	1.16033	0.00023	-0.02207	0.12112	0.09923	1.25956
D40	-3.06248	0.00040	-0.01528	0.09963	0.08463	-2.97785
D41	-0.90010	0.00015	-0.02422	0.11151	0.08737	-0.81273
D42	-1.63441	-0.00030	0.02116	-0.10709	-0.08444	-1.71885
D43	2.57042	-0.00046	0.01614	-0.11000	-0.09298	2.47744
D44	0.48797	-0.00022	0.01392	-0.09893	-0.08435	0.40363
D45	-0.07676	-0.00023	-0.00565	0.07039	0.06101	-0.01574
D46	-0.05375	-0.00026	0.01726	-0.12491	-0.10761	-0.16136
D47	-2.80339	-0.00006	0.04112	-0.27447	-0.23909	-3.04248
D48	-3.13309	-0.00005	-0.00054	0.00087	0.00033	-3.13276
D49	0.00962	-0.00004	-0.00095	0.00318	0.00222	0.01184
D50	0.00373	0.00002	-0.00017	0.00325	0.00308	0.00681
D51	-3.13675	0.00003	-0.00058	0.00555	0.00497	-3.13178
D52	-2.77547	-0.00011	0.01087	0.00542	0.01410	-2.76137
D53	-3.07106	0.00024	-0.04050	0.14218	0.09495	-2.97611
D54	-2.39584	-0.00037	0.02763	-0.23083	-0.19835	-2.59420
D55	-0.74961	-0.00029	0.03751	-0.32502	-0.28707	-1.03668
D56	-2.72074	-0.00036	-0.00045	-0.01158	-0.01183	-2.73258

D57	-0.00931	-0.00060	-0.00530	-0.00101	-0.00653	-0.01584
D58	-0.03398	0.00051	0.00875	-0.00488	0.00376	-0.03022
D59	2.67746	0.00027	0.00390	0.00570	0.00906	2.68652
D60	0.76809	-0.00014	0.04327	-0.30572	-0.26766	0.50043
D61	0.16886	-0.00032	-0.00268	-0.05132	-0.05080	0.11806
D62	-1.63018	0.00002	0.04937	-0.28967	-0.24528	-1.87546
D63	-2.22941	-0.00016	0.00342	-0.03527	-0.02842	-2.25782
D64	2.00437	-0.00004	-0.01610	0.07668	0.06361	2.06798
D65	-0.39523	0.00041	-0.01353	0.08335	0.07274	-0.32249
D66	2.54752	-0.00006	-0.01069	0.02415	0.01341	2.56094
D67	-1.65070	-0.00003	-0.00951	0.02446	0.01491	-1.63579
D68	0.44600	-0.00002	-0.00856	0.01878	0.01021	0.45621
D69	1.34709	-0.00011	-0.01247	0.02557	0.01294	1.36003
D70	-2.85114	-0.00007	-0.01129	0.02589	0.01444	-2.83670
D71	-0.75444	-0.00007	-0.01033	0.02020	0.00974	-0.74470
D72	-1.02146	-0.00004	-0.01369	0.03570	0.02218	-0.99928
D73	1.06350	0.00000	-0.01251	0.03601	0.02367	1.08717
D74	-3.12299	0.00000	-0.01155	0.03032	0.01898	-3.10401

Item	Value	Threshold	Converged?
Maximum Force	0.003950	0.000450	NO
RMS Force	0.000574	0.000300	NO
Maximum Displacement	0.867896	0.001800	NO
RMS Displacement	0.251549	0.001200	NO

Predicted change in Energy=-8.394767D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.408919	-1.820408	-0.170233
2	6	0	-2.640495	-1.254643	-0.214222
3	7	0	-2.481725	0.077758	0.156332
4	6	0	-1.175256	0.312205	0.393949
5	7	0	-0.509243	-0.826525	0.191806
6	6	0	0.959231	-0.964935	0.260540
7	6	0	1.589280	-1.116052	-1.137436
8	1	0	-1.096954	-2.831730	-0.366425
9	1	0	-3.595617	-1.681522	-0.459923
10	1	0	1.334101	-0.064213	0.752331
11	1	0	1.187084	-1.843749	0.866229
12	1	0	1.034638	-1.870511	-1.710985
13	1	0	1.496346	-0.162344	-1.671325

14	35	0	0.755094	2.833454	0.872776
15	1	0	-0.678065	1.287290	0.654335
16	6	0	-3.472269	1.089492	0.279096
17	6	0	-4.777581	0.885457	0.155056
18	1	0	-3.038394	2.059980	0.486283
19	1	0	-5.455172	1.721545	0.257316
20	1	0	-5.213113	-0.085506	-0.043294
21	8	0	2.915635	-1.546270	-1.017655
22	1	0	3.538772	-0.799374	-1.089437
23	6	0	5.329647	1.716002	-0.745176
24	6	0	6.192685	0.542749	-0.603685
25	8	0	4.914084	0.447419	-1.293463
26	1	0	4.745076	2.056143	0.103183
27	1	0	5.545800	2.472186	-1.492271
28	1	0	7.031564	0.447981	-1.289340
29	6	0	6.314107	-0.204782	0.697312
30	1	0	6.470076	-1.270873	0.516082
31	1	0	7.167454	0.174607	1.267553
32	1	0	5.408597	-0.075217	1.293446

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.356026	0.000000			
3	N	2.204675	1.392053	0.000000		
4	C	2.218319	2.229756	1.348439	0.000000	
5	N	1.388630	2.211421	2.170178	1.334594	0.000000
6	C	2.554512	3.642438	3.596977	2.490968	1.476583
7	C	3.228126	4.331574	4.435325	3.468101	2.500902
8	H	1.076376	2.211987	3.264351	3.235526	2.162839
9	H	2.210172	1.074641	2.171541	3.249953	3.268253
10	H	3.385189	4.260137	3.864700	2.562617	2.072010
11	H	2.795358	4.020545	4.201940	3.232930	2.089764
12	H	2.889187	4.015744	4.432543	3.752151	2.663474
13	H	3.666472	4.519925	4.384407	3.409987	2.816874
14	Br	5.237294	5.424401	4.310934	3.211265	3.931630
15	H	3.297248	3.326702	2.228040	1.125073	2.170402
16	C	3.595390	2.535780	1.421216	2.427681	3.529627
17	C	4.333060	3.046889	2.433790	3.655466	4.599016
18	H	4.259533	3.411123	2.085174	2.556272	3.849056
19	H	5.394478	4.123403	3.399061	4.508057	5.564096
20	H	4.183048	2.830982	2.743535	4.080887	4.767680
21	O	4.415319	5.621489	5.757362	4.709772	3.702785
22	H	5.134889	6.257524	6.210288	5.065383	4.246027

23	C	7.631843	8.522313	8.032067	6.751446	6.437003
24	C	7.972250	9.022603	8.720048	7.438749	6.886476
25	O	6.810657	7.818788	7.545631	6.320262	5.765539
26	H	7.278328	8.099921	7.492896	6.178689	5.993788
27	H	8.279025	9.085048	8.537701	7.307253	7.097968
28	H	8.811341	9.879450	9.629626	8.378771	7.789861
29	C	7.937758	9.061898	8.816981	7.513313	6.870240
30	H	7.927898	9.139809	9.059965	7.808467	7.000963
31	H	8.921966	10.021691	9.713437	8.389454	7.816084
32	H	7.187946	8.273572	7.973306	6.656299	6.066210

		6	7	8	9	10
6	C	0.000000				
7	C	1.540823	0.000000			
8	H	2.847087	3.279308	0.000000		
9	H	4.666820	5.259462	2.752279	0.000000	
10	H	1.092559	2.177775	3.849779	5.327980	0.000000
11	H	1.091371	2.169327	2.777116	4.965806	1.789227
12	H	2.170868	1.098087	2.697308	4.800015	3.069254
13	H	2.159802	1.096920	3.943804	5.450090	2.431062
14	Br	3.852825	4.509481	6.087694	6.410131	2.957403
15	H	2.812174	3.758636	4.264240	4.309005	2.425897
16	C	4.884589	5.700024	4.629773	2.870519	4.965500
17	C	6.028772	6.798051	5.257037	2.892165	6.213797
18	H	5.018175	5.842860	5.331522	3.899313	4.868439
19	H	6.954261	7.721502	6.333674	3.943759	7.037627
20	H	6.242078	6.966471	4.958722	2.310224	6.595414
21	O	2.408163	1.399519	4.263494	6.536495	2.798320
22	H	2.916141	1.975628	5.113039	7.216230	2.965324
23	C	5.224885	4.707945	7.882038	9.554312	4.623427
24	C	5.514439	4.922179	8.036307	10.038870	5.080651
25	O	4.477782	3.677378	6.909761	8.811481	4.154915
26	H	4.846060	4.643383	7.631589	9.157205	4.068422
27	H	5.993560	5.353075	8.574686	10.093787	5.404625
28	H	6.424305	5.664603	8.813687	10.870129	6.073866
29	C	5.426168	5.149825	7.934495	10.085762	4.982293
30	H	5.525243	5.155604	7.776569	10.121235	5.281105
31	H	6.391766	6.210137	8.944741	11.057717	5.860930
32	H	4.653531	4.645396	7.257805	9.312915	4.110285

		11	12	13	14	15
11	H	0.000000				
12	H	2.581858	0.000000			
13	H	3.059729	1.769910	0.000000		
14	Br	4.697115	5.374129	3.999589	0.000000	
15	H	3.650627	4.301139	3.498313	2.119501	0.000000

16	C	5.536984	5.747544	5.482552	4.611340	2.826218
17	C	6.597845	6.697714	6.617833	5.909341	4.149311
18	H	5.765251	6.071766	5.491618	3.890783	2.489266
19	H	7.563177	7.674289	7.456024	6.338969	4.813206
20	H	6.699341	6.708340	6.904580	6.706639	4.789354
21	O	2.573985	2.030761	2.087323	5.236760	4.872298
22	H	3.231994	2.793625	2.217184	4.979617	5.017630
23	C	5.694671	5.678289	4.368081	4.979258	6.183448
24	C	5.736903	5.801326	4.867506	6.082324	7.024540
25	O	4.878960	4.538417	3.492210	5.261460	5.980922
26	H	5.333920	5.698875	4.315648	4.137203	5.505031
27	H	6.571774	6.265576	4.834345	5.354889	6.689424
28	H	6.637503	6.443315	5.581850	7.054028	7.995042
29	C	5.385268	6.037163	5.368712	6.337531	7.149727
30	H	5.325485	5.904521	5.545410	7.045122	7.593367
31	H	6.324528	7.117979	6.396250	6.952963	7.947721
32	H	4.596889	5.601893	4.909498	5.503855	6.269955

		16	17	18	19	20
16	C	0.000000				
17	C	1.326972	0.000000			
18	H	1.083061	2.124615	0.000000		
19	H	2.081314	1.081032	2.451077	0.000000	
20	H	2.124875	1.082497	3.100478	1.847808	0.000000
21	O	7.030941	8.153167	7.121611	9.076044	8.316234
22	H	7.388869	8.576080	7.342882	9.437150	8.843048
23	C	8.883433	10.181173	8.465159	10.831312	10.718575
24	C	9.720575	11.001812	9.418219	11.738971	11.436825
25	O	8.556642	9.809101	8.307212	10.561713	10.217977
26	H	8.275876	9.594488	7.792894	10.206898	10.186935
27	H	9.293824	10.573722	8.818899	11.164493	11.153274
28	H	10.639645	11.905191	10.351591	12.646449	12.319470
29	C	9.880446	11.158325	9.625121	11.933995	11.551602
30	H	10.221434	11.458180	10.075042	12.297685	11.756483
31	H	10.724634	12.017772	10.407899	12.757127	12.452486
32	H	9.014169	10.294516	8.749985	11.059990	10.705498

		21	22	23	24	25
21	O	0.000000				
22	H	0.975349	0.000000			
23	C	4.067446	3.106906	0.000000		
24	C	3.908251	3.013388	1.463345	0.000000	
25	O	2.836312	1.867513	1.443126	1.455919	0.000000
26	H	4.192912	3.321369	1.084957	2.210338	2.137095
27	H	4.826077	3.859215	1.084752	2.220534	2.130322
28	H	4.581672	3.714223	2.191008	1.087576	2.117484

29	C	4.036126	3.353878	2.596026	1.505370	2.519646
30	H	3.881010	3.375285	3.436971	2.149429	2.940763
31	H	5.124603	4.435243	3.131216	2.141783	3.422120
32	H	3.704057	3.114287	2.714900	2.143777	2.685105

		26	27	28	29	30
26	H	0.000000				
27	H	1.832955	0.000000			
28	H	3.123033	2.519143	0.000000		
29	C	2.815427	3.542701	2.210799	0.000000	
30	H	3.770298	4.347212	2.555244	1.092575	0.000000
31	H	3.280831	3.940210	2.575053	1.094218	1.772133
32	H	2.529759	3.777341	3.094922	1.091838	1.777815

		31	32
31	H	0.000000	
32	H	1.776700	0.000000

Stoichiometry C10H17BrN2O2
Framework group C1[X(C10H17BrN2O2)]
Deg. of freedom 90
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.375793	2.361065	-0.291699
2	6	0	-3.592373	1.838811	0.001543
3	7	0	-3.441606	0.454978	0.010740
4	6	0	-2.152762	0.154423	-0.247790
5	7	0	-1.490551	1.299516	-0.424934
6	6	0	-0.033262	1.403243	-0.639055
7	6	0	0.695278	1.938465	0.608704
8	1	0	-2.065201	3.384580	-0.412261
9	1	0	-4.533093	2.323944	0.187410
10	1	0	0.317762	0.397919	-0.883577
11	1	0	0.136622	2.073964	-1.483071
12	1	0	0.173131	2.827721	0.986039
13	1	0	0.655774	1.174750	1.395095
14	35	0	-0.225817	-2.412148	-0.139075
15	1	0	-1.661702	-0.857763	-0.259108
16	6	0	-4.423489	-0.543750	0.252197
17	6	0	-5.719057	-0.304421	0.410567
18	1	0	-3.991736	-1.536102	0.295187

19	1	0	-6.389945	-1.130918	0.598831
20	1	0	-6.153117	0.685904	0.359113
21	8	0	2.002810	2.308675	0.274101
22	1	0	2.640454	1.608284	0.506841
23	6	0	4.438093	-0.913771	0.753011
24	6	0	5.271080	0.166199	0.222752
25	8	0	4.045219	0.460670	0.950937
26	1	0	3.797975	-1.475577	0.080884
27	1	0	4.719534	-1.429876	1.664665
28	1	0	6.156478	0.445030	0.789449
29	6	0	5.285793	0.515515	-1.241455
30	1	0	5.438924	1.588378	-1.380146
31	1	0	6.100533	-0.014947	-1.743571
32	1	0	4.341025	0.228996	-1.707749

Rotational constants (GHZ): 0.5686975 0.1862884 0.1466522

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.

475 basis functions, 751 primitive gaussians, 492 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1258.5445469231 Hartrees.

NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 475 RedAO= T EigKep= 3.84D-06 NBF= 475

NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999592 0.027886 -0.001529 0.006028 Ang= 3.27 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3225.51826339 A.U. after 14 cycles
NFock= 14 Conv=0.54D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.001029112	0.001060520	-0.002145948
2	6	-0.000863034	-0.000512098	0.003057969
3	7	0.000591399	0.000453160	-0.001084772
4	6	0.001574098	0.000042908	-0.001283786
5	7	-0.001238735	-0.000250989	0.000285410
6	6	0.000276192	0.000708328	0.001380225
7	6	-0.006231082	0.002524750	-0.001046667
8	1	0.000046362	0.000165596	-0.000636590
9	1	-0.000095949	-0.000078044	0.000323518
10	1	0.000162535	-0.000860684	0.000475851
11	1	0.000431514	0.000034759	-0.000134503
12	1	0.000692186	0.000007300	0.000565582
13	1	0.001155803	-0.000497256	0.000125817
14	35	0.002504637	0.001700624	0.000285614
15	1	-0.002081796	-0.003298670	-0.000856924
16	6	-0.000186598	0.000191176	-0.000142903
17	6	0.000354927	0.000023199	0.000063561
18	1	-0.000055260	-0.000022541	0.000108041
19	1	0.000005608	0.000026799	0.000018474
20	1	-0.000187354	0.000010828	-0.000065694
21	8	0.005878546	-0.000670228	0.000320991
22	1	-0.001762789	-0.000205054	0.000498010
23	6	-0.002969746	0.001947702	-0.000849367
24	6	-0.002797950	-0.002684694	-0.000649557
25	8	0.003563050	-0.000905021	0.001585581
26	1	-0.000931058	0.000343795	0.000834465
27	1	0.000741195	0.000474169	-0.000598895
28	1	0.000406889	0.000476708	-0.000035835
29	6	-0.000304517	0.000978220	-0.001747156
30	1	-0.000162075	-0.000454043	0.000459484

```
      31        1             -0.000004927     -0.000184487      0.000173423
      32        1              0.000458815     -0.000546733      0.000716584
 ---------------------------------------------------------------------
 Cartesian Forces:  Max        0.006231082 RMS        0.001426171

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 GSVD:  received Info=                1 from GESDD.
 Internal  Forces:  Max        0.003936499 RMS        0.000788474
 Search for a local minimum.
 Step number  14 out of a maximum of  177
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swapping is turned off.
 Update second derivatives using D2CorX and points    13    14
 DE= -1.23D-03 DEPred=-8.39D-04 R= 1.47D+00
 TightC=F SS=  1.41D+00  RLast= 1.08D+00 DXNew= 4.0363D+00 3.2330D+00
 Trust test= 1.47D+00 RLast= 1.08D+00 DXMaxT set to 3.00D+00
 ITU=  1  1  1  1  1  1  1  1  1  0  1  0  1  0
      Eigenvalues ---    0.00068    0.00181    0.00237    0.00322    0.00401
      Eigenvalues ---    0.00772    0.00967    0.01398    0.01410    0.01533
      Eigenvalues ---    0.01774    0.01865    0.02054    0.02086    0.02149
      Eigenvalues ---    0.02179    0.02316    0.02388    0.02602    0.02763
      Eigenvalues ---    0.03062    0.03066    0.03383    0.03745    0.03903
      Eigenvalues ---    0.04544    0.05226    0.05392    0.05551    0.05615
      Eigenvalues ---    0.05901    0.06040    0.06673    0.09360    0.09867
      Eigenvalues ---    0.10925    0.11323    0.11858    0.12011    0.13045
      Eigenvalues ---    0.14014    0.15263    0.15525    0.15997    0.16000
      Eigenvalues ---    0.16001    0.16001    0.16003    0.16057    0.16105
      Eigenvalues ---    0.17299    0.17858    0.19479    0.22024    0.22087
      Eigenvalues ---    0.22836    0.23565    0.23664    0.25033    0.27003
      Eigenvalues ---    0.27853    0.28906    0.31876    0.32947    0.33058
      Eigenvalues ---    0.33174    0.34099    0.34338    0.34531    0.34765
      Eigenvalues ---    0.34973    0.35685    0.35691    0.35859    0.36436
      Eigenvalues ---    0.36658    0.36824    0.37236    0.37321    0.37778
      Eigenvalues ---    0.40660    0.42222    0.42520    0.45051    0.46446
      Eigenvalues ---    0.49373    0.53699    0.54787    0.56256    0.60366
 En-DIIS/RFO-DIIS IScMMF=              0 using points:    14    13    12    11    10
 RFO step:  Lambda=-2.62894829D-04.
 EnCoef did    100 forward-backward iterations
 DidBck=T  Rises=F    En-DIIS  coefs:          0.77036          0.00000          0.00257          0.00339
0.22368
```

New curvilinear step failed, DQL= 6.19D+00 SP=-6.15D-02.
ITry= 1 IFail=1 DXMaxC= 0.00D+00 DCOld= 1.00D+10 DXMaxT= 3.00D+00 DXLimC= 3.00D+00 Rises=F
New curvilinear step failed, DQL= 6.17D+00 SP=-9.89D-02.
ITry= 2 IFail=1 DXMaxC= 0.00D+00 DCOld= 1.00D+10 DXMaxT= 3.00D+00 DXLimC= 3.00D+00 Rises=F
Iteration 1 RMS(Cart)= 0.02003922 RMS(Int)= 0.06124148
Iteration 2 RMS(Cart)= 0.00181772 RMS(Int)= 0.06076657
Iteration 3 RMS(Cart)= 0.00178918 RMS(Int)= 0.06029930
Iteration 4 RMS(Cart)= 0.00175308 RMS(Int)= 0.05984177
Iteration 5 RMS(Cart)= 0.00171822 RMS(Int)= 0.05939362
Iteration 6 RMS(Cart)= 0.00168453 RMS(Int)= 0.05895454
Iteration 7 RMS(Cart)= 0.00165195 RMS(Int)= 0.05852423
Iteration 8 RMS(Cart)= 0.00162044 RMS(Int)= 0.05810239
Iteration 9 RMS(Cart)= 0.00158994 RMS(Int)= 0.05768875
Iteration 10 RMS(Cart)= 0.00156041 RMS(Int)= 0.05728304
Iteration 11 RMS(Cart)= 0.00153180 RMS(Int)= 0.05688501
Iteration 12 RMS(Cart)= 0.00150407 RMS(Int)= 0.05649443
Iteration 13 RMS(Cart)= 0.00147718 RMS(Int)= 0.05611106
Iteration 14 RMS(Cart)= 0.00145109 RMS(Int)= 0.05573468
Iteration 15 RMS(Cart)= 0.00142577 RMS(Int)= 0.05536509
Iteration 16 RMS(Cart)= 0.00140119 RMS(Int)= 0.05500209
Iteration 17 RMS(Cart)= 0.00137732 RMS(Int)= 0.05464547
New curvilinear step failed, DQL= 6.15D+00 SP=-1.89D-01.
ITry= 3 IFail=1 DXMaxC= 1.75D-01 DCOld= 1.00D+10 DXMaxT= 3.00D+00 DXLimC= 3.00D+00 Rises=F
Iteration 1 RMS(Cart)= 0.05739928 RMS(Int)= 0.03953379
Iteration 2 RMS(Cart)= 0.06449424 RMS(Int)= 0.02320920
Iteration 3 RMS(Cart)= 0.06446922 RMS(Int)= 0.00747933
Iteration 4 RMS(Cart)= 0.02407371 RMS(Int)= 0.00259115
Iteration 5 RMS(Cart)= 0.00600779 RMS(Int)= 0.00131233
Iteration 6 RMS(Cart)= 0.00254780 RMS(Int)= 0.00117902
Iteration 7 RMS(Cart)= 0.00004697 RMS(Int)= 0.00117734
Iteration 8 RMS(Cart)= 0.00000046 RMS(Int)= 0.00117734
ITry= 4 IFail=0 DXMaxC= 7.57D-01 DCOld= 1.00D+10 DXMaxT= 3.00D+00 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56252	0.00044	0.00073	0.00015	0.00122	2.56374
R2	2.62413	-0.00045	-0.00139	0.00305	0.00072	2.62484
R3	2.03406	-0.00003	0.00004	-0.00027	-0.00015	2.03391
R4	2.63060	-0.00032	-0.00029	0.00007	0.00001	2.63061
R5	2.03078	0.00004	-0.00003	0.00016	0.00008	2.03086
R6	2.54818	-0.00053	-0.00011	-0.00171	-0.00154	2.54664

R7	2.68571	0.00022	-0.00009	0.00109	0.00068	2.68638
R8	2.52202	-0.00120	-0.00141	0.00213	-0.00027	2.52175
R9	2.12608	-0.00170	-0.00848	0.02042	0.00506	2.13114
R10	2.79034	0.00011	0.00093	0.00080	0.00227	2.79261
R11	2.91173	-0.00039	-0.00043	0.00432	0.00199	2.91373
R12	2.06464	-0.00044	-0.00072	0.00110	0.00004	2.06468
R13	2.06239	-0.00001	-0.00028	0.00004	-0.00025	2.06214
R14	2.07508	-0.00065	-0.00129	0.00094	-0.00064	2.07445
R15	2.07288	-0.00059	-0.00091	0.00082	-0.00034	2.07254
R16	2.64471	0.00394	0.00491	0.00248	0.00740	2.65211
R17	4.00528	0.00218	0.05581	-0.06225	0.01145	4.01673
R18	9.94272	-0.00138	-0.34778	0.55510	0.04075	9.98347
R19	2.50761	-0.00018	-0.00012	0.00004	-0.00010	2.50752
R20	2.04669	-0.00002	-0.00017	0.00077	0.00037	2.04706
R21	2.04285	0.00002	0.00003	-0.00002	0.00001	2.04287
R22	2.04562	0.00007	0.00005	0.00017	0.00017	2.04580
R23	1.84314	-0.00226	-0.00068	-0.00041	-0.00049	1.84265
R24	3.52909	-0.00089	0.02826	0.03886	0.05594	3.58503
R25	2.76532	0.00251	0.00289	-0.00994	-0.00369	2.76163
R26	2.72711	-0.00038	-0.00287	0.01810	0.00956	2.73667
R27	2.05027	0.00126	0.00091	-0.00468	-0.00237	2.04790
R28	2.04988	0.00089	0.00073	-0.00526	-0.00295	2.04693
R29	2.75129	-0.00367	-0.00795	0.01534	0.00266	2.75394
R30	2.05522	0.00030	0.00077	-0.00106	0.00003	2.05525
R31	2.84474	-0.00024	0.00034	0.01251	0.00910	2.85384
R32	2.06467	0.00035	0.00035	-0.00141	-0.00064	2.06403
R33	2.06777	0.00002	0.00013	-0.00034	-0.00011	2.06766
R34	2.06328	-0.00005	0.00010	-0.00111	-0.00068	2.06260
A1	1.87367	0.00005	0.00042	-0.00135	-0.00064	1.87303
A2	2.27749	-0.00006	0.00015	-0.00034	-0.00004	2.27745
A3	2.13201	0.00002	-0.00057	0.00171	0.00069	2.13270
A4	1.86202	-0.00035	-0.00021	0.00058	0.00035	1.86236
A5	2.27693	0.00021	0.00016	0.00021	0.00024	2.27717
A6	2.14413	0.00015	0.00007	-0.00076	-0.00053	2.14360
A7	1.90057	-0.00010	-0.00095	0.00140	-0.00040	1.90017
A8	2.24577	0.00042	0.00040	0.00130	0.00151	2.24728
A9	2.13682	-0.00032	0.00056	-0.00264	-0.00109	2.13574
A10	1.88438	0.00054	0.00126	-0.00075	0.00132	1.88570
A11	2.23907	-0.00121	0.00035	-0.00504	-0.00107	2.23801
A12	2.15797	0.00069	-0.00141	0.00615	0.00025	2.15822
A13	1.90377	-0.00010	-0.00046	0.00004	-0.00050	1.90327
A14	2.20108	0.00055	0.00242	0.00700	0.00841	2.20949
A15	2.17636	-0.00046	-0.00196	-0.00537	-0.00691	2.16945
A16	1.95370	-0.00082	-0.00208	0.01371	0.00613	1.95983

A17	1.85970	0.00042	0.00213	-0.00491	-0.00134	1.85836
A18	1.88488	0.00045	-0.00074	0.00522	0.00381	1.88869
A19	1.92725	0.00042	-0.00386	0.00816	0.00289	1.93014
A20	1.91685	-0.00007	0.00371	-0.00993	-0.00361	1.91323
A21	1.92027	-0.00040	0.00086	-0.01247	-0.00806	1.91221
A22	1.91213	0.00002	0.00159	0.00034	-0.00001	1.91212
A23	1.89830	0.00094	0.00093	0.00467	0.00461	1.90291
A24	1.91774	-0.00050	-0.00069	0.00140	0.00323	1.92097
A25	1.87586	0.00018	0.00649	-0.01330	-0.00252	1.87333
A26	1.88829	-0.00002	-0.00358	0.00978	0.00285	1.89114
A27	1.97058	-0.00060	-0.00456	-0.00314	-0.00819	1.96239
A28	1.73274	-0.00157	0.07706	-0.21483	-0.07574	1.65701
A29	2.84016	0.00102	-0.04327	0.16291	0.06739	2.90755
A30	2.17494	0.00032	0.00102	-0.00190	-0.00031	2.17463
A31	1.95541	-0.00011	0.00024	-0.00138	-0.00073	1.95468
A32	2.15283	-0.00020	-0.00125	0.00329	0.00105	2.15387
A33	2.08152	-0.00016	-0.00048	-0.00007	-0.00053	2.08099
A34	2.15414	0.00026	0.00092	-0.00051	0.00057	2.15471
A35	2.04753	-0.00010	-0.00044	0.00058	-0.00004	2.04749
A36	1.94312	-0.00180	-0.00806	-0.00083	-0.01023	1.93290
A37	2.99857	-0.00030	-0.09448	0.33606	0.13926	3.13782
A38	2.08693	0.00041	-0.00058	0.01114	0.00652	2.09345
A39	2.10364	0.00005	-0.00019	0.00646	0.00496	2.10860
A40	2.00150	0.00031	-0.00027	-0.00827	-0.00621	1.99530
A41	1.99161	0.00071	0.00171	-0.01313	-0.00731	1.98430
A42	2.01236	-0.00014	0.00104	-0.00543	-0.00293	2.00943
A43	2.05309	-0.00020	-0.00189	0.01882	0.01081	2.06390
A44	2.12854	0.00042	0.00251	-0.01042	-0.00429	2.12424
A45	1.95303	0.00017	0.00389	0.00554	0.00758	1.96061
A46	2.03507	-0.00001	0.00097	-0.00573	-0.00286	2.03222
A47	2.02569	-0.00026	-0.00254	-0.00807	-0.00816	2.01753
A48	1.24047	0.00133	-0.04850	0.20362	0.09519	1.33567
A49	1.23720	-0.00266	0.10901	-0.40168	-0.17302	1.06417
A50	2.43017	-0.00118	0.02345	-0.09278	-0.04131	2.38886
A51	2.26361	-0.00111	0.00335	-0.03550	-0.02090	2.24271
A52	1.93125	0.00046	-0.00071	-0.01116	-0.00854	1.92271
A53	1.91890	0.00001	0.00132	-0.00263	-0.00051	1.91839
A54	1.92415	0.00130	0.00276	-0.01481	-0.00761	1.91653
A55	1.88960	-0.00033	-0.00025	0.00875	0.00587	1.89547
A56	1.90154	-0.00086	-0.00288	0.01692	0.00893	1.91047
A57	1.89769	-0.00065	-0.00037	0.00377	0.00228	1.89997
A58	3.50408	0.00022	-0.04515	0.16813	0.07429	3.57837
A59	4.34376	0.00003	-0.16503	0.62390	0.27311	4.61687
D1	-0.02561	0.00145	0.00675	-0.00169	0.00538	-0.02023

D2	3.13140	0.00066	0.00360	-0.00422	0.00068	3.13208
D3	3.12050	0.00047	0.00450	-0.00717	-0.00068	3.11982
D4	-0.00567	-0.00033	0.00135	-0.00969	-0.00538	-0.01105
D5	0.02347	-0.00141	-0.00749	0.00642	-0.00292	0.02055
D6	-3.05303	-0.00132	-0.00738	-0.02083	-0.02214	-3.07517
D7	-3.12218	-0.00053	-0.00547	0.01133	0.00253	-3.11966
D8	0.08451	-0.00044	-0.00537	-0.01592	-0.01670	0.06781
D9	0.01932	-0.00101	-0.00380	-0.00351	-0.00605	0.01326
D10	-3.12986	-0.00066	-0.00281	0.00517	0.00109	-3.12876
D11	-3.13624	-0.00029	-0.00095	-0.00121	-0.00179	-3.13803
D12	-0.00223	0.00006	0.00004	0.00746	0.00536	0.00313
D13	-0.00486	0.00013	-0.00083	0.00755	0.00429	-0.00057
D14	3.07400	0.00048	0.00324	0.01433	0.01407	3.08808
D15	-3.13944	-0.00020	-0.00175	-0.00049	-0.00232	3.14143
D16	-0.06057	0.00015	0.00232	0.00629	0.00746	-0.05312
D17	0.10160	-0.00026	-0.01179	0.02564	0.00611	0.10771
D18	-3.03816	-0.00031	-0.01123	0.02087	0.00334	-3.03482
D19	-3.04849	0.00014	-0.01068	0.03538	0.01413	-3.03436
D20	0.09493	0.00009	-0.01012	0.03061	0.01136	0.10628
D21	-0.01132	0.00078	0.00510	-0.00863	-0.00090	-0.01222
D22	3.06631	0.00073	0.00519	0.01871	0.01848	3.08479
D23	-3.09378	0.00053	0.00120	-0.01454	-0.01006	-3.10384
D24	-0.01615	0.00049	0.00130	0.01280	0.00932	-0.00683
D25	-2.67798	-0.00009	-0.00406	-0.12080	-0.08755	-2.76553
D26	0.39193	0.00029	0.00067	-0.11336	-0.07636	0.31557
D27	1.21359	-0.00004	0.05776	-0.12833	-0.03305	1.18054
D28	-2.96108	0.00027	0.05319	-0.11346	-0.02675	-2.98784
D29	-0.89858	0.00026	0.05494	-0.12796	-0.03494	-0.93352
D30	-1.85316	0.00004	0.05780	-0.15996	-0.05540	-1.90856
D31	0.25536	0.00035	0.05323	-0.14509	-0.04911	0.20625
D32	2.31786	0.00034	0.05498	-0.15959	-0.05729	2.26057
D33	-0.83401	-0.00025	-0.04947	0.07371	0.00191	-0.83209
D34	1.21177	0.00052	-0.04013	0.06060	0.00153	1.21329
D35	-2.90629	0.00006	-0.04564	0.06070	-0.00352	-2.90982
D36	-2.90287	-0.00053	-0.04832	0.06567	-0.00230	-2.90517
D37	-0.85710	0.00024	-0.03898	0.05256	-0.00269	-0.85978
D38	1.30803	-0.00022	-0.04449	0.05266	-0.00774	1.30029
D39	1.25956	-0.00026	-0.04928	0.08248	0.00825	1.26781
D40	-2.97785	0.00050	-0.03994	0.06937	0.00787	-2.96999
D41	-0.81273	0.00005	-0.04545	0.06947	0.00282	-0.80991
D42	-1.71885	-0.00029	0.03757	-0.13990	-0.06306	-1.78191
D43	2.47744	-0.00001	0.03818	-0.14702	-0.06667	2.41077
D44	0.40363	0.00015	0.03521	-0.13505	-0.06046	0.34317
D45	-0.01574	-0.00010	-0.01673	0.19626	0.12593	0.11019

D46	-0.16136	-0.00062	0.03602	-0.23950	-0.12526	-0.28661
D47	-3.04248	-0.00076	0.08929	-0.49745	-0.25316	2.98755
D48	-3.13276	-0.00004	-0.00040	-0.00106	-0.00114	-3.13390
D49	0.01184	-0.00007	-0.00139	0.00095	-0.00072	0.01112
D50	0.00681	0.00002	-0.00102	0.00422	0.00193	0.00874
D51	-3.13178	-0.00002	-0.00201	0.00623	0.00236	-3.12942
D52	-2.76137	-0.00026	0.00553	0.06851	0.05732	-2.70404
D53	-2.97611	0.00031	-0.05506	0.11900	0.03092	-2.94519
D54	-2.59420	-0.00084	0.07722	-0.36885	-0.18111	-2.77531
D55	-1.03668	0.00028	0.10998	-0.50490	-0.24219	-1.27887
D56	-2.73258	-0.00037	0.00410	-0.01314	-0.00497	-2.73755
D57	-0.01584	-0.00053	-0.00156	-0.01387	-0.01114	-0.02697
D58	-0.03022	0.00043	0.00505	0.01706	0.01724	-0.01298
D59	2.68652	0.00027	-0.00061	0.01633	0.01107	2.69759
D60	0.50043	-0.00012	0.10616	-0.48655	-0.23618	0.26425
D61	0.11806	0.00048	0.01333	-0.08211	-0.04297	0.07509
D62	-1.87546	-0.00105	0.10286	-0.45389	-0.21675	-2.09221
D63	-2.25782	-0.00045	0.01002	-0.04945	-0.02354	-2.28137
D64	2.06798	0.00064	-0.02911	0.10597	0.04449	2.11246
D65	-0.32249	0.00086	-0.03075	0.11877	0.05184	-0.27065
D66	2.56094	0.00011	-0.01242	0.00429	-0.00937	2.55157
D67	-1.63579	0.00000	-0.01234	0.00643	-0.00779	-1.64358
D68	0.45621	0.00003	-0.01016	0.00010	-0.01006	0.44614
D69	1.36003	-0.00009	-0.01339	0.00222	-0.01186	1.34817
D70	-2.83670	-0.00020	-0.01330	0.00436	-0.01028	-2.84698
D71	-0.74470	-0.00017	-0.01113	-0.00197	-0.01256	-0.75726
D72	-0.99928	-0.00004	-0.01787	0.00971	-0.01108	-1.01036
D73	1.08717	-0.00015	-0.01779	0.01185	-0.00950	1.07767
D74	-3.10401	-0.00012	-0.01562	0.00552	-0.01177	-3.11579

Item	Value	Threshold	Converged?
Maximum Force	0.003936	0.000450	NO
RMS Force	0.000788	0.000300	NO
Maximum Displacement	0.757357	0.001800	NO
RMS Displacement	0.217989	0.001200	NO

Predicted change in Energy=-8.648920D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.395215	-1.817314	-0.289692
2	6	0	-2.595297	-1.184583	-0.286228

3	7	0	-2.362701	0.112096	0.163605
4	6	0	-1.045706	0.258745	0.408790
5	7	0	-0.442088	-0.898333	0.130269
6	6	0	1.017582	-1.115816	0.207188
7	6	0	1.659140	-1.276364	-1.185656
8	1	0	-1.139824	-2.829905	-0.550172
9	1	0	-3.573333	-1.542479	-0.551374
10	1	0	1.433422	-0.247639	0.723987
11	1	0	1.197800	-2.014480	0.799408
12	1	0	1.072940	-1.988983	-1.780297
13	1	0	1.627735	-0.312032	-1.707118
14	35	0	0.932611	2.700214	1.169598
15	1	0	-0.496298	1.186909	0.738164
16	6	0	-3.295470	1.166716	0.360048
17	6	0	-4.611322	1.039852	0.245331
18	1	0	-2.806325	2.098116	0.618261
19	1	0	-5.241061	1.903476	0.407272
20	1	0	-5.101652	0.106898	-0.001999
21	8	0	2.964985	-1.774898	-1.059681
22	1	0	3.619554	-1.060696	-1.170365
23	6	0	5.084250	1.676079	-0.903533
24	6	0	6.048334	0.636448	-0.549457
25	8	0	4.897947	0.324035	-1.387789
26	1	0	4.344300	1.996855	-0.179660
27	1	0	5.303016	2.392401	-1.686046
28	1	0	6.985045	0.593743	-1.100465
29	6	0	6.069949	0.008367	0.823755
30	1	0	6.362266	-1.041642	0.752941
31	1	0	6.791261	0.529307	1.460554
32	1	0	5.080622	0.080521	1.279118

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.356672	0.000000			
3	N	2.205478	1.392059	0.000000		
4	C	2.218120	2.228783	1.347626	0.000000	
5	N	1.389008	2.211722	2.170445	1.334451	0.000000
6	C	2.561362	3.647064	3.596662	2.487412	1.477786
7	C	3.228694	4.349440	4.463579	3.494998	2.507933
8	H	1.076297	2.212499	3.265009	3.235464	2.163517
9	H	2.210930	1.074685	2.171278	3.248880	3.268678
10	H	3.390076	4.257813	3.854086	2.549873	2.072062
11	H	2.819351	4.031739	4.195681	3.217679	2.093505

12	H	2.888453	4.041690	4.471791	3.785901	2.671159
13	H	3.662403	4.540294	4.427535	3.456897	2.829118
14	Br	5.287378	5.445843	4.309229	3.233163	3.989931
15	H	3.299985	3.328536	2.229080	1.127752	2.172720
16	C	3.596883	2.537030	1.421573	2.426566	3.529733
17	C	4.335089	3.048774	2.433866	3.653828	4.599164
18	H	4.259837	3.411561	2.085135	2.554788	3.847917
19	H	5.396348	4.125181	3.399025	4.506234	5.563902
20	H	4.186053	2.833818	2.743958	4.079522	4.768597
21	O	4.427869	5.644770	5.782855	4.730513	3.713825
22	H	5.147422	6.278647	6.240375	5.098951	4.267897
23	C	7.386749	8.218266	7.683873	6.427083	6.183588
24	C	7.841865	8.837296	8.457476	7.168424	6.703966
25	O	6.737586	7.722568	7.427566	6.209587	5.684599
26	H	6.892171	7.634848	6.975242	5.693809	5.602471
27	H	8.033543	8.782805	8.208789	7.017628	6.865433
28	H	8.757814	9.777953	9.445115	8.178205	7.674849
29	C	7.765407	8.817124	8.459086	7.132141	6.611328
30	H	7.865574	9.018772	8.820628	7.529110	6.834289
31	H	8.694157	9.700316	9.254791	7.911856	7.491939
32	H	6.928160	7.935397	7.526514	6.190406	5.725237

		6	7	8	9	10
6	C	0.000000				
7	C	1.541878	0.000000			
8	H	2.857639	3.263669	0.000000		
9	H	4.672682	5.277491	2.753077	0.000000	
10	H	1.092582	2.180816	3.861759	5.326420	0.000000
11	H	1.091238	2.167518	2.819712	4.981075	1.784078
12	H	2.171539	1.097750	2.667711	4.826746	3.071427
13	H	2.164006	1.096742	3.916324	5.468167	2.439707
14	Br	3.936437	4.678486	6.151002	6.423840	3.023114
15	H	2.806476	3.796671	4.267170	4.310524	2.404568
16	C	4.882185	5.736375	4.631230	2.871870	4.949269
17	C	6.027679	6.836028	5.259196	2.894926	6.198844
18	H	5.012046	5.880613	5.331778	3.900036	4.846566
19	H	6.951745	7.762833	6.335751	3.946508	7.019710
20	H	6.243702	7.001626	4.961995	2.314739	6.584827
21	O	2.414896	1.403437	4.268735	6.562164	2.803511
22	H	2.944647	1.972300	5.115312	7.235530	3.004796
23	C	5.056300	4.530771	7.692065	9.243207	4.435996
24	C	5.380651	4.829971	7.980302	9.865303	4.868335
25	O	4.435578	3.618287	6.863208	8.714703	4.097480
26	H	4.572245	4.351559	7.315088	8.680666	3.785174
27	H	5.852937	5.195003	8.370955	9.775497	5.268001

28	H	6.343750	5.645336	8.833894	10.786301	5.903987
29	C	5.212519	5.014329	7.869199	9.863519	4.644661
30	H	5.372988	5.092410	7.821595	10.033355	4.992473
31	H	6.132921	6.049920	8.844741	10.759413	5.463754
32	H	4.369044	4.429761	7.107097	8.993095	3.703772

		11	12	13	14	15
11	H	0.000000				
12	H	2.582851	0.000000			
13	H	3.060367	1.767856	0.000000		
14	Br	4.736634	5.541673	4.222833	0.000000	
15	H	3.622514	4.346429	3.568998	2.125561	0.000000
16	C	5.522908	5.798493	5.540561	4.569864	2.824667
17	C	6.586489	6.751877	6.675738	5.860568	4.147039
18	H	5.742759	6.124227	5.556716	3.827028	2.486142
19	H	7.547389	7.733260	7.520604	6.271376	4.809962
20	H	6.695192	6.758746	6.954681	6.671601	4.787855
21	O	2.576151	2.035916	2.085039	5.396930	4.897451
22	H	3.264139	2.778304	2.194526	5.180688	5.063047
23	C	5.623587	5.503817	4.067657	4.752139	5.837548
24	C	5.689863	5.758680	4.667064	5.777967	6.692771
25	O	4.893217	4.487180	3.346765	5.283024	5.861920
26	H	5.191324	5.399142	3.878635	3.735617	4.992975
27	H	6.515435	6.090891	4.563124	5.229713	6.400161
28	H	6.626051	6.487344	5.467104	6.798702	7.726765
29	C	5.275447	5.978343	5.122620	5.810154	6.671723
30	H	5.255501	5.940683	5.385165	6.607287	7.211557
31	H	6.180192	7.038756	6.115880	6.254700	7.352741
32	H	4.437956	5.450172	4.581935	4.907217	5.711283

		16	17	18	19	20
16	C	0.000000				
17	C	1.326922	0.000000			
18	H	1.083256	2.125326	0.000000		
19	H	2.080954	1.081038	2.451599	0.000000	
20	H	2.125226	1.082589	3.101322	1.847871	0.000000
21	O	7.061304	8.186959	7.150087	9.111617	8.350478
22	H	7.424357	8.611841	7.380325	9.475534	8.876248
23	C	8.489746	9.784109	8.047058	10.410666	10.345419
24	C	9.402928	10.696854	9.050140	11.400488	11.175971
25	O	8.420043	9.675002	8.156433	10.417118	10.097502
26	H	7.703668	9.016631	7.195719	9.603768	9.634807
27	H	8.923159	10.190864	8.435512	10.760976	10.785020
28	H	10.399537	11.682718	10.054257	12.388153	12.146270
29	C	9.448167	10.746538	9.121268	11.476230	11.202511
30	H	9.914791	11.180783	9.692228	11.976243	11.546017

31	H	10.166589	11.478515	9.761367	12.156254	11.989948
32	H	8.496082	9.794018	8.167702	10.517624	10.262585

		21	22	23	24	25
21	O	0.000000				
22	H	0.975088	0.000000			
23	C	4.052766	3.115521	0.000000		
24	C	3.947399	3.027342	1.461391	0.000000	
25	O	2.872197	1.897114	1.448184	1.457325	0.000000
26	H	4.111333	3.294748	1.083704	2.211603	2.136452
27	H	4.819243	3.876062	1.083191	2.220520	2.128657
28	H	4.666155	3.750811	2.196191	1.087594	2.123977
29	C	4.045759	3.335243	2.595456	1.510186	2.522729
30	H	3.919794	3.349916	3.429758	2.147272	2.931216
31	H	5.128482	4.416963	3.133350	2.145591	3.426344
32	H	3.659027	3.071980	2.703661	2.142243	2.684225

		26	27	28	29	30
26	H	0.000000				
27	H	1.828878	0.000000			
28	H	3.128919	2.531264	0.000000		
29	C	2.817586	3.545547	2.209680	0.000000	
30	H	3.764889	4.343192	2.549009	1.092238	0.000000
31	H	3.291142	3.948048	2.569148	1.094158	1.775565
32	H	2.518440	3.766490	3.090734	1.091481	1.782898

		31	32
31	H	0.000000	
32	H	1.777812	0.000000

Stoichiometry C10H17BrN2O2
Framework group C1[X(C10H17BrN2O2)]
Deg. of freedom 90
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.401565	2.347853	-0.314460
2	6	0	-3.587765	1.776070	0.011961
3	7	0	-3.370239	0.401897	0.058450
4	6	0	-2.074401	0.156110	-0.218115
5	7	0	-1.469621	1.325256	-0.437427
6	6	0	-0.024249	1.477983	-0.704681
7	6	0	0.722181	2.134856	0.473771

8	1	0	-2.142960	3.381078	-0.469327
9	1	0	-4.547601	2.220608	0.201823
10	1	0	0.363702	0.474225	-0.893619
11	1	0	0.094210	2.090055	-1.600302
12	1	0	0.173069	3.025480	0.805916
13	1	0	0.747555	1.433449	1.316521
14	35	0	-0.122656	-2.421091	-0.172633
15	1	0	-1.537597	-0.835683	-0.221942
16	6	0	-4.298315	-0.637000	0.341711
17	6	0	-5.602954	-0.458015	0.504811
18	1	0	-3.815930	-1.604537	0.409693
19	1	0	-6.229368	-1.311061	0.725176
20	1	0	-6.087402	0.506942	0.426278
21	8	0	2.005801	2.532507	0.069013
22	1	0	2.678562	1.901193	0.384656
23	6	0	4.161994	-0.759611	1.037361
24	6	0	5.078228	0.060629	0.247814
25	8	0	3.992419	0.678087	0.998521
26	1	0	3.372710	-1.315604	0.545104
27	1	0	4.453237	-1.137409	2.009857
28	1	0	6.054557	0.291503	0.667741
29	6	0	4.981564	0.133886	-1.257493
30	1	0	5.261451	1.130946	-1.604651
31	1	0	5.658921	-0.596323	-1.710443
32	1	0	3.960788	-0.088092	-1.573838

Rotational constants (GHZ): 0.5432681 0.1970733 0.1523192

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.

475 basis functions, 751 primitive gaussians, 492 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1263.9798971871 Hartrees.

NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 475 RedAO= T EigKep= 3.79D-06 NBF= 475

NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999827 0.017989 -0.000929 -0.004562 Ang= 2.13 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3225.51937871 A.U. after 12 cycles

NFock= 12 Conv=0.73D-08 -V/T= 2.0018

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000985967	0.001002932	-0.001452601
2	6	-0.000301346	-0.000604163	0.002434549
3	7	0.000654759	0.000248764	-0.000509659
4	6	0.003280447	0.001458525	-0.001588399
5	7	-0.000581029	-0.000208482	0.000239049
6	6	0.001387385	0.000244569	0.001025886
7	6	-0.004627143	0.002778436	-0.001687376
8	1	0.000014696	0.000158231	-0.000647543
9	1	-0.000052288	-0.000106657	0.000258014
10	1	-0.000218379	-0.000742951	0.000447742
11	1	0.000066625	-0.000231442	-0.000088299
12	1	0.000535359	-0.000316961	0.000554014
13	1	0.000538976	-0.000491415	0.000327152
14	35	0.002414802	0.000564392	-0.000241040
15	1	-0.003182164	-0.003410214	-0.001051287
16	6	-0.000296608	0.000330286	-0.000007882
17	6	0.000478322	-0.000002681	-0.000037332
18	1	-0.000087782	-0.000067082	0.000137789
19	1	-0.000012083	0.000022183	0.000022301

20	1	-0.000185755	0.000047533	-0.000071253
21	8	0.003753799	-0.000325895	0.000611543
22	1	-0.002149735	0.000862338	0.000957430
23	6	-0.004568648	0.000499747	-0.002814618
24	6	-0.002089185	-0.004343069	0.002371513
25	8	0.004019350	-0.000829314	0.002602345
26	1	-0.000959114	0.000866189	0.002364210
27	1	0.001858832	0.001316408	-0.001116658
28	1	-0.000231738	0.000974518	-0.000973899
29	6	-0.000736725	0.002375719	-0.005067405
30	1	-0.000185045	-0.000692984	0.001326935
31	1	-0.000128791	-0.000440449	0.000175650
32	1	0.000604235	-0.000937011	0.001499130

Cartesian Forces: Max 0.005067405 RMS 0.001614591

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.004237656 RMS 0.000917720

Search for a local minimum.

Step number 15 out of a maximum of 177

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 14 15

DE= -1.12D-03 DEPred=-8.65D-04 R= 1.29D+00

TightC=F SS= 1.41D+00 RLast= 7.07D-01 DXNew= 5.0454D+00 2.1208D+00

Trust test= 1.29D+00 RLast= 7.07D-01 DXMaxT set to 3.00D+00

ITU= 1 1 1 1 1 1 1 1 1 1 0 1 0 1 0

Eigenvalues ---	0.00101	0.00145	0.00234	0.00279	0.00419
Eigenvalues ---	0.00675	0.00963	0.01394	0.01443	0.01571
Eigenvalues ---	0.01701	0.01865	0.02054	0.02123	0.02167
Eigenvalues ---	0.02221	0.02318	0.02390	0.02670	0.02828
Eigenvalues ---	0.03061	0.03069	0.03331	0.03746	0.03969
Eigenvalues ---	0.04501	0.05011	0.05256	0.05612	0.05655
Eigenvalues ---	0.05909	0.06000	0.06565	0.09423	0.09793
Eigenvalues ---	0.10866	0.11113	0.11851	0.11931	0.12965
Eigenvalues ---	0.14087	0.15428	0.15581	0.15994	0.16000
Eigenvalues ---	0.16000	0.16001	0.16003	0.16014	0.16088
Eigenvalues ---	0.17208	0.17804	0.19545	0.22014	0.22199
Eigenvalues ---	0.22881	0.23550	0.23952	0.25016	0.26159
Eigenvalues ---	0.27755	0.29038	0.31282	0.32924	0.33055

Eigenvalues --- 0.33190 0.34090 0.34210 0.34545 0.34766
Eigenvalues --- 0.34958 0.35685 0.35690 0.35859 0.36434
Eigenvalues --- 0.36657 0.36892 0.37230 0.37385 0.37802
Eigenvalues --- 0.39038 0.42181 0.42543 0.45204 0.47264
Eigenvalues --- 0.49221 0.53207 0.54686 0.56248 0.60363
En-DIIS/RFO-DIIS IScMMF= 0 using points: 15 14 13 12 11
RFO step: Lambda=-3.73758171D-04.
EnCoef did 100 forward-backward iterations
DidBck=T Rises=F En-DIIS coefs: 0.73942 0.00000 0.00325 0.00100 0.25633
New curvilinear step failed, DQL= 6.19D+00 SP=-1.84D-01.
ITry= 1 IFail=1 DXMaxC= 0.00D+00 DCOld= 1.00D+10 DXMaxT= 3.00D+00 DXLimC= 3.00D+00 Rises=F
New curvilinear step failed, DQL= 6.20D+00 SP=-1.96D-01.
ITry= 2 IFail=1 DXMaxC= 0.00D+00 DCOld= 1.00D+10 DXMaxT= 3.00D+00 DXLimC= 3.00D+00 Rises=F
New curvilinear step failed, DQL= 6.21D+00 SP=-4.45D-02.
ITry= 3 IFail=1 DXMaxC= 0.00D+00 DCOld= 1.00D+10 DXMaxT= 3.00D+00 DXLimC= 3.00D+00 Rises=F
New curvilinear step failed, DQL= 6.23D+00 SP=-3.80D-02.
ITry= 4 IFail=1 DXMaxC= 0.00D+00 DCOld= 1.00D+10 DXMaxT= 3.00D+00 DXLimC= 3.00D+00 Rises=F
Iteration 1 RMS(Cart)= 0.07969274 RMS(Int)= 0.03505351
Iteration 2 RMS(Cart)= 0.02497046 RMS(Int)= 0.01727998
Iteration 3 RMS(Cart)= 0.02365226 RMS(Int)= 0.00356838
Iteration 4 RMS(Cart)= 0.00213067 RMS(Int)= 0.00330009
Iteration 5 RMS(Cart)= 0.00000332 RMS(Int)= 0.00330009
Iteration 6 RMS(Cart)= 0.00000002 RMS(Int)= 0.00330009
ITry= 5 IFail=0 DXMaxC= 4.69D-01 DCOld= 1.00D+10 DXMaxT= 3.00D+00 DXLimC= 3.00D+00 Rises=F

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56374	-0.00008	0.00023	0.00324	0.00239	2.56613
R2	2.62484	-0.00071	-0.00142	-0.00091	-0.00201	2.62283
R3	2.03391	0.00001	0.00006	-0.00022	-0.00007	2.03383
R4	2.63061	-0.00027	-0.00023	-0.00006	-0.00009	2.63052
R5	2.03086	0.00002	-0.00001	0.00021	0.00012	2.03098
R6	2.54664	-0.00059	0.00020	-0.00417	-0.00241	2.54424
R7	2.68638	0.00031	-0.00027	0.00178	0.00079	2.68718
R8	2.52175	-0.00105	-0.00135	-0.00427	-0.00537	2.51638
R9	2.13114	-0.00325	-0.01049	-0.00564	-0.01488	2.11627
R10	2.79261	-0.00118	0.00001	0.00253	0.00120	2.79381
R11	2.91373	-0.00149	-0.00194	0.00078	-0.00337	2.91036
R12	2.06468	-0.00046	-0.00097	-0.00158	-0.00191	2.06277

R13	2.06214	0.00015	0.00000	-0.00026	-0.00016	2.06198
R14	2.07445	-0.00038	-0.00084	-0.00213	-0.00212	2.07232
R15	2.07254	-0.00060	-0.00094	-0.00197	-0.00212	2.07042
R16	2.65211	0.00151	0.00211	0.01948	0.01342	2.66553
R17	4.01673	0.00134	0.04685	0.06934	0.08775	4.10447
R18	9.98347	-0.00202	-0.27426	-0.58945	-0.62640	9.35707
R19	2.50752	-0.00027	-0.00015	-0.00063	-0.00053	2.50698
R20	2.04706	-0.00007	-0.00030	0.00048	-0.00001	2.04705
R21	2.04287	0.00002	0.00004	0.00008	0.00009	2.04296
R22	2.04580	0.00006	0.00001	0.00060	0.00037	2.04616
R23	1.84265	-0.00260	-0.00038	-0.00305	-0.00199	1.84066
R24	3.58503	-0.00168	-0.03119	0.20492	0.09196	3.67699
R25	2.76163	0.00256	0.00495	-0.00150	0.00977	2.77140
R26	2.73667	-0.00003	-0.00599	0.01714	0.00169	2.73836
R27	2.04790	0.00249	0.00218	-0.00082	0.00169	2.04960
R28	2.04693	0.00205	0.00209	-0.00302	0.00028	2.04721
R29	2.75394	-0.00424	-0.00829	-0.00445	-0.01415	2.73979
R30	2.05525	0.00025	0.00050	0.00083	0.00100	2.05625
R31	2.85384	-0.00201	-0.00427	0.01381	0.00401	2.85785
R32	2.06403	0.00053	0.00096	0.00122	0.00170	2.06573
R33	2.06766	-0.00019	0.00044	0.00111	0.00111	2.06877
R34	2.06260	0.00002	0.00056	-0.00032	0.00037	2.06297
A1	1.87303	-0.00005	0.00071	-0.00131	-0.00040	1.87263
A2	2.27745	-0.00007	-0.00015	-0.00048	-0.00032	2.27713
A3	2.13270	0.00011	-0.00059	0.00177	0.00060	2.13330
A4	1.86236	-0.00022	-0.00047	0.00027	-0.00044	1.86193
A5	2.27717	0.00009	0.00010	0.00044	0.00038	2.27754
A6	2.14360	0.00014	0.00037	-0.00050	0.00008	2.14368
A7	1.90017	-0.00006	-0.00070	-0.00194	-0.00228	1.89789
A8	2.24728	0.00032	0.00007	0.00416	0.00274	2.25003
A9	2.13574	-0.00026	0.00063	-0.00221	-0.00051	2.13523
A10	1.88570	0.00017	0.00089	0.00416	0.00385	1.88955
A11	2.23801	-0.00143	-0.00030	0.00250	0.00268	2.24069
A12	2.15822	0.00127	-0.00056	-0.00514	-0.00574	2.15248
A13	1.90327	0.00018	-0.00045	-0.00044	-0.00054	1.90273
A14	2.20949	-0.00020	-0.00129	0.02332	0.01403	2.22352
A15	2.16945	0.00002	0.00125	-0.02140	-0.01302	2.15644
A16	1.95983	-0.00211	-0.00623	0.00315	-0.00397	1.95586
A17	1.85836	0.00060	0.00349	-0.00164	0.00251	1.86087
A18	1.88869	0.00066	-0.00174	0.00661	0.00204	1.89073
A19	1.93014	0.00088	-0.00199	0.00532	0.00126	1.93140
A20	1.91323	0.00043	0.00308	0.00229	0.00424	1.91748
A21	1.91221	-0.00045	0.00349	-0.01640	-0.00631	1.90591
A22	1.91212	0.00042	-0.00074	-0.00140	-0.00228	1.90984

A23	1.90291	0.00083	-0.00036	0.01118	0.00696	1.90986
A24	1.92097	-0.00211	-0.00100	0.00238	0.00060	1.92157
A25	1.87333	0.00011	0.00726	0.00272	0.00889	1.88222
A26	1.89114	0.00040	-0.00396	0.00151	-0.00316	1.88798
A27	1.96239	0.00042	-0.00110	-0.01631	-0.01088	1.95151
A28	1.65701	-0.00184	0.08195	-0.05933	0.05281	1.70981
A29	2.90755	0.00012	-0.06163	0.10008	-0.00261	2.90494
A30	2.17463	0.00021	0.00102	0.00031	0.00120	2.17583
A31	1.95468	-0.00005	0.00038	-0.00163	-0.00060	1.95408
A32	2.15387	-0.00016	-0.00140	0.00132	-0.00061	2.15326
A33	2.08099	-0.00013	-0.00034	-0.00195	-0.00151	2.07948
A34	2.15471	0.00025	0.00078	0.00310	0.00264	2.15734
A35	2.04749	-0.00012	-0.00044	-0.00115	-0.00113	2.04636
A36	1.93290	-0.00180	-0.00254	-0.02713	-0.01621	1.91668
A37	3.13782	-0.00085	-0.13163	0.21879	-0.00766	3.13016
A38	2.09345	0.00005	-0.00364	0.00635	0.00508	2.09852
A39	2.10860	-0.00019	-0.00271	0.00181	-0.00596	2.10263
A40	1.99530	0.00110	0.00224	-0.00056	0.00032	1.99562
A41	1.98430	0.00066	0.00439	-0.01029	0.00098	1.98528
A42	2.00943	0.00011	0.00296	-0.00012	0.00276	2.01219
A43	2.06390	-0.00095	-0.00605	0.01507	-0.00312	2.06079
A44	2.12424	0.00038	0.00422	-0.00505	0.00811	2.13235
A45	1.96061	-0.00073	0.00036	0.01452	0.01097	1.97158
A46	2.03222	0.00023	0.00166	-0.00035	0.00005	2.03227
A47	2.01753	0.00053	0.00103	-0.01622	-0.00907	2.00845
A48	1.33567	0.00076	-0.07649	0.17999	0.02981	1.36548
A49	1.06417	-0.00205	0.15255	-0.28537	-0.02877	1.03540
A50	2.38886	-0.00118	0.03338	-0.06430	0.00665	2.39551
A51	2.24271	-0.00112	0.01216	-0.05502	-0.01618	2.22653
A52	1.92271	0.00150	0.00365	-0.01200	-0.00353	1.91918
A53	1.91839	-0.00012	0.00106	0.00168	0.00209	1.92048
A54	1.91653	0.00236	0.00711	-0.00537	0.00393	1.92046
A55	1.89547	-0.00090	-0.00329	0.00613	0.00039	1.89587
A56	1.91047	-0.00180	-0.00707	0.01089	-0.00050	1.90998
A57	1.89997	-0.00112	-0.00186	-0.00101	-0.00243	1.89754
A58	3.57837	-0.00036	-0.06433	0.12497	0.01364	3.59201
A59	4.61687	-0.00018	-0.23258	0.44785	0.05269	4.66956
D1	-0.02023	0.00117	0.01149	0.03096	0.03006	0.00983
D2	3.13208	0.00055	0.00553	0.00862	0.01096	-3.14014
D3	3.11982	0.00041	0.00778	0.01234	0.01478	3.13460
D4	-0.01105	-0.00021	0.00182	-0.00999	-0.00432	-0.01537
D5	0.02055	-0.00122	-0.01134	-0.02916	-0.02921	-0.00866
D6	-3.07517	-0.00106	-0.00279	-0.06346	-0.04187	-3.11704
D7	-3.11966	-0.00054	-0.00801	-0.01243	-0.01546	-3.13512

D8	0.06781	-0.00038	0.00054	-0.04673	-0.02813	0.03968
D9	0.01326	-0.00072	-0.00785	-0.02258	-0.02101	-0.00775
D10	-3.12876	-0.00049	-0.00704	-0.00656	-0.01076	-3.13952
D11	-3.13803	-0.00016	-0.00245	-0.00235	-0.00372	3.14143
D12	0.00313	0.00006	-0.00164	0.01366	0.00653	0.00965
D13	-0.00057	-0.00004	0.00086	0.00460	0.00299	0.00242
D14	3.08808	0.00041	0.00148	0.03632	0.02353	3.11161
D15	3.14143	-0.00025	0.00011	-0.01018	-0.00645	3.13498
D16	-0.05312	0.00020	0.00074	0.02154	0.01409	-0.03902
D17	0.10771	-0.00028	-0.01435	-0.00960	-0.02001	0.08770
D18	-3.03482	-0.00031	-0.01309	-0.01648	-0.02288	-3.05771
D19	-3.03436	-0.00003	-0.01344	0.00834	-0.00853	-3.04289
D20	0.10628	-0.00005	-0.01218	0.00146	-0.01140	0.09489
D21	-0.01222	0.00077	0.00640	0.01494	0.01601	0.00379
D22	3.08479	0.00061	-0.00205	0.04970	0.02894	3.11373
D23	-3.10384	0.00045	0.00581	-0.01526	-0.00355	-3.10739
D24	-0.00683	0.00028	-0.00265	0.01950	0.00937	0.00254
D25	-2.76553	-0.00020	0.02975	-0.27831	-0.13340	-2.89893
D26	0.31557	0.00027	0.03050	-0.24178	-0.10974	0.20583
D27	1.18054	-0.00003	0.05719	0.03661	0.07918	1.25972
D28	-2.98784	0.00019	0.05332	0.04396	0.08002	-2.90782
D29	-0.93352	0.00031	0.05836	0.02728	0.07500	-0.85852
D30	-1.90856	0.00015	0.06708	-0.00341	0.06437	-1.84419
D31	0.20625	0.00037	0.06320	0.00393	0.06520	0.27145
D32	2.26057	0.00049	0.06825	-0.01274	0.06019	2.32076
D33	-0.83209	-0.00040	-0.03812	-0.07664	-0.08408	-0.91617
D34	1.21329	0.00044	-0.02999	-0.06771	-0.07061	1.14268
D35	-2.90982	0.00013	-0.03225	-0.07908	-0.07919	-2.98900
D36	-2.90517	-0.00038	-0.03720	-0.08021	-0.08549	-2.99066
D37	-0.85978	0.00047	-0.02906	-0.07128	-0.07203	-0.93181
D38	1.30029	0.00016	-0.03133	-0.08265	-0.08060	1.21969
D39	1.26781	-0.00065	-0.04228	-0.06468	-0.08120	1.18661
D40	-2.96999	0.00019	-0.03414	-0.05575	-0.06774	-3.03773
D41	-0.80991	-0.00012	-0.03641	-0.06712	-0.07631	-0.88622
D42	-1.78191	-0.00004	0.05111	-0.09510	-0.00753	-1.78943
D43	2.41077	0.00046	0.05495	-0.09573	-0.00319	2.40758
D44	0.34317	-0.00019	0.04920	-0.09027	-0.00564	0.33753
D45	0.11019	-0.00010	-0.06219	0.35347	0.15942	0.26961
D46	-0.28661	-0.00007	0.07909	-0.21903	-0.05618	-0.34279
D47	2.98755	-0.00060	0.16429	-0.45361	-0.09576	2.89179
D48	-3.13390	-0.00003	-0.00031	-0.00526	-0.00347	-3.13737
D49	0.01112	-0.00007	-0.00131	-0.00494	-0.00427	0.00685
D50	0.00874	-0.00001	-0.00171	0.00238	-0.00028	0.00846
D51	-3.12942	-0.00005	-0.00271	0.00271	-0.00108	-3.13050

D52	-2.70404	-0.00002	-0.02022	0.18443	0.09499	-2.60905
D53	-2.94519	0.00030	-0.05499	-0.05249	-0.07057	-3.01575
D54	-2.77531	-0.00080	0.12417	-0.39318	-0.12252	-2.89783
D55	-1.27887	0.00047	0.17759	-0.50034	-0.12326	-1.40213
D56	-2.73755	-0.00002	0.00572	0.00816	0.00992	-2.72763
D57	-0.02697	-0.00001	0.00374	-0.01193	-0.00306	-0.03003
D58	-0.01298	-0.00005	-0.00247	0.03042	0.01582	0.00283
D59	2.69759	-0.00005	-0.00445	0.01033	0.00284	2.70043
D60	0.26425	0.00035	0.16914	-0.42479	-0.07686	0.18739
D61	0.07509	0.00132	0.03237	-0.08312	-0.02202	0.05307
D62	-2.09221	-0.00171	0.15696	-0.41291	-0.08252	-2.17473
D63	-2.28137	-0.00074	0.02019	-0.07124	-0.02768	-2.30905
D64	2.11246	0.00099	-0.03942	0.06628	-0.00523	2.10723
D65	-0.27065	0.00073	-0.04338	0.07556	-0.00362	-0.27427
D66	2.55157	0.00042	-0.00774	-0.03843	-0.03089	2.52068
D67	-1.64358	0.00017	-0.00884	-0.03731	-0.03130	-1.67488
D68	0.44614	0.00019	-0.00593	-0.04086	-0.03053	0.41561
D69	1.34817	-0.00020	-0.00752	-0.04694	-0.03519	1.31298
D70	-2.84698	-0.00044	-0.00862	-0.04582	-0.03560	-2.88258
D71	-0.75726	-0.00043	-0.00571	-0.04937	-0.03483	-0.79209
D72	-1.01036	0.00008	-0.01134	-0.05086	-0.04229	-1.05265
D73	1.07767	-0.00016	-0.01244	-0.04975	-0.04270	1.03498
D74	-3.11579	-0.00015	-0.00954	-0.05330	-0.04193	3.12547

Item	Value	Threshold	Converged?
Maximum Force	0.004238	0.000450	NO
RMS Force	0.000918	0.000300	NO
Maximum Displacement	0.468655	0.001800	NO
RMS Displacement	0.118173	0.001200	NO

Predicted change in Energy=-1.068467D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.441167	-1.863779	-0.300702
2	6	0	-2.613015	-1.178824	-0.260737
3	7	0	-2.305942	0.114555	0.152260
4	6	0	-0.978957	0.197388	0.364189
5	7	0	-0.438959	-0.990422	0.098311
6	6	0	1.010488	-1.267601	0.187763
7	6	0	1.665306	-1.377356	-1.201863
8	1	0	-1.239335	-2.888100	-0.562165

9	1	0	-3.613954	-1.494133	-0.492655
10	1	0	1.450723	-0.446987	0.757245
11	1	0	1.148276	-2.200181	0.737241
12	1	0	1.109203	-2.100011	-1.811052
13	1	0	1.616337	-0.405617	-1.705558
14	35	0	1.180613	2.529331	1.138234
15	1	0	-0.379087	1.089956	0.676617
16	6	0	-3.179024	1.218478	0.355105
17	6	0	-4.501334	1.161309	0.264562
18	1	0	-2.637054	2.124111	0.599094
19	1	0	-5.079919	2.058856	0.433069
20	1	0	-5.047454	0.256054	0.030707
21	8	0	2.993100	-1.836713	-1.077078
22	1	0	3.611385	-1.090769	-1.177271
23	6	0	4.985578	1.749868	-0.913847
24	6	0	5.968488	0.736075	-0.517714
25	8	0	4.861628	0.385499	-1.386034
26	1	0	4.207898	2.056074	-0.222610
27	1	0	5.216577	2.462944	-1.696011
28	1	0	6.928843	0.726514	-1.029217
29	6	0	5.969151	0.109590	0.858729
30	1	0	6.265493	-0.940409	0.790689
31	1	0	6.679028	0.631852	1.508176
32	1	0	4.973554	0.178061	1.301280

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357936	0.000000			
3	N	2.206087	1.392009	0.000000		
4	C	2.214527	2.225901	1.346352	0.000000	
5	N	1.387943	2.211545	2.170141	1.331609	0.000000
6	C	2.569948	3.652233	3.593094	2.476936	1.478420
7	C	3.270913	4.385107	4.453118	3.453182	2.503618
8	H	1.076258	2.213477	3.265577	3.232053	2.162871
9	H	2.212350	1.074749	2.171334	3.246327	3.268572
10	H	3.389628	4.252745	3.846279	2.544220	2.073744
11	H	2.809929	4.023237	4.199027	3.226860	2.095486
12	H	2.973441	4.136057	4.519083	3.790795	2.696972
13	H	3.667177	4.535722	4.371080	3.373873	2.796459
14	Br	5.314479	5.486268	4.354233	3.271215	4.011623
15	H	3.287509	3.319100	2.222414	1.119880	2.160091
16	C	3.598686	2.539032	1.421993	2.425491	3.528901
17	C	4.339966	3.052525	2.434759	3.653247	4.600052

18	H	4.259466	3.413102	2.085092	2.552788	3.844831
19	H	5.400556	4.129110	3.399133	4.504186	5.563153
20	H	4.196288	2.840829	2.747851	4.082563	4.774568
21	O	4.501801	5.703310	5.779149	4.689568	3.725154
22	H	5.185962	6.292133	6.183464	5.010658	4.247643
23	C	7.398476	8.169602	7.548317	6.294382	6.161108
24	C	7.855528	8.796309	8.324742	7.023882	6.664507
25	O	6.779559	7.719046	7.335790	6.100089	5.673857
26	H	6.876284	7.549229	6.807358	5.540984	5.565735
27	H	8.061822	8.753570	8.094401	6.910991	6.865159
28	H	8.791895	9.760529	9.330147	8.047040	7.648771
29	C	7.755725	8.750244	8.305196	6.966239	6.546154
30	H	7.838134	8.943726	8.659678	7.345647	6.740293
31	H	8.685492	9.630662	9.101416	7.755140	7.435403
32	H	6.919833	7.863654	7.369894	6.025852	5.666373

		6	7	8	9	10
6	C	0.000000				
7	C	1.540095	0.000000			
8	H	2.872300	3.335941	0.000000		
9	H	4.679717	5.327965	2.754413	0.000000	
10	H	1.091570	2.179390	3.864750	5.320688	0.000000
11	H	1.091154	2.168983	2.803992	4.968902	1.779204
12	H	2.167466	1.096627	2.774245	4.941000	3.073317
13	H	2.166733	1.095620	3.952839	5.478316	2.468712
14	Br	3.917785	4.579649	6.172201	6.468070	3.012736
15	H	2.779923	3.714278	4.254355	4.302218	2.391003
16	C	4.874485	5.712272	4.633332	2.875086	4.936603
17	C	6.023760	6.828080	5.265152	2.900377	6.185170
18	H	4.997746	5.832154	5.331454	3.903580	4.831715
19	H	6.943958	7.744587	6.341368	3.953447	7.002401
20	H	6.248588	7.017721	4.973828	2.322064	6.576353
21	O	2.419599	1.410537	4.391361	6.641692	2.770380
22	H	2.942661	1.967222	5.209438	7.268902	2.970736
23	C	5.110774	4.570196	7.770712	9.200701	4.484854
24	C	5.393902	4.842729	8.067796	9.838580	4.841008
25	O	4.476701	3.654866	6.972586	8.727350	4.113508
26	H	4.630189	4.383167	7.364272	8.594083	3.850642
27	H	5.929313	5.253914	8.461565	9.751144	5.354234
28	H	6.362741	5.671058	8.944424	10.787481	5.880336
29	C	5.189912	4.998012	7.935197	9.809897	4.553709
30	H	5.299590	5.032186	7.870588	9.977828	4.840102
31	H	6.122398	6.043065	8.909368	10.699001	5.391007
32	H	4.362998	4.430525	7.174521	8.930830	3.618977

		11	12	13	14	15

11	H	0.000000				
12	H	2.550560	0.000000			
13	H	3.067052	1.771803	0.000000		
14	Br	4.746591	5.489462	4.109857	0.000000	
15	H	3.627880	4.310382	3.448654	2.171993	0.000000
16	C	5.528000	5.838964	5.466215	4.619314	2.821265
17	C	6.590989	6.813406	6.615325	5.909256	4.143404
18	H	5.748679	6.138929	5.459146	3.876784	2.484733
19	H	7.551313	7.787007	7.448973	6.317662	4.805819
20	H	6.702190	6.844526	6.917986	6.721846	4.786046
21	O	2.612898	2.038899	2.082906	5.220637	4.797133
22	H	3.311051	2.771491	2.174566	4.937139	4.910839
23	C	5.749249	5.536499	4.077341	4.392762	5.634243
24	C	5.781951	5.773106	4.653563	5.374167	6.468645
25	O	4.998302	4.520961	3.355573	4.951547	5.675904
26	H	5.329006	5.422001	3.869786	3.352659	4.773094
27	H	6.649551	6.140384	4.603310	4.932175	6.231045
28	H	6.715719	6.516803	5.473745	6.402355	7.513176
29	C	5.347021	5.969016	5.078188	5.372464	6.426073
30	H	5.270274	5.890760	5.303951	6.165702	6.948801
31	H	6.261307	7.035858	6.085660	5.828366	7.121681
32	H	4.539485	5.459801	4.544519	4.465586	5.465576

		16	17	18	19	20
16	C	0.000000				
17	C	1.326639	0.000000			
18	H	1.083251	2.124722	0.000000		
19	H	2.079835	1.081086	2.449370	0.000000	
20	H	2.126623	1.082784	3.102052	1.847443	0.000000
21	O	7.034234	8.182583	7.084935	9.090084	8.381966
22	H	7.334198	8.542070	7.248029	9.383608	8.845826
23	C	8.279695	9.577920	7.780332	10.159915	10.187511
24	C	9.201712	10.507614	8.788017	11.167857	11.040025
25	O	8.269069	9.538941	7.949448	10.244198	10.010684
26	H	7.456671	8.768618	6.894432	9.310932	9.432167
27	H	8.731660	9.998794	8.189128	10.522076	10.639654
28	H	10.214077	11.511380	9.803625	12.170611	12.032309
29	C	9.228888	10.539934	8.842650	11.227768	11.048649
30	H	9.697908	10.982649	9.417182	11.740606	11.401397
31	H	9.942580	11.261767	9.478536	11.893907	11.825164
32	H	8.272983	9.582018	7.886794	10.264672	10.101536

		21	22	23	24	25
21	O	0.000000				
22	H	0.974037	0.000000			
23	C	4.106115	3.166546	0.000000		

24	C	3.973042	3.054228	1.466563	0.000000	
25	O	2.919773	1.945779	1.449078	1.449835	0.000000
26	H	4.166490	3.342129	1.084600	2.220171	2.138162
27	H	4.879957	3.933778	1.083337	2.221673	2.130224
28	H	4.697074	3.785494	2.199282	1.088122	2.125321
29	C	4.048744	3.338445	2.607672	1.512310	2.518272
30	H	3.873044	3.307531	3.432377	2.147261	2.909809
31	H	5.134532	4.426000	3.159735	2.149409	3.426381
32	H	3.692980	3.099782	2.716157	2.147094	2.697631

		26	27	28	29	30
26	H	0.000000				
27	H	1.831362	0.000000			
28	H	3.133989	2.528173	0.000000		
29	C	2.839033	3.554060	2.205889	0.000000	
30	H	3.773510	4.343583	2.555528	1.093135	0.000000
31	H	3.336242	3.969694	2.551417	1.094744	1.777021
32	H	2.536809	3.776705	3.091144	1.091675	1.783475

		31	32
31	H	0.000000	
32	H	1.776900	0.000000

Stoichiometry C10H17BrN2O2
Framework group C1[X(C10H17BrN2O2)]
Deg. of freedom 90
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.576781	2.278202	-0.303283
2	6	0	-3.716986	1.609259	0.007262
3	7	0	-3.381634	0.260191	0.079686
4	6	0	-2.069875	0.125350	-0.191917
5	7	0	-1.566339	1.335042	-0.429148
6	6	0	-0.140168	1.581810	-0.730589
7	6	0	0.602589	2.212073	0.462296
8	1	0	-2.403314	3.329211	-0.456971
9	1	0	-4.712762	1.972403	0.185146
10	1	0	0.296173	0.615130	-0.988780
11	1	0	-0.081891	2.244364	-1.595599
12	1	0	0.057838	3.100835	0.802795
13	1	0	0.631446	1.497525	1.292340

14	35	0	0.133319	-2.292532	-0.217052
15	1	0	-1.453657	-0.809726	-0.198349
16	6	0	-4.216567	-0.853449	0.370819
17	6	0	-5.530824	-0.787596	0.539227
18	1	0	-3.652795	-1.776048	0.437192
19	1	0	-6.079073	-1.692301	0.762112
20	1	0	-6.099407	0.130809	0.463947
21	8	0	1.896992	2.612760	0.070398
22	1	0	2.553251	1.967839	0.390005
23	6	0	4.031223	-0.744070	1.088693
24	6	0	4.938677	0.064385	0.267879
25	8	0	3.879272	0.695827	1.030090
26	1	0	3.222499	-1.298176	0.624700
27	1	0	4.346647	-1.110387	2.058197
28	1	0	5.930376	0.279158	0.660834
29	6	0	4.817367	0.132482	-1.238019
30	1	0	5.070663	1.136702	-1.587773
31	1	0	5.503712	-0.582935	-1.702317
32	1	0	3.797878	-0.111799	-1.542522

Rotational constants (GHZ): 0.5612566 0.2024467 0.1573615

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.

475 basis functions, 751 primitive gaussians, 492 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1273.0273552407 Hartrees.

NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 475 RedAO= T EigKep= 3.77D-06 NBF= 475

NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999790 -0.006304 0.000459 -0.019475 Ang= -2.35 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3225.52085213 A.U. after 12 cycles
NFock= 12 Conv=0.96D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000088110	-0.000113560	0.001102040
2	6	0.000887938	0.000054450	-0.000544879
3	7	-0.000126004	-0.000122029	0.000566124
4	6	0.002625156	0.002279437	-0.000367954
5	7	0.001123054	-0.000395138	-0.000562552
6	6	0.001954399	-0.000793145	-0.000169760
7	6	-0.000081787	0.000867515	-0.001214360
8	1	-0.000022754	-0.000061543	-0.000131429
9	1	0.000063928	-0.000029977	-0.000027609
10	1	0.000020352	0.000315438	-0.000165053
11	1	-0.000444026	-0.000395836	-0.000223362
12	1	0.000108804	-0.000237961	-0.000185715
13	1	-0.000397742	-0.000043279	0.000521013
14	35	0.001191040	-0.000759439	-0.000671770
15	1	-0.002234815	-0.000832750	-0.000161819
16	6	-0.000187662	0.000093173	0.000196883
17	6	0.000145738	0.000013099	-0.000160296
18	1	-0.000141357	-0.000070644	0.000069317
19	1	-0.000028706	0.000012634	0.000002019
20	1	0.000022311	0.000068901	-0.000038631
21	8	-0.000408847	0.001346496	0.000479921
22	1	-0.000758680	0.000811138	0.001102666
23	6	-0.002946682	-0.001539305	-0.000709248
24	6	-0.001820013	-0.001883823	0.004327695
25	8	0.002112299	-0.001871587	0.000632172

26	1	-0.000882866	0.000398943	0.002219790
27	1	0.001798092	0.001145064	-0.001297992
28	1	-0.000566423	0.000491824	-0.001763225
29	6	-0.001042321	0.002921916	-0.005055453
30	1	-0.000114183	-0.000268193	0.001316459
31	1	-0.000300408	-0.000594398	-0.000218844
32	1	0.000540274	-0.000807419	0.001133854

Cartesian Forces: Max 0.005055453 RMS 0.001200784

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.003097955 RMS 0.000888581
Search for a local minimum.
Step number 16 out of a maximum of 177
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 15 16
DE= -1.47D-03 DEPred=-1.07D-03 R= 1.38D+00
TightC=F SS= 1.41D+00 RLast= 8.06D-01 DXNew= 5.0454D+00 2.4189D+00
Trust test= 1.38D+00 RLast= 8.06D-01 DXMaxT set to 3.00D+00
ITU= 1 1 1 1 1 1 1 1 1 1 1 0 1 0 1 0

Eigenvalues ---	0.00067	0.00171	0.00233	0.00268	0.00418
Eigenvalues ---	0.00652	0.00972	0.01347	0.01438	0.01531
Eigenvalues ---	0.01614	0.01861	0.02055	0.02103	0.02185
Eigenvalues ---	0.02224	0.02319	0.02389	0.02628	0.02945
Eigenvalues ---	0.03061	0.03068	0.03528	0.03657	0.03889
Eigenvalues ---	0.04519	0.05087	0.05285	0.05606	0.05639
Eigenvalues ---	0.05809	0.05984	0.06668	0.09405	0.09561
Eigenvalues ---	0.10852	0.11307	0.11845	0.12248	0.13050
Eigenvalues ---	0.14012	0.15360	0.15518	0.15960	0.15996
Eigenvalues ---	0.16000	0.16001	0.16003	0.16006	0.16081
Eigenvalues ---	0.16678	0.17777	0.19570	0.21734	0.22039
Eigenvalues ---	0.22902	0.23541	0.24257	0.25059	0.25243
Eigenvalues ---	0.27739	0.29703	0.30940	0.32827	0.33060
Eigenvalues ---	0.33163	0.34100	0.34187	0.34593	0.34767
Eigenvalues ---	0.34980	0.35598	0.35686	0.35706	0.35859
Eigenvalues ---	0.36438	0.36660	0.37225	0.37300	0.37784
Eigenvalues ---	0.37892	0.42181	0.42505	0.45195	0.47678
Eigenvalues ---	0.49881	0.52764	0.54497	0.56931	0.60356

En-DIIS/RFO-DIIS IScMMF= 0 using points: 16 15 14 13 12

RFO step: Lambda=-4.17005111D-04.
DidBck=F Rises=F En-DIIS coefs: 1.00000 0.00000 0.00000 0.00000 0.00000
New curvilinear step failed, DQL= 6.23D+00 SP=-1.20D-01.
ITry= 1 IFail=1 DXMaxC= 0.00D+00 DCOld= 1.00D+10 DXMaxT= 3.00D+00 DXLimC= 3.00D+00 Rises=F
New curvilinear step failed, DQL= 6.22D+00 SP=-1.40D-01.
ITry= 2 IFail=1 DXMaxC= 0.00D+00 DCOld= 1.00D+10 DXMaxT= 3.00D+00 DXLimC= 3.00D+00 Rises=F
New curvilinear step failed, DQL= 6.21D+00 SP=-1.58D-01.
ITry= 3 IFail=1 DXMaxC= 0.00D+00 DCOld= 1.00D+10 DXMaxT= 3.00D+00 DXLimC= 3.00D+00 Rises=F
New curvilinear step failed, DQL= 6.20D+00 SP=-1.73D-01.
ITry= 4 IFail=1 DXMaxC= 0.00D+00 DCOld= 1.00D+10 DXMaxT= 3.00D+00 DXLimC= 3.00D+00 Rises=F
New curvilinear step failed, DQL= 6.19D+00 SP=-1.91D-01.
ITry= 5 IFail=1 DXMaxC= 0.00D+00 DCOld= 1.00D+10 DXMaxT= 3.00D+00 DXLimC= 3.00D+00 Rises=F
New curvilinear step failed, DQL= 6.19D+00 SP=-2.11D-01.
ITry= 6 IFail=1 DXMaxC= 0.00D+00 DCOld= 1.00D+10 DXMaxT= 3.00D+00 DXLimC= 3.00D+00 Rises=F
New curvilinear step failed, DQL= 6.17D+00 SP=-1.19D-01.
ITry= 7 IFail=1 DXMaxC= 0.00D+00 DCOld= 1.00D+10 DXMaxT= 3.00D+00 DXLimC= 3.00D+00 Rises=F
New curvilinear step failed, DQL= 6.15D+00 SP=-1.70D-01.
ITry= 8 IFail=1 DXMaxC= 0.00D+00 DCOld= 1.00D+10 DXMaxT= 3.00D+00 DXLimC= 3.00D+00 Rises=F
New curvilinear step failed, DQL= 6.19D+00 SP=-1.81D-01.
ITry= 9 IFail=1 DXMaxC= 0.00D+00 DCOld= 1.00D+10 DXMaxT= 3.00D+00 DXLimC= 3.00D+00 Rises=F
New curvilinear step failed, DQL= 6.23D+00 SP=-1.95D-01.
ITry=10 IFail=1 DXMaxC= 0.00D+00 DCOld= 1.00D+10 DXMaxT= 3.00D+00 DXLimC= 3.00D+00 Rises=F
RedQX1 iteration 1 Try 1 RMS(Cart)= 0.12902103 RMS(Int)= 0.54022596 XScale= 0.38489970
RedQX1 iteration 2 Try 1 RMS(Cart)= 0.02580421 RMS(Int)= 0.17403451 XScale= 13.95862654
RedQX1 iteration 2 Try 2 RMS(Cart)= 0.02580297 RMS(Int)= 0.55072618 XScale= 0.38175528
RedQX1 iteration 3 Try 1 RMS(Cart)= 0.02477085 RMS(Int)= 0.55088601 XScale= 0.38170805
RedQX1 iteration 4 Try 1 RMS(Cart)= 0.00495417 RMS(Int)= 0.23771362 XScale= 0.76331983
RedQX1 iteration 5 Try 1 RMS(Cart)= 0.00099083 RMS(Int)= 0.17283416 XScale=

11.57664337
RedQX1 iteration 5 Try 2 RMS(Cart)= 0.00099082 RMS(Int)= 0.17112732 XScale= 9.01487982
RedQX1 iteration 5 Try 3 RMS(Cart)= 0.00099078 RMS(Int)= 0.16840367 XScale= 6.26018799
RedQX1 iteration 5 Try 4 RMS(Cart)= 0.00099072 RMS(Int)= 0.16390457 XScale= 3.34556956
RedQX1 iteration 5 Try 5 RMS(Cart)= 0.00099054 RMS(Int)= 0.23720062 XScale= 0.76555435
RedQX1 iteration 6 Try 1 RMS(Cart)= 0.00098420 RMS(Int)= 0.23520094 XScale= 0.77443973
RedQX1 iteration 7 Try 1 RMS(Cart)= 0.00019684 RMS(Int)= 0.16327570 XScale= 2.76766814
RedQX1 iteration 7 Try 2 RMS(Cart)= 0.00019682 RMS(Int)= 0.16390131 XScale= 2.19706644
RedQX1 iteration 7 Try 3 RMS(Cart)= 0.00019680 RMS(Int)= 0.16876827 XScale= 1.64749030
RedQX1 iteration 7 Try 4 RMS(Cart)= 0.00019676 RMS(Int)= 0.18699412 XScale= 1.15157876
RedQX1 iteration 7 Try 5 RMS(Cart)= 0.00019670 RMS(Int)= 0.23478475 XScale= 0.77632261
RedQX1 iteration 8 Try 1 RMS(Cart)= 0.00019644 RMS(Int)= 0.23470311 XScale= 0.77669365
RedQX1 iteration 9 Try 1 RMS(Cart)= 0.00003929 RMS(Int)= 0.19372293 XScale= 1.06467179
RedQX1 iteration 9 Try 2 RMS(Cart)= 0.00003929 RMS(Int)= 0.20184068 XScale= 0.98311396
RedQX1 iteration 10 Try 1 RMS(Cart)= 0.00003928 RMS(Int)= 0.20184011 XScale= 0.98311900
RedQX1 iteration 11 Try 1 RMS(Cart)= 0.00000786 RMS(Int)= 0.19523046 XScale= 1.04792640
RedQX1 iteration 11 Try 2 RMS(Cart)= 0.00000786 RMS(Int)= 0.19679456 XScale= 1.03139926
RedQX1 iteration 11 Try 3 RMS(Cart)= 0.00000786 RMS(Int)= 0.19841596 XScale= 1.01509606
RedQX1 iteration 11 Try 4 RMS(Cart)= 0.00000786 RMS(Int)= 0.20009523 XScale= 0.99902244
RedQX1 iteration 11 Try 5 RMS(Cart)= 0.00000786 RMS(Int)= 0.20183281 XScale= 0.98318393
RedQX1 iteration 12 Try 1 RMS(Cart)= 0.00000786 RMS(Int)= 0.20183272 XScale= 0.98318473
RedQX1 iteration 13 Try 1 RMS(Cart)= 0.00000157 RMS(Int)= 0.20043799 XScale= 0.99583648
RedQX1 iteration 14 Try 1 RMS(Cart)= 0.00000031 RMS(Int)= 0.20016359 XScale=

0.99838452
RedQX1 iteration 15 Try 1 RMS(Cart)= 0.00000006 RMS(Int)= 0.20010889 XScale= 0.99889482
RedQX1 iteration 16 Try 1 RMS(Cart)= 0.00000001 RMS(Int)= 0.20009796 XScale= 0.99899691
RedQX1 iteration 17 Try 1 RMS(Cart)= 0.00000000 RMS(Int)= 0.20009577 XScale= 0.99901733
TrRot= 0.000000 0.000000 0.000000 0.000000 0.000000 0.000000

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56613	-0.00070	0.00000	0.00402	0.00031	2.56643
R2	2.62283	-0.00045	0.00000	-0.00374	-0.00007	2.62276
R3	2.03383	0.00009	0.00000	0.00007	0.00009	2.03393
R4	2.63052	-0.00011	0.00000	-0.00022	0.00010	2.63061
R5	2.03098	-0.00004	0.00000	0.00022	0.00010	2.03108
R6	2.54424	0.00002	0.00000	-0.00654	-0.00020	2.54404
R7	2.68718	0.00022	0.00000	0.00342	0.00029	2.68747
R8	2.51638	0.00111	0.00000	-0.00918	-0.00033	2.51604
R9	2.11627	-0.00262	0.00000	-0.03446	-0.00154	2.11473
R10	2.79381	-0.00129	0.00000	0.00126	0.00014	2.79395
R11	2.91036	-0.00189	0.00000	-0.00840	-0.00039	2.90997
R12	2.06277	0.00016	0.00000	-0.00185	0.00001	2.06278
R13	2.06198	0.00017	0.00000	0.00021	0.00009	2.06207
R14	2.07232	0.00021	0.00000	-0.00286	-0.00012	2.07220
R15	2.07042	-0.00026	0.00000	-0.00356	-0.00015	2.07027
R16	2.66553	-0.00223	0.00000	0.02713	0.00130	2.66683
R17	4.10447	-0.00077	0.00000	0.12168	0.00591	4.11038
R18	9.35707	-0.00180	0.00000	-1.28849	-0.06086	9.29620
R19	2.50698	-0.00013	0.00000	-0.00135	0.00004	2.50703
R20	2.04705	-0.00011	0.00000	0.00011	0.00010	2.04715
R21	2.04296	0.00003	0.00000	0.00032	0.00012	2.04307
R22	2.04616	-0.00006	0.00000	0.00069	0.00013	2.04629
R23	1.84066	-0.00264	0.00000	-0.00500	-0.00024	1.84043
R24	3.67699	-0.00266	0.00000	0.07171	0.00362	3.68061
R25	2.77140	0.00009	0.00000	0.00898	0.00105	2.77246
R26	2.73836	-0.00028	0.00000	0.01960	0.00152	2.73988
R27	2.04960	0.00216	0.00000	0.00417	0.00078	2.05038
R28	2.04721	0.00207	0.00000	0.00057	0.00007	2.04728
R29	2.73979	-0.00262	0.00000	-0.02053	-0.00011	2.73969
R30	2.05625	0.00032	0.00000	0.00207	0.00062	2.05687
R31	2.85785	-0.00308	0.00000	0.00759	0.00064	2.85849
R32	2.06573	0.00015	0.00000	0.00493	0.00049	2.06622
R33	2.06877	-0.00061	0.00000	0.00265	0.00056	2.06932
R34	2.06297	-0.00008	0.00000	0.00120	0.00043	2.06340

A1	1.87263	0.00009	0.00000	-0.00188	-0.00009	1.87254
A2	2.27713	-0.00010	0.00000	-0.00159	-0.00007	2.27706
A3	2.13330	0.00001	0.00000	0.00321	0.00015	2.13345
A4	1.86193	0.00037	0.00000	0.00038	0.00002	1.86194
A5	2.27754	-0.00024	0.00000	-0.00045	-0.00002	2.27752
A6	2.14368	-0.00013	0.00000	-0.00011	-0.00001	2.14368
A7	1.89789	-0.00003	0.00000	-0.00549	-0.00026	1.89762
A8	2.25003	-0.00011	0.00000	0.00702	0.00033	2.25036
A9	2.13523	0.00014	0.00000	-0.00162	-0.00007	2.13516
A10	1.88955	-0.00042	0.00000	0.00838	0.00040	1.88995
A11	2.24069	-0.00088	0.00000	0.00117	0.00006	2.24074
A12	2.15248	0.00131	0.00000	-0.00754	-0.00036	2.15212
A13	1.90273	0.00000	0.00000	-0.00185	-0.00009	1.90265
A14	2.22352	-0.00154	0.00000	0.03214	0.00153	2.22505
A15	2.15644	0.00154	0.00000	-0.02922	-0.00139	2.15504
A16	1.95586	-0.00175	0.00000	-0.00759	-0.00039	1.95546
A17	1.86087	0.00064	0.00000	0.00416	0.00021	1.86108
A18	1.89073	0.00028	0.00000	0.00327	0.00018	1.89091
A19	1.93140	0.00031	0.00000	0.01031	0.00050	1.93189
A20	1.91748	0.00051	0.00000	0.00554	0.00025	1.91773
A21	1.90591	0.00004	0.00000	-0.01633	-0.00077	1.90514
A22	1.90984	0.00104	0.00000	-0.00041	-0.00002	1.90983
A23	1.90986	0.00012	0.00000	0.01449	0.00069	1.91055
A24	1.92157	-0.00310	0.00000	-0.00889	-0.00043	1.92114
A25	1.88222	-0.00016	0.00000	0.01115	0.00053	1.88275
A26	1.88798	0.00072	0.00000	0.00075	0.00004	1.88802
A27	1.95151	0.00146	0.00000	-0.01665	-0.00079	1.95072
A28	1.70981	-0.00166	0.00000	-0.04923	-0.00243	1.70738
A29	2.90494	-0.00128	0.00000	0.10208	0.00484	2.90978
A30	2.17583	0.00001	0.00000	0.00123	0.00006	2.17589
A31	1.95408	0.00009	0.00000	-0.00212	-0.00010	1.95399
A32	2.15326	-0.00010	0.00000	0.00088	0.00004	2.15330
A33	2.07948	0.00001	0.00000	-0.00336	-0.00016	2.07932
A34	2.15734	0.00001	0.00000	0.00589	0.00027	2.15762
A35	2.04636	-0.00002	0.00000	-0.00252	-0.00012	2.04624
A36	1.91668	-0.00165	0.00000	-0.04440	-0.00211	1.91457
A37	3.13016	-0.00029	0.00000	0.24002	0.01130	3.14145
A38	2.09852	-0.00046	0.00000	0.00588	0.00046	2.09899
A39	2.10263	-0.00019	0.00000	-0.01272	-0.00072	2.10191
A40	1.99562	0.00111	0.00000	0.00387	0.00038	1.99600
A41	1.98528	-0.00037	0.00000	-0.01446	-0.00091	1.98437
A42	2.01219	0.00052	0.00000	0.01415	0.00060	2.01279
A43	2.06079	-0.00057	0.00000	0.00992	0.00074	2.06153
A44	2.13235	-0.00074	0.00000	0.00043	-0.00010	2.13225

A45	1.97158	-0.00145	0.00000	0.01398	0.00066	1.97224
A46	2.03227	0.00048	0.00000	0.00525	0.00040	2.03267
A47	2.00845	0.00126	0.00000	-0.01960	-0.00109	2.00737
A48	1.36548	0.00136	0.00000	0.25743	0.01221	1.37769
A49	1.03540	-0.00250	0.00000	-0.38725	-0.01820	1.01720
A50	2.39551	-0.00108	0.00000	-0.08255	-0.00397	2.39154
A51	2.22653	-0.00070	0.00000	-0.06753	-0.00316	2.22337
A52	1.91918	0.00154	0.00000	-0.00870	-0.00058	1.91860
A53	1.92048	-0.00028	0.00000	0.00273	0.00031	1.92079
A54	1.92046	0.00187	0.00000	0.00843	0.00030	1.92076
A55	1.89587	-0.00087	0.00000	-0.00090	-0.00010	1.89577
A56	1.90998	-0.00153	0.00000	0.00591	0.00047	1.91045
A57	1.89754	-0.00080	0.00000	-0.00755	-0.00040	1.89714
A58	3.59201	0.00067	0.00000	0.18989	0.00905	3.60106
A59	4.66956	0.00115	0.00000	0.66033	0.03137	4.70094
D1	0.00983	-0.00035	0.00000	0.03968	0.00188	0.01171
D2	-3.14014	-0.00014	0.00000	0.01431	0.00068	-3.13947
D3	3.13460	-0.00002	0.00000	0.02216	0.00105	3.13565
D4	-0.01537	0.00019	0.00000	-0.00322	-0.00015	-0.01552
D5	-0.00866	0.00029	0.00000	-0.05093	-0.00242	-0.01107
D6	-3.11704	0.00030	0.00000	-0.08617	-0.00409	-3.12113
D7	-3.13512	-0.00001	0.00000	-0.03511	-0.00167	-3.13679
D8	0.03968	0.00001	0.00000	-0.07036	-0.00334	0.03634
D9	-0.00775	0.00030	0.00000	-0.01548	-0.00073	-0.00848
D10	-3.13952	0.00019	0.00000	-0.00514	-0.00024	-3.13977
D11	3.14143	0.00011	0.00000	0.00748	0.00036	-3.14140
D12	0.00965	0.00000	0.00000	0.01783	0.00085	0.01050
D13	0.00242	-0.00012	0.00000	-0.01615	-0.00077	0.00165
D14	3.11161	0.00009	0.00000	0.05332	0.00254	3.11414
D15	3.13498	-0.00003	0.00000	-0.02561	-0.00122	3.13376
D16	-0.03902	0.00018	0.00000	0.04386	0.00209	-0.03694
D17	0.08770	-0.00016	0.00000	-0.04209	-0.00200	0.08570
D18	-3.05771	-0.00009	0.00000	-0.04582	-0.00218	-3.05989
D19	-3.04289	-0.00028	0.00000	-0.03049	-0.00145	-3.04434
D20	0.09489	-0.00021	0.00000	-0.03422	-0.00163	0.09326
D21	0.00379	-0.00010	0.00000	0.04127	0.00196	0.00575
D22	3.11373	-0.00018	0.00000	0.07626	0.00362	3.11735
D23	-3.10739	-0.00025	0.00000	-0.02408	-0.00115	-3.10854
D24	0.00254	-0.00034	0.00000	0.01091	0.00051	0.00305
D25	-2.89893	-0.00033	0.00000	-0.38955	-0.01873	-2.91766
D26	0.20583	-0.00013	0.00000	-0.31029	-0.01496	0.19086
D27	1.25972	0.00000	0.00000	0.11799	0.00560	1.26532
D28	-2.90782	-0.00024	0.00000	0.12890	0.00611	-2.90170
D29	-0.85852	0.00029	0.00000	0.11366	0.00542	-0.85310

D30	-1.84419	0.00006	0.00000	0.07730	0.00367	-1.84053
D31	0.27145	-0.00018	0.00000	0.08821	0.00418	0.27563
D32	2.32076	0.00034	0.00000	0.07297	0.00348	2.32424
D33	-0.91617	-0.00018	0.00000	-0.12955	-0.00615	-0.92232
D34	1.14268	0.00031	0.00000	-0.10779	-0.00512	1.13756
D35	-2.98900	0.00018	0.00000	-0.12486	-0.00593	-2.99493
D36	-2.99066	-0.00004	0.00000	-0.13675	-0.00649	-2.99715
D37	-0.93181	0.00045	0.00000	-0.11498	-0.00546	-0.93727
D38	1.21969	0.00032	0.00000	-0.13205	-0.00627	1.21342
D39	1.18661	-0.00062	0.00000	-0.12663	-0.00601	1.18059
D40	-3.03773	-0.00014	0.00000	-0.10487	-0.00498	-3.04270
D41	-0.88622	-0.00027	0.00000	-0.12194	-0.00579	-0.89201
D42	-1.78943	0.00033	0.00000	-0.08355	-0.00397	-1.79340
D43	2.40758	0.00044	0.00000	-0.07831	-0.00372	2.40385
D44	0.33753	-0.00068	0.00000	-0.08263	-0.00393	0.33360
D45	0.26961	-0.00033	0.00000	0.45156	0.02172	0.29133
D46	-0.34279	0.00049	0.00000	-0.21108	-0.01008	-0.35287
D47	2.89179	0.00014	0.00000	-0.60679	-0.02917	2.86262
D48	-3.13737	0.00003	0.00000	-0.00421	-0.00020	-3.13757
D49	0.00685	-0.00001	0.00000	-0.00795	-0.00038	0.00647
D50	0.00846	-0.00004	0.00000	-0.00005	0.00000	0.00846
D51	-3.13050	-0.00008	0.00000	-0.00379	-0.00018	-3.13068
D52	-2.60905	-0.00003	0.00000	0.23973	1.18202	-1.42703
D53	-3.01575	0.00062	0.00000	-0.10978	-1.17581	2.09162
D54	-2.89783	-0.00014	0.00000	-0.65030	-1.20147	2.18388
D55	-1.40213	-0.00053	0.00000	-0.77011	-1.20718	-2.60931
D56	-2.72763	-0.00023	0.00000	0.01210	0.00063	-2.72700
D57	-0.03003	-0.00002	0.00000	-0.01646	-0.00078	-0.03081
D58	0.00283	-0.00046	0.00000	0.03590	0.00172	0.00455
D59	2.70043	-0.00025	0.00000	0.00733	0.00031	2.70074
D60	0.18739	0.00039	0.00000	-0.66675	-0.03213	0.15526
D61	0.05307	0.00102	0.00000	-0.08849	-0.00430	0.04877
D62	-2.17473	-0.00122	0.00000	-0.67703	-0.03248	-2.20720
D63	-2.30905	-0.00060	0.00000	-0.09877	-0.00464	-2.31369
D64	2.10723	0.00085	0.00000	0.08823	0.00396	2.11119
D65	-0.27427	-0.00002	0.00000	0.09718	0.00447	-0.26981
D66	2.52068	0.00040	0.00000	-0.07332	-0.00345	2.51724
D67	-1.67488	0.00011	0.00000	-0.07816	-0.00374	-1.67862
D68	0.41561	0.00012	0.00000	-0.08048	-0.00385	0.41176
D69	1.31298	-0.00010	0.00000	-0.08875	-0.00414	1.30884
D70	-2.88258	-0.00039	0.00000	-0.09360	-0.00443	-2.88702
D71	-0.79209	-0.00038	0.00000	-0.09591	-0.00454	-0.79663
D72	-1.05265	0.00019	0.00000	-0.09432	-0.00439	-1.05704
D73	1.03498	-0.00009	0.00000	-0.09916	-0.00469	1.03029

D74	3.12547	-0.00008	0.00000	-0.10148	-0.00480	3.12067

Item	Value	Threshold	Converged?
Maximum Force	0.003098	0.000450	NO
RMS Force	0.000889	0.000300	NO
Maximum Displacement	0.120209	0.001800	NO
RMS Displacement	0.030625	0.001200	NO

Predicted change in Energy=-1.477541D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.437776	-1.866148	-0.307632
2	6	0	-2.604158	-1.172072	-0.260284
3	7	0	-2.284939	0.117989	0.154051
4	6	0	-0.956503	0.189402	0.360312
5	7	0	-0.427231	-1.002184	0.090673
6	6	0	1.020252	-1.290326	0.178492
7	6	0	1.673779	-1.396057	-1.211826
8	1	0	-1.245228	-2.891246	-0.573218
9	1	0	-3.608589	-1.478790	-0.488841
10	1	0	1.466438	-0.476801	0.753501
11	1	0	1.151494	-2.227181	0.722366
12	1	0	1.116075	-2.115542	-1.823185
13	1	0	1.627315	-0.422506	-1.712074
14	35	0	1.220120	2.505403	1.147639
15	1	0	-0.348606	1.075092	0.673874
16	6	0	-3.148050	1.228679	0.363589
17	6	0	-4.471114	1.183101	0.277243
18	1	0	-2.597514	2.128789	0.609065
19	1	0	-5.041353	2.085057	0.450973
20	1	0	-5.025981	0.283521	0.041772
21	8	0	3.001402	-1.858551	-1.089070
22	1	0	3.619506	-1.112802	-1.190615
23	6	0	4.950802	1.748496	-0.928749
24	6	0	5.939897	0.750622	-0.506396
25	8	0	4.855611	0.378578	-1.393959
26	1	0	4.154977	2.048740	-0.255125
27	1	0	5.187778	2.458732	-1.711757
28	1	0	6.910962	0.750867	-0.998081
29	6	0	5.922400	0.133724	0.874628
30	1	0	6.230914	-0.913759	0.818810

31	1	0	6.615416	0.667694	1.533199
32	1	0	4.918371	0.195095	1.299380

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.358098	0.000000			
3	N	2.206272	1.392061	0.000000		
4	C	2.214285	2.225650	1.346249	0.000000	
5	N	1.387905	2.211570	2.170226	1.331432	0.000000
6	C	2.570951	3.652787	3.592803	2.475927	1.478494
7	C	3.274191	4.388205	4.453022	3.450172	2.503175
8	H	1.076308	2.213635	3.265795	3.231909	2.162967
9	H	2.212535	1.074800	2.171420	3.246149	3.268643
10	H	3.389800	4.252166	3.845250	2.543436	2.073970
11	H	2.809903	4.022906	4.199033	3.227167	2.095717
12	H	2.980143	4.144023	4.523828	3.791571	2.698928
13	H	3.667607	4.535957	4.368099	3.368283	2.794115
14	Br	5.319086	5.489187	4.355731	3.274359	4.016728
15	H	3.286417	3.318119	2.221631	1.119065	2.159023
16	C	3.599101	2.539418	1.422146	2.425486	3.529035
17	C	4.340638	3.053080	2.434954	3.653331	4.600355
18	H	4.259676	3.413429	2.085199	2.552649	3.844717
19	H	5.401228	4.129733	3.399314	4.504189	5.563361
20	H	4.197425	2.841693	2.748330	4.083011	4.775346
21	O	4.507438	5.707928	5.779054	4.686132	3.725679
22	H	5.188765	6.293093	6.179437	5.004095	4.246176
23	C	7.366503	8.127360	7.495796	6.244094	6.126067
24	C	7.830520	8.761175	8.275526	6.973269	6.630922
25	O	6.769462	7.703109	7.311067	6.074037	5.658538
26	H	6.827004	7.487293	6.735558	5.473858	5.515826
27	H	8.035802	8.718015	8.049958	6.869900	6.837764
28	H	8.776497	9.735479	9.289377	8.003592	7.622837
29	C	7.718122	8.700305	8.238925	6.898327	6.497898
30	H	7.809271	8.904474	8.603845	7.286024	6.698425
31	H	8.640770	9.570886	9.023333	7.677134	7.380261
32	H	6.872540	7.803213	7.294202	5.949455	5.609804

		6	7	8	9	10
6	C	0.000000				
7	C	1.539890	0.000000			
8	H	2.874093	3.341259	0.000000		
9	H	4.680493	5.332256	2.754565	0.000000	
10	H	1.091577	2.179572	3.865600	5.320084	0.000000
11	H	1.091201	2.169020	2.804246	4.968450	1.778760

12	H	2.167227	1.096563	2.782065	4.950593	3.073685
13	H	2.166997	1.095540	3.955145	5.479664	2.471414
14	Br	3.922595	4.581951	6.177630	6.470570	3.018205
15	H	2.777477	3.708435	4.253353	4.301361	2.389372
16	C	4.873847	5.711498	4.633802	2.875608	4.934997
17	C	6.023511	6.828550	5.265922	2.901120	6.183576
18	H	4.996396	5.829591	5.331719	3.904138	4.829666
19	H	6.943378	7.744421	6.342170	3.954373	7.000427
20	H	6.249210	7.019920	4.975083	2.322992	6.575420
21	O	2.419617	1.411223	4.400730	6.648042	2.767746
22	H	2.943143	1.966351	5.216289	7.271298	2.969812
23	C	5.090152	4.550520	7.748832	9.158169	4.463486
24	C	5.370051	4.827590	8.055661	9.805313	4.806843
25	O	4.468537	3.647816	6.970337	8.712734	4.102408
26	H	4.600423	4.351810	7.325767	8.530594	3.824124
27	H	5.915805	5.239992	8.444057	9.714714	5.342586
28	H	6.344388	5.664191	8.942535	10.765298	5.849620
29	C	5.152046	4.974364	7.913380	9.762120	4.499223
30	H	5.263345	5.012342	7.857537	9.942083	4.784916
31	H	6.080702	6.017808	8.882160	10.640785	5.331957
32	H	4.319513	4.400602	7.142973	8.871790	3.558829

		11	12	13	14	15
11	H	0.000000				
12	H	2.548244	0.000000			
13	H	3.067532	1.772028	0.000000		
14	Br	4.752149	5.494520	4.112957	0.000000	
15	H	3.627349	4.308218	3.440903	2.175119	0.000000
16	C	5.527908	5.843677	5.462499	4.617971	2.820771
17	C	6.591045	6.819789	6.612578	5.907301	4.142952
18	H	5.748249	6.141737	5.453987	3.873787	2.484364
19	H	7.551185	7.792993	7.445654	6.314116	4.805370
20	H	6.702837	6.852622	6.916704	6.721122	4.785809
21	O	2.615215	2.039467	2.082900	5.217272	4.789237
22	H	3.315481	2.769981	2.171923	4.931114	4.899909
23	C	5.741684	5.516877	4.046284	4.336160	5.577240
24	C	5.771132	5.763513	4.629065	5.300130	6.406527
25	O	4.998929	4.515418	3.341381	4.919339	5.643132
26	H	5.316004	5.388412	3.823458	3.284764	4.700350
27	H	6.646377	6.124962	4.580221	4.890873	6.185244
28	H	6.708217	6.517500	5.459259	6.329944	7.456667
29	C	5.325279	5.952995	5.044618	5.273598	6.344446
30	H	5.247369	5.880985	5.276345	6.075101	6.875072
31	H	6.236361	7.018152	6.049916	5.712710	7.028657
32	H	4.515498	5.435706	4.503480	4.363211	5.376495

		16	17	18	19	20
16	C	0.000000				
17	C	1.326662	0.000000			
18	H	1.083303	2.124807	0.000000		
19	H	2.079811	1.081147	2.449337	0.000000	
20	H	2.126856	1.082852	3.102303	1.847489	0.000000
21	O	7.032564	8.182722	7.080283	9.088986	8.384876
22	H	7.327884	8.537207	7.238653	9.377184	8.843808
23	C	8.217770	9.515597	7.712754	10.092575	10.130364
24	C	9.142001	10.449415	8.719575	11.103383	10.989502
25	O	8.238339	9.509362	7.913559	10.211059	9.985801
26	H	7.374924	8.685746	6.808037	9.223468	9.353830
27	H	8.677910	9.943719	8.130551	10.461938	10.589017
28	H	10.161996	11.461454	9.741289	12.113531	11.991260
29	C	9.150581	10.463421	8.754413	11.144104	10.981035
30	H	9.631315	10.918952	9.340355	11.670141	11.347024
31	H	9.849262	11.169342	9.373735	11.792387	11.742831
32	H	8.186033	9.496491	7.791292	10.172897	10.023948

		21	22	23	24	25
21	O	0.000000				
22	H	0.973913	0.000000			
23	C	4.103249	3.166694	0.000000		
24	C	3.972662	3.053640	1.467120	0.000000	
25	O	2.921609	1.947696	1.449881	1.449779	0.000000
26	H	4.158500	3.340242	1.085014	2.221303	2.139456
27	H	4.879233	3.935343	1.083372	2.221760	2.130345
28	H	4.701277	3.787350	2.200522	1.088450	2.125979
29	C	4.044441	3.335023	2.608383	1.512646	2.518825
30	H	3.868124	3.301039	3.432237	2.147330	2.908253
31	H	5.130235	4.423212	3.162319	2.150152	3.427646
32	H	3.687401	3.098019	2.716370	2.147779	2.700311

		26	27	28	29	30
26	H	0.000000				
27	H	1.832089	0.000000			
28	H	3.135588	2.528932	0.000000		
29	C	2.840319	3.554535	2.205711	0.000000	
30	H	3.773493	4.343454	2.556275	1.093397	0.000000
31	H	3.340532	3.971865	2.549833	1.095039	1.777410
32	H	2.536781	3.776716	3.091542	1.091904	1.784173

		31	32
31	H	0.000000	
32	H	1.777072	0.000000

Stoichiometry C10H17BrN2O2

Framework group C1[X(C10H17BrN2O2)]

Deg. of freedom 90

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.588999	2.269704	-0.304360
2	6	0	-3.722138	1.588774	0.006701
3	7	0	-3.371858	0.243654	0.082793
4	6	0	-2.058669	0.123013	-0.188067
5	7	0	-1.568605	1.337249	-0.429271
6	6	0	-0.145535	1.596296	-0.735397
7	6	0	0.595488	2.231219	0.455829
8	1	0	-2.426993	3.322363	-0.459610
9	1	0	-4.721923	1.941364	0.183637
10	1	0	0.298036	0.633783	-0.996843
11	1	0	-0.095619	2.260222	-1.599938
12	1	0	0.047656	3.118457	0.795151
13	1	0	0.628806	1.518330	1.287026
14	35	0	0.165271	-2.279991	-0.221054
15	1	0	-1.432759	-0.804622	-0.194074
16	6	0	-4.194313	-0.878870	0.376061
17	6	0	-5.509106	-0.827375	0.545471
18	1	0	-3.620256	-1.795128	0.442963
19	1	0	-6.047019	-1.737987	0.769781
20	1	0	-6.088136	0.084535	0.469882
21	8	0	1.888569	2.636333	0.061653
22	1	0	2.546372	1.995320	0.385542
23	6	0	3.989177	-0.728720	1.110708
24	6	0	4.899432	0.052749	0.266207
25	8	0	3.861886	0.713498	1.033519
26	1	0	3.164249	-1.275297	0.665733
27	1	0	4.311899	-1.085994	2.081224
28	1	0	5.900671	0.255499	0.641886
29	6	0	4.759082	0.101451	-1.239126
30	1	0	5.021326	1.097583	-1.605821
31	1	0	5.429868	-0.629527	-1.702623
32	1	0	3.732433	-0.133615	-1.527207

Rotational constants (GHZ): 0.5609390 0.2044951 0.1586841

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.
There are 475 symmetry adapted basis functions of A symmetry.
475 basis functions, 751 primitive gaussians, 492 cartesian basis functions
71 alpha electrons 71 beta electrons
nuclear repulsion energy 1275.2628642389 Hartrees.
NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 475 RedAO= T EigKep= 3.76D-06 NBF= 475
NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999998 0.000744 -0.000056 -0.002013 Ang= 0.25 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3225.52108426 A.U. after 11 cycles
NFock= 11 Conv=0.33D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Atomic Forces (Hartrees/Bohr)
Number Number X Y Z
---
1 6 -0.000177636 -0.000186374 0.001284072
2 6 0.000982602 0.000080018 -0.000716052
3 7 -0.000165429 -0.000124541 0.000557231

4	6	0.002522309	0.002139833	-0.000209471
5	7	0.001194127	-0.000345529	-0.000636397
6	6	0.001933875	-0.000911005	-0.000270502
7	6	0.000399916	0.000654515	-0.001145205
8	1	-0.000033596	-0.000043460	-0.000072693
9	1	0.000100248	-0.000019188	-0.000037793
10	1	-0.000009867	0.000349293	-0.000249379
11	1	-0.000486153	-0.000368951	-0.000255317
12	1	0.000065817	-0.000225777	-0.000223934
13	1	-0.000462917	-0.000010269	0.000539457
14	35	0.001121934	-0.000860919	-0.000736172
15	1	-0.002166953	-0.000515118	-0.000043156
16	6	-0.000186742	0.000066935	0.000182923
17	6	0.000131147	0.000016173	-0.000175048
18	1	-0.000159211	-0.000096253	0.000062231
19	1	-0.000007804	-0.000021660	0.000001648
20	1	0.000074131	0.000096412	-0.000026517
21	8	-0.000883888	0.001423416	0.000400082
22	1	-0.000603859	0.000932447	0.001154525
23	6	-0.002742041	-0.001853632	-0.000656610
24	6	-0.001914335	-0.001629647	0.004426814
25	8	0.002076862	-0.001763551	0.000782105
26	1	-0.000717297	0.000304660	0.002149304
27	1	0.001832557	0.001158744	-0.001262348
28	1	-0.000764727	0.000497516	-0.001802823
29	6	-0.001054053	0.002836953	-0.005072607
30	1	-0.000167580	-0.000129531	0.001343954
31	1	-0.000417334	-0.000662465	-0.000380488
32	1	0.000685896	-0.000789049	0.001088165

Cartesian Forces: Max 0.005072607 RMS 0.001199902

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.003265178 RMS 0.000902153
Search for a local minimum.
Step number 17 out of a maximum of 177
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 16 17
DE= -2.32D-04 DEPred=-1.48D-02 R= 1.57D-02

Trust test= 1.57D-02 RLast= 2.39D+00 DXMaxT set to 1.50D+00

ITU= -1 1 1 1 1 1 1 1 1 1 1 1 0 1 0 1 0

Eigenvalues ---	0.00000	0.00105	0.00233	0.00276	0.00417
Eigenvalues ---	0.00483	0.00976	0.01252	0.01408	0.01509
Eigenvalues ---	0.01767	0.01894	0.02050	0.02148	0.02187
Eigenvalues ---	0.02237	0.02320	0.02389	0.02622	0.03042
Eigenvalues ---	0.03062	0.03090	0.03538	0.03705	0.03994
Eigenvalues ---	0.04566	0.05105	0.05267	0.05610	0.05636
Eigenvalues ---	0.05953	0.06248	0.07667	0.09410	0.09537
Eigenvalues ---	0.10325	0.10981	0.11689	0.11967	0.12883
Eigenvalues ---	0.13917	0.15083	0.15529	0.15968	0.15996
Eigenvalues ---	0.16000	0.16001	0.16002	0.16006	0.16064
Eigenvalues ---	0.16829	0.17995	0.19798	0.21821	0.22036
Eigenvalues ---	0.22897	0.23568	0.24222	0.25056	0.25305
Eigenvalues ---	0.27763	0.29756	0.31038	0.32810	0.33093
Eigenvalues ---	0.33221	0.34100	0.34267	0.34576	0.34768
Eigenvalues ---	0.34980	0.35685	0.35698	0.35713	0.35866
Eigenvalues ---	0.36443	0.36661	0.37228	0.37316	0.37795
Eigenvalues ---	0.38052	0.42196	0.42493	0.45224	0.47969
Eigenvalues ---	0.50114	0.52613	0.54505	0.56833	0.60365

Eigenvalue 1 is 2.38D-06 Eigenvector:

	D54	D53	D55	D52	R18
1	-0.50051	-0.50025	-0.49965	0.49932	-0.01354
	A37	D30	D32	D27	D29
1	-0.00298	0.00258	0.00255	0.00254	0.00250

En-DIIS/RFO-DIIS IScMMF= 0 using points: 17 16 15 14 13

RFO step: Lambda=-3.72594456D-04.

DidBck=F Rises=F En-DIIS coefs: 1.00000 0.00000 0.00000 0.00000 0.00000

Iteration 1 RMS(Cart)= 0.16725076 RMS(Int)= 0.05857914

Iteration 2 RMS(Cart)= 0.01273881 RMS(Int)= 0.05352344

Iteration 3 RMS(Cart)= 0.00816103 RMS(Int)= 0.04994957

Iteration 4 RMS(Cart)= 0.00183922 RMS(Int)= 0.04908604

Iteration 5 RMS(Cart)= 0.00081023 RMS(Int)= 0.04869972

Iteration 6 RMS(Cart)= 0.00062902 RMS(Int)= 0.04839776

Iteration 7 RMS(Cart)= 0.00055132 RMS(Int)= 0.04813169

Iteration 8 RMS(Cart)= 0.00050705 RMS(Int)= 0.04788585

Iteration 9 RMS(Cart)= 0.00047760 RMS(Int)= 0.04765331

Iteration 10 RMS(Cart)= 0.00045587 RMS(Int)= 0.04743046

Iteration 11 RMS(Cart)= 0.00043874 RMS(Int)= 0.04721519

Iteration 12 RMS(Cart)= 0.00042460 RMS(Int)= 0.04700610

Iteration 13 RMS(Cart)= 0.00041253 RMS(Int)= 0.04680225

Iteration 14 RMS(Cart)= 0.00040195 RMS(Int)= 0.04660295

Iteration 15 RMS(Cart)= 0.00039252 RMS(Int)= 0.04640770

Iteration 16 RMS(Cart)= 0.00038398 RMS(Int)= 0.04621610
Iteration 17 RMS(Cart)= 0.00037615 RMS(Int)= 0.04602782
Iteration 18 RMS(Cart)= 0.00036891 RMS(Int)= 0.04584262
Iteration 19 RMS(Cart)= 0.00036216 RMS(Int)= 0.04566027
Iteration 20 RMS(Cart)= 0.00035583 RMS(Int)= 0.04548060
Iteration 21 RMS(Cart)= 0.00034986 RMS(Int)= 0.04530345
Iteration 22 RMS(Cart)= 0.00034420 RMS(Int)= 0.04512869
Iteration 23 RMS(Cart)= 0.00033883 RMS(Int)= 0.04495620
Iteration 24 RMS(Cart)= 0.00033370 RMS(Int)= 0.04478587
Iteration 25 RMS(Cart)= 0.00032880 RMS(Int)= 0.04461762
Iteration 26 RMS(Cart)= 0.00032410 RMS(Int)= 0.04445135
Iteration 27 RMS(Cart)= 0.00031958 RMS(Int)= 0.04428700
Iteration 28 RMS(Cart)= 0.00031524 RMS(Int)= 0.04412449
Iteration 29 RMS(Cart)= 0.00031105 RMS(Int)= 0.04396376
Iteration 30 RMS(Cart)= 0.00030701 RMS(Int)= 0.04380475
Iteration 31 RMS(Cart)= 0.00030310 RMS(Int)= 0.04364741
Iteration 32 RMS(Cart)= 0.00029931 RMS(Int)= 0.04349169
Iteration 33 RMS(Cart)= 0.00029565 RMS(Int)= 0.04333753
Iteration 34 RMS(Cart)= 0.00029209 RMS(Int)= 0.04318490
Iteration 35 RMS(Cart)= 0.00028864 RMS(Int)= 0.04303376
Iteration 36 RMS(Cart)= 0.00028529 RMS(Int)= 0.04288406
Iteration 37 RMS(Cart)= 0.00028203 RMS(Int)= 0.04273577
Iteration 38 RMS(Cart)= 0.00027886 RMS(Int)= 0.04258885
Iteration 39 RMS(Cart)= 0.00027577 RMS(Int)= 0.04244327
Iteration 40 RMS(Cart)= 0.00027276 RMS(Int)= 0.04229900
Iteration 41 RMS(Cart)= 0.00026983 RMS(Int)= 0.04215601
Iteration 42 RMS(Cart)= 0.00026697 RMS(Int)= 0.04201426
Iteration 43 RMS(Cart)= 0.00026418 RMS(Int)= 0.04187374
Iteration 44 RMS(Cart)= 0.00026146 RMS(Int)= 0.04173441
Iteration 45 RMS(Cart)= 0.00025880 RMS(Int)= 0.04159626
Iteration 46 RMS(Cart)= 0.00025620 RMS(Int)= 0.04145925
Iteration 47 RMS(Cart)= 0.00025366 RMS(Int)= 0.04132336
Iteration 48 RMS(Cart)= 0.00025118 RMS(Int)= 0.04118858
Iteration 49 RMS(Cart)= 0.00024875 RMS(Int)= 0.04105487
Iteration 50 RMS(Cart)= 0.00024637 RMS(Int)= 0.04092222
Iteration 51 RMS(Cart)= 0.00024404 RMS(Int)= 0.04079061
Iteration 52 RMS(Cart)= 0.00024177 RMS(Int)= 0.04066002
Iteration 53 RMS(Cart)= 0.00023954 RMS(Int)= 0.04053043
Iteration 54 RMS(Cart)= 0.00023735 RMS(Int)= 0.04040182
Iteration 55 RMS(Cart)= 0.00023521 RMS(Int)= 0.04027418
Iteration 56 RMS(Cart)= 0.00023311 RMS(Int)= 0.04014749
Iteration 57 RMS(Cart)= 0.00023105 RMS(Int)= 0.04002172
Iteration 58 RMS(Cart)= 0.00022904 RMS(Int)= 0.03989687
Iteration 59 RMS(Cart)= 0.00022706 RMS(Int)= 0.03977293

Iteration 60 RMS(Cart)= 0.00022511 RMS(Int)= 0.03964986
Iteration 61 RMS(Cart)= 0.00022321 RMS(Int)= 0.03952767
Iteration 62 RMS(Cart)= 0.00022134 RMS(Int)= 0.03940634
Iteration 63 RMS(Cart)= 0.00021950 RMS(Int)= 0.03928584
Iteration 64 RMS(Cart)= 0.00021770 RMS(Int)= 0.03916618
Iteration 65 RMS(Cart)= 0.00021593 RMS(Int)= 0.03904733
Iteration 66 RMS(Cart)= 0.00021419 RMS(Int)= 0.03892929
Iteration 67 RMS(Cart)= 0.00021248 RMS(Int)= 0.03881204
Iteration 68 RMS(Cart)= 0.00021080 RMS(Int)= 0.03869556
Iteration 69 RMS(Cart)= 0.00020914 RMS(Int)= 0.03857986
Iteration 70 RMS(Cart)= 0.00020752 RMS(Int)= 0.03846491
Iteration 71 RMS(Cart)= 0.00020592 RMS(Int)= 0.03835070
Iteration 72 RMS(Cart)= 0.00020435 RMS(Int)= 0.03823723
Iteration 73 RMS(Cart)= 0.00020281 RMS(Int)= 0.03812448
Iteration 74 RMS(Cart)= 0.00020129 RMS(Int)= 0.03801245
Iteration 75 RMS(Cart)= 0.00019980 RMS(Int)= 0.03790111
Iteration 76 RMS(Cart)= 0.00019833 RMS(Int)= 0.03779048
Iteration 77 RMS(Cart)= 0.00019688 RMS(Int)= 0.03768052
Iteration 78 RMS(Cart)= 0.00019546 RMS(Int)= 0.03757124
Iteration 79 RMS(Cart)= 0.00019405 RMS(Int)= 0.03746262
Iteration 80 RMS(Cart)= 0.00019267 RMS(Int)= 0.03735466
Iteration 81 RMS(Cart)= 0.00019131 RMS(Int)= 0.03724734
Iteration 82 RMS(Cart)= 0.00018998 RMS(Int)= 0.03714067
Iteration 83 RMS(Cart)= 0.00018866 RMS(Int)= 0.03703462
Iteration 84 RMS(Cart)= 0.00018736 RMS(Int)= 0.03692919
Iteration 85 RMS(Cart)= 0.00018608 RMS(Int)= 0.03682438
Iteration 86 RMS(Cart)= 0.00018482 RMS(Int)= 0.03672017
Iteration 87 RMS(Cart)= 0.00018358 RMS(Int)= 0.03661656
Iteration 88 RMS(Cart)= 0.00018235 RMS(Int)= 0.03651354
Iteration 89 RMS(Cart)= 0.00018115 RMS(Int)= 0.03641111
Iteration 90 RMS(Cart)= 0.00017996 RMS(Int)= 0.03630924
Iteration 91 RMS(Cart)= 0.00017878 RMS(Int)= 0.03620795
Iteration 92 RMS(Cart)= 0.00017763 RMS(Int)= 0.03610722
Iteration 93 RMS(Cart)= 0.00017649 RMS(Int)= 0.03600704
Iteration 94 RMS(Cart)= 0.00017536 RMS(Int)= 0.03590741
Iteration 95 RMS(Cart)= 0.00017425 RMS(Int)= 0.03580832
Iteration 96 RMS(Cart)= 0.00017316 RMS(Int)= 0.03570976
Iteration 97 RMS(Cart)= 0.00017208 RMS(Int)= 0.03561173
Iteration 98 RMS(Cart)= 0.00017102 RMS(Int)= 0.03551423
Iteration 99 RMS(Cart)= 0.00016997 RMS(Int)= 0.03541723
Iteration100 RMS(Cart)= 0.00016893 RMS(Int)= 0.03532075
New curvilinear step not converged.
ITry= 1 IFail=1 DXMaxC= 8.29D-01 DCOld= 1.00D+10 DXMaxT= 1.50D+00 DXLimC= 3.00D+00
Rises=F

Iteration 1 RMS(Cart)= 0.16289103 RMS(Int)= 0.05043767
Iteration 2 RMS(Cart)= 0.01373342 RMS(Int)= 0.04365137
Iteration 3 RMS(Cart)= 0.00020927 RMS(Int)= 0.04353642
Iteration 4 RMS(Cart)= 0.00020675 RMS(Int)= 0.04342270
Iteration 5 RMS(Cart)= 0.00020435 RMS(Int)= 0.04331016
Iteration 6 RMS(Cart)= 0.00020214 RMS(Int)= 0.04319869
Iteration 7 RMS(Cart)= 0.00020005 RMS(Int)= 0.04308824
Iteration 8 RMS(Cart)= 0.00019808 RMS(Int)= 0.04297874
Iteration 9 RMS(Cart)= 0.00019620 RMS(Int)= 0.04287015
Iteration 10 RMS(Cart)= 0.00019440 RMS(Int)= 0.04276243
Iteration 11 RMS(Cart)= 0.00019271 RMS(Int)= 0.04265552
Iteration 12 RMS(Cart)= 0.00019101 RMS(Int)= 0.04254944
Iteration 13 RMS(Cart)= 0.00018940 RMS(Int)= 0.04244412
Iteration 14 RMS(Cart)= 0.00018785 RMS(Int)= 0.04233955
Iteration 15 RMS(Cart)= 0.00018634 RMS(Int)= 0.04223570
Iteration 16 RMS(Cart)= 0.00018487 RMS(Int)= 0.04213256
Iteration 17 RMS(Cart)= 0.00018345 RMS(Int)= 0.04203010
Iteration 18 RMS(Cart)= 0.00018206 RMS(Int)= 0.04192830
Iteration 19 RMS(Cart)= 0.00018071 RMS(Int)= 0.04182716
Iteration 20 RMS(Cart)= 0.00017941 RMS(Int)= 0.04172664
Iteration 21 RMS(Cart)= 0.00017812 RMS(Int)= 0.04162674
Iteration 22 RMS(Cart)= 0.00017686 RMS(Int)= 0.04152744
Iteration 23 RMS(Cart)= 0.00017562 RMS(Int)= 0.04142875
Iteration 24 RMS(Cart)= 0.00017441 RMS(Int)= 0.04133063
Iteration 25 RMS(Cart)= 0.00017322 RMS(Int)= 0.04123309
Iteration 26 RMS(Cart)= 0.00017206 RMS(Int)= 0.04113611
Iteration 27 RMS(Cart)= 0.00017092 RMS(Int)= 0.04103967
Iteration 28 RMS(Cart)= 0.00016980 RMS(Int)= 0.04094379
Iteration 29 RMS(Cart)= 0.00016870 RMS(Int)= 0.04084843
Iteration 30 RMS(Cart)= 0.00016762 RMS(Int)= 0.04075360
Iteration 31 RMS(Cart)= 0.00016655 RMS(Int)= 0.04065928
Iteration 32 RMS(Cart)= 0.00016551 RMS(Int)= 0.04056547
Iteration 33 RMS(Cart)= 0.00016448 RMS(Int)= 0.04047216
Iteration 34 RMS(Cart)= 0.00016347 RMS(Int)= 0.04037934
Iteration 35 RMS(Cart)= 0.00016248 RMS(Int)= 0.04028700
Iteration 36 RMS(Cart)= 0.00016150 RMS(Int)= 0.04019514
Iteration 37 RMS(Cart)= 0.00016053 RMS(Int)= 0.04010376
Iteration 38 RMS(Cart)= 0.00015958 RMS(Int)= 0.04001284
Iteration 39 RMS(Cart)= 0.00015864 RMS(Int)= 0.03992237
Iteration 40 RMS(Cart)= 0.00015772 RMS(Int)= 0.03983236
Iteration 41 RMS(Cart)= 0.00015681 RMS(Int)= 0.03974279
Iteration 42 RMS(Cart)= 0.00015592 RMS(Int)= 0.03965367
Iteration 43 RMS(Cart)= 0.00015503 RMS(Int)= 0.03956498
Iteration 44 RMS(Cart)= 0.00015416 RMS(Int)= 0.03947672

Iteration 45 RMS(Cart)= 0.00015330 RMS(Int)= 0.03938888
Iteration 46 RMS(Cart)= 0.00015245 RMS(Int)= 0.03930146
Iteration 47 RMS(Cart)= 0.00015161 RMS(Int)= 0.03921445
Iteration 48 RMS(Cart)= 0.00015079 RMS(Int)= 0.03912785
Iteration 49 RMS(Cart)= 0.00014997 RMS(Int)= 0.03904166
Iteration 50 RMS(Cart)= 0.00014917 RMS(Int)= 0.03895586
Iteration 51 RMS(Cart)= 0.00014837 RMS(Int)= 0.03887046
Iteration 52 RMS(Cart)= 0.00014759 RMS(Int)= 0.03878545
Iteration 53 RMS(Cart)= 0.00014681 RMS(Int)= 0.03870083
Iteration 54 RMS(Cart)= 0.00014605 RMS(Int)= 0.03861658
Iteration 55 RMS(Cart)= 0.00014529 RMS(Int)= 0.03853272
Iteration 56 RMS(Cart)= 0.00014454 RMS(Int)= 0.03844922
Iteration 57 RMS(Cart)= 0.00014381 RMS(Int)= 0.03836610
Iteration 58 RMS(Cart)= 0.00014308 RMS(Int)= 0.03828333
Iteration 59 RMS(Cart)= 0.00014236 RMS(Int)= 0.03820094
Iteration 60 RMS(Cart)= 0.00014165 RMS(Int)= 0.03811889
Iteration 61 RMS(Cart)= 0.00014094 RMS(Int)= 0.03803720
Iteration 62 RMS(Cart)= 0.00014025 RMS(Int)= 0.03795586
Iteration 63 RMS(Cart)= 0.00013956 RMS(Int)= 0.03787487
Iteration 64 RMS(Cart)= 0.00013888 RMS(Int)= 0.03779422
Iteration 65 RMS(Cart)= 0.00013821 RMS(Int)= 0.03771391
Iteration 66 RMS(Cart)= 0.00013754 RMS(Int)= 0.03763393
Iteration 67 RMS(Cart)= 0.00013688 RMS(Int)= 0.03755429
Iteration 68 RMS(Cart)= 0.00013623 RMS(Int)= 0.03747497
Iteration 69 RMS(Cart)= 0.00013559 RMS(Int)= 0.03739598
Iteration 70 RMS(Cart)= 0.00013495 RMS(Int)= 0.03731732
Iteration 71 RMS(Cart)= 0.00013433 RMS(Int)= 0.03723897
Iteration 72 RMS(Cart)= 0.00013370 RMS(Int)= 0.03716094
Iteration 73 RMS(Cart)= 0.00013309 RMS(Int)= 0.03708322
Iteration 74 RMS(Cart)= 0.00013248 RMS(Int)= 0.03700582
Iteration 75 RMS(Cart)= 0.00013187 RMS(Int)= 0.03692872
Iteration 76 RMS(Cart)= 0.00013128 RMS(Int)= 0.03685193
Iteration 77 RMS(Cart)= 0.00013069 RMS(Int)= 0.03677543
Iteration 78 RMS(Cart)= 0.00013010 RMS(Int)= 0.03669924
Iteration 79 RMS(Cart)= 0.00012952 RMS(Int)= 0.03662334
Iteration 80 RMS(Cart)= 0.00012895 RMS(Int)= 0.03654774
Iteration 81 RMS(Cart)= 0.00012838 RMS(Int)= 0.03647243
Iteration 82 RMS(Cart)= 0.00012782 RMS(Int)= 0.03639740
Iteration 83 RMS(Cart)= 0.00012727 RMS(Int)= 0.03632267
Iteration 84 RMS(Cart)= 0.00012672 RMS(Int)= 0.03624821
Iteration 85 RMS(Cart)= 0.00012617 RMS(Int)= 0.03617404
Iteration 86 RMS(Cart)= 0.00012563 RMS(Int)= 0.03610014
Iteration 87 RMS(Cart)= 0.00012510 RMS(Int)= 0.03602652
Iteration 88 RMS(Cart)= 0.00012457 RMS(Int)= 0.03595318

Iteration 89 RMS(Cart)= 0.00012405 RMS(Int)= 0.03588010
Iteration 90 RMS(Cart)= 0.00012353 RMS(Int)= 0.03580729
Iteration 91 RMS(Cart)= 0.00012301 RMS(Int)= 0.03573475
Iteration 92 RMS(Cart)= 0.00012251 RMS(Int)= 0.03566248
Iteration 93 RMS(Cart)= 0.00012200 RMS(Int)= 0.03559046
Iteration 94 RMS(Cart)= 0.00012150 RMS(Int)= 0.03551871
Iteration 95 RMS(Cart)= 0.00012101 RMS(Int)= 0.03544721
Iteration 96 RMS(Cart)= 0.00012052 RMS(Int)= 0.03537597
Iteration 97 RMS(Cart)= 0.00012003 RMS(Int)= 0.03530498
Iteration 98 RMS(Cart)= 0.00011955 RMS(Int)= 0.03523424
Iteration 99 RMS(Cart)= 0.00011907 RMS(Int)= 0.03516376
Iteration100 RMS(Cart)= 0.00011859 RMS(Int)= 0.03509352
New curvilinear step not converged.
ITry= 2 IFail=1 DXMaxC= 7.34D-01 DCOld= 1.00D+10 DXMaxT= 1.50D+00 DXLimC= 3.00D+00 Rises=F
Iteration 1 RMS(Cart)= 0.15117646 RMS(Int)= 0.04314419
Iteration 2 RMS(Cart)= 0.02359686 RMS(Int)= 0.03023030
Iteration 3 RMS(Cart)= 0.00013233 RMS(Int)= 0.03014600
Iteration 4 RMS(Cart)= 0.00013172 RMS(Int)= 0.03006208
Iteration 5 RMS(Cart)= 0.00013112 RMS(Int)= 0.02997853
Iteration 6 RMS(Cart)= 0.00013052 RMS(Int)= 0.02989536
Iteration 7 RMS(Cart)= 0.00012993 RMS(Int)= 0.02981256
Iteration 8 RMS(Cart)= 0.00012934 RMS(Int)= 0.02973011
Iteration 9 RMS(Cart)= 0.00012876 RMS(Int)= 0.02964803
Iteration 10 RMS(Cart)= 0.00012819 RMS(Int)= 0.02956631
Iteration 11 RMS(Cart)= 0.00012762 RMS(Int)= 0.02948494
Iteration 12 RMS(Cart)= 0.00012706 RMS(Int)= 0.02940392
Iteration 13 RMS(Cart)= 0.00012650 RMS(Int)= 0.02932325
Iteration 14 RMS(Cart)= 0.00012595 RMS(Int)= 0.02924292
Iteration 15 RMS(Cart)= 0.00012540 RMS(Int)= 0.02916293
Iteration 16 RMS(Cart)= 0.00006341 RMS(Int)= 0.02912248
Iteration 17 RMS(Cart)= 0.00006327 RMS(Int)= 0.02908212
Iteration 18 RMS(Cart)= 0.00006313 RMS(Int)= 0.02904185
Iteration 19 RMS(Cart)= 0.00006299 RMS(Int)= 0.02900166
Iteration 20 RMS(Cart)= 0.00006285 RMS(Int)= 0.02896156
Iteration 21 RMS(Cart)= 0.00006271 RMS(Int)= 0.02892155
Iteration 22 RMS(Cart)= 0.00006257 RMS(Int)= 0.02888162
Iteration 23 RMS(Cart)= 0.00006244 RMS(Int)= 0.02884178
Iteration 24 RMS(Cart)= 0.00006230 RMS(Int)= 0.02880202
Iteration 25 RMS(Cart)= 0.00006217 RMS(Int)= 0.02876235
Iteration 26 RMS(Cart)= 0.00006203 RMS(Int)= 0.02872276
Iteration 27 RMS(Cart)= 0.00006190 RMS(Int)= 0.02868326
Iteration 28 RMS(Cart)= 0.00006176 RMS(Int)= 0.02864383
Iteration 29 RMS(Cart)= 0.00006163 RMS(Int)= 0.02860450

Iteration 30 RMS(Cart)= 0.00006150 RMS(Int)= 0.02856524
Iteration 31 RMS(Cart)= 0.00006136 RMS(Int)= 0.02852607
Iteration 32 RMS(Cart)= 0.00006123 RMS(Int)= 0.02848698
Iteration 33 RMS(Cart)= 0.00006110 RMS(Int)= 0.02844797
Iteration 34 RMS(Cart)= 0.00006097 RMS(Int)= 0.02840904
Iteration 35 RMS(Cart)= 0.00006084 RMS(Int)= 0.02837020
Iteration 36 RMS(Cart)= 0.00006071 RMS(Int)= 0.02833143
Iteration 37 RMS(Cart)= 0.00006058 RMS(Int)= 0.02829275
Iteration 38 RMS(Cart)= 0.00006046 RMS(Int)= 0.02825414
Iteration 39 RMS(Cart)= 0.00006033 RMS(Int)= 0.02821562
Iteration 40 RMS(Cart)= 0.00006020 RMS(Int)= 0.02817717
Iteration 41 RMS(Cart)= 0.00006007 RMS(Int)= 0.02813880
Iteration 42 RMS(Cart)= 0.00005995 RMS(Int)= 0.02810051
Iteration 43 RMS(Cart)= 0.00005982 RMS(Int)= 0.02806230
Iteration 44 RMS(Cart)= 0.00005970 RMS(Int)= 0.02802417
Iteration 45 RMS(Cart)= 0.00005958 RMS(Int)= 0.02798612
Iteration 46 RMS(Cart)= 0.00005945 RMS(Int)= 0.02794814
Iteration 47 RMS(Cart)= 0.00005933 RMS(Int)= 0.02791024
Iteration 48 RMS(Cart)= 0.00005921 RMS(Int)= 0.02787241
Iteration 49 RMS(Cart)= 0.00005908 RMS(Int)= 0.02783466
Iteration 50 RMS(Cart)= 0.00005896 RMS(Int)= 0.02779699
Iteration 51 RMS(Cart)= 0.00005884 RMS(Int)= 0.02775940
Iteration 52 RMS(Cart)= 0.00005872 RMS(Int)= 0.02772188
Iteration 53 RMS(Cart)= 0.00005860 RMS(Int)= 0.02768443
Iteration 54 RMS(Cart)= 0.00005848 RMS(Int)= 0.02764706
Iteration 55 RMS(Cart)= 0.00005836 RMS(Int)= 0.02760976
Iteration 56 RMS(Cart)= 0.00005824 RMS(Int)= 0.02757254
Iteration 57 RMS(Cart)= 0.00005813 RMS(Int)= 0.02753539
Iteration 58 RMS(Cart)= 0.00005801 RMS(Int)= 0.02749832
Iteration 59 RMS(Cart)= 0.00005789 RMS(Int)= 0.02746131
Iteration 60 RMS(Cart)= 0.00005777 RMS(Int)= 0.02742438
Iteration 61 RMS(Cart)= 0.00005766 RMS(Int)= 0.02738753
Iteration 62 RMS(Cart)= 0.00005754 RMS(Int)= 0.02735074
Iteration 63 RMS(Cart)= 0.00005743 RMS(Int)= 0.02731403
Iteration 64 RMS(Cart)= 0.00005731 RMS(Int)= 0.02727739
Iteration 65 RMS(Cart)= 0.00005720 RMS(Int)= 0.02724082
Iteration 66 RMS(Cart)= 0.00005709 RMS(Int)= 0.02720433
Iteration 67 RMS(Cart)= 0.00005697 RMS(Int)= 0.02716790
Iteration 68 RMS(Cart)= 0.00005686 RMS(Int)= 0.02713154
Iteration 69 RMS(Cart)= 0.00005675 RMS(Int)= 0.02709526
Iteration 70 RMS(Cart)= 0.00005664 RMS(Int)= 0.02705904
Iteration 71 RMS(Cart)= 0.00005652 RMS(Int)= 0.02702290
Iteration 72 RMS(Cart)= 0.00005641 RMS(Int)= 0.02698682
Iteration 73 RMS(Cart)= 0.00005630 RMS(Int)= 0.02695081

Iteration 74 RMS(Cart)= 0.00005619 RMS(Int)= 0.02691487
Iteration 75 RMS(Cart)= 0.00005608 RMS(Int)= 0.02687900
Iteration 76 RMS(Cart)= 0.00005597 RMS(Int)= 0.02684320
Iteration 77 RMS(Cart)= 0.00005586 RMS(Int)= 0.02680747
Iteration 78 RMS(Cart)= 0.00005576 RMS(Int)= 0.02677181
Iteration 79 RMS(Cart)= 0.00005565 RMS(Int)= 0.02673621
Iteration 80 RMS(Cart)= 0.00005554 RMS(Int)= 0.02670068
Iteration 81 RMS(Cart)= 0.00005543 RMS(Int)= 0.02666522
Iteration 82 RMS(Cart)= 0.00005533 RMS(Int)= 0.02662982
Iteration 83 RMS(Cart)= 0.00005522 RMS(Int)= 0.02659449
Iteration 84 RMS(Cart)= 0.00005511 RMS(Int)= 0.02655923
Iteration 85 RMS(Cart)= 0.00005501 RMS(Int)= 0.02652404
Iteration 86 RMS(Cart)= 0.00005490 RMS(Int)= 0.02648891
Iteration 87 RMS(Cart)= 0.00005480 RMS(Int)= 0.02645384
Iteration 88 RMS(Cart)= 0.00005469 RMS(Int)= 0.02641884
Iteration 89 RMS(Cart)= 0.00005459 RMS(Int)= 0.02638391
Iteration 90 RMS(Cart)= 0.00005448 RMS(Int)= 0.02634904
Iteration 91 RMS(Cart)= 0.00005438 RMS(Int)= 0.02631424
Iteration 92 RMS(Cart)= 0.00005428 RMS(Int)= 0.02627950
Iteration 93 RMS(Cart)= 0.00005417 RMS(Int)= 0.02624483
Iteration 94 RMS(Cart)= 0.00005407 RMS(Int)= 0.02621022
Iteration 95 RMS(Cart)= 0.00005397 RMS(Int)= 0.02617567
Iteration 96 RMS(Cart)= 0.00005387 RMS(Int)= 0.02614119
Iteration 97 RMS(Cart)= 0.00005377 RMS(Int)= 0.02610677
Iteration 98 RMS(Cart)= 0.00005366 RMS(Int)= 0.02607242
Iteration 99 RMS(Cart)= 0.00005356 RMS(Int)= 0.02603813
Iteration100 RMS(Cart)= 0.00005346 RMS(Int)= 0.02600390
New curvilinear step not converged.
ITry= 3 IFail=1 DXMaxC= 6.92D-01 DCOld= 1.00D+10 DXMaxT= 1.50D+00 DXLimC= 3.00D+00 Rises=F
Iteration 1 RMS(Cart)= 0.12311906 RMS(Int)= 0.03809950
Iteration 2 RMS(Cart)= 0.00367158 RMS(Int)= 0.03625658
Iteration 3 RMS(Cart)= 0.00049326 RMS(Int)= 0.03600480
Iteration 4 RMS(Cart)= 0.00047917 RMS(Int)= 0.03575953
Iteration 5 RMS(Cart)= 0.00046672 RMS(Int)= 0.03551996
Iteration 6 RMS(Cart)= 0.00045566 RMS(Int)= 0.03528543
Iteration 7 RMS(Cart)= 0.00044565 RMS(Int)= 0.03505543
Iteration 8 RMS(Cart)= 0.00043644 RMS(Int)= 0.03482961
Iteration 9 RMS(Cart)= 0.00042786 RMS(Int)= 0.03460767
Iteration 10 RMS(Cart)= 0.00041967 RMS(Int)= 0.03438940
Iteration 11 RMS(Cart)= 0.00041219 RMS(Int)= 0.03417454
Iteration 12 RMS(Cart)= 0.00040496 RMS(Int)= 0.03396294
Iteration 13 RMS(Cart)= 0.00039807 RMS(Int)= 0.03375447
Iteration 14 RMS(Cart)= 0.00039148 RMS(Int)= 0.03354898

Iteration 15 RMS(Cart)= 0.00038516 RMS(Int)= 0.03334635
Iteration 16 RMS(Cart)= 0.00037908 RMS(Int)= 0.03314649
Iteration 17 RMS(Cart)= 0.00037324 RMS(Int)= 0.03294929
Iteration 18 RMS(Cart)= 0.00036760 RMS(Int)= 0.03275466
Iteration 19 RMS(Cart)= 0.00036216 RMS(Int)= 0.03256252
Iteration 20 RMS(Cart)= 0.00035689 RMS(Int)= 0.03237279
Iteration 21 RMS(Cart)= 0.00035180 RMS(Int)= 0.03218539
Iteration 22 RMS(Cart)= 0.00034687 RMS(Int)= 0.03200026
Iteration 23 RMS(Cart)= 0.00034209 RMS(Int)= 0.03181734
Iteration 24 RMS(Cart)= 0.00033745 RMS(Int)= 0.03163655
Iteration 25 RMS(Cart)= 0.00033294 RMS(Int)= 0.03145786
Iteration 26 RMS(Cart)= 0.00032856 RMS(Int)= 0.03128119
Iteration 27 RMS(Cart)= 0.00032431 RMS(Int)= 0.03110650
Iteration 28 RMS(Cart)= 0.00032017 RMS(Int)= 0.03093374
Iteration 29 RMS(Cart)= 0.00031613 RMS(Int)= 0.03076286
Iteration 30 RMS(Cart)= 0.00031221 RMS(Int)= 0.03059382
Iteration 31 RMS(Cart)= 0.00030839 RMS(Int)= 0.03042657
Iteration 32 RMS(Cart)= 0.00030466 RMS(Int)= 0.03026107
Iteration 33 RMS(Cart)= 0.00030102 RMS(Int)= 0.03009728
Iteration 34 RMS(Cart)= 0.00029748 RMS(Int)= 0.02993517
Iteration 35 RMS(Cart)= 0.00029401 RMS(Int)= 0.02977469
Iteration 36 RMS(Cart)= 0.00029063 RMS(Int)= 0.02961582
Iteration 37 RMS(Cart)= 0.00028733 RMS(Int)= 0.02945851
Iteration 38 RMS(Cart)= 0.00028411 RMS(Int)= 0.02930273
Iteration 39 RMS(Cart)= 0.00028095 RMS(Int)= 0.02914846
Iteration 40 RMS(Cart)= 0.00027787 RMS(Int)= 0.02899566
Iteration 41 RMS(Cart)= 0.00027485 RMS(Int)= 0.02884430
Iteration 42 RMS(Cart)= 0.00027190 RMS(Int)= 0.02869436
Iteration 43 RMS(Cart)= 0.00026901 RMS(Int)= 0.02854581
Iteration 44 RMS(Cart)= 0.00026618 RMS(Int)= 0.02839862
Iteration 45 RMS(Cart)= 0.00026340 RMS(Int)= 0.02825276
Iteration 46 RMS(Cart)= 0.00026069 RMS(Int)= 0.02810822
Iteration 47 RMS(Cart)= 0.00025802 RMS(Int)= 0.02796496
Iteration 48 RMS(Cart)= 0.00025541 RMS(Int)= 0.02782297
Iteration 49 RMS(Cart)= 0.00025285 RMS(Int)= 0.02768222
Iteration 50 RMS(Cart)= 0.00025033 RMS(Int)= 0.02754269
Iteration 51 RMS(Cart)= 0.00024786 RMS(Int)= 0.02740437
Iteration 52 RMS(Cart)= 0.00024543 RMS(Int)= 0.02726722
Iteration 53 RMS(Cart)= 0.00024304 RMS(Int)= 0.02713124
Iteration 54 RMS(Cart)= 0.00011480 RMS(Int)= 0.02706700
Iteration 55 RMS(Cart)= 0.00011434 RMS(Int)= 0.02700299
Iteration 56 RMS(Cart)= 0.00011389 RMS(Int)= 0.02693919
Iteration 57 RMS(Cart)= 0.00011344 RMS(Int)= 0.02687560
Iteration 58 RMS(Cart)= 0.00011299 RMS(Int)= 0.02681224

Iteration 59 RMS(Cart)= 0.00011255 RMS(Int)= 0.02674908
Iteration 60 RMS(Cart)= 0.00011210 RMS(Int)= 0.02668614
Iteration 61 RMS(Cart)= 0.00011166 RMS(Int)= 0.02662341
Iteration 62 RMS(Cart)= 0.00011123 RMS(Int)= 0.02656089
Iteration 63 RMS(Cart)= 0.00011079 RMS(Int)= 0.02649858
Iteration 64 RMS(Cart)= 0.00011036 RMS(Int)= 0.02643647
Iteration 65 RMS(Cart)= 0.00010993 RMS(Int)= 0.02637457
Iteration 66 RMS(Cart)= 0.00010951 RMS(Int)= 0.02631287
Iteration 67 RMS(Cart)= 0.00010908 RMS(Int)= 0.02625138
Iteration 68 RMS(Cart)= 0.00010866 RMS(Int)= 0.02619008
Iteration 69 RMS(Cart)= 0.00010824 RMS(Int)= 0.02612899
Iteration 70 RMS(Cart)= 0.00010782 RMS(Int)= 0.02606809
Iteration 71 RMS(Cart)= 0.00010740 RMS(Int)= 0.02600739
Iteration 72 RMS(Cart)= 0.00010698 RMS(Int)= 0.02594689
Iteration 73 RMS(Cart)= 0.00010656 RMS(Int)= 0.02588657
Iteration 74 RMS(Cart)= 0.00010614 RMS(Int)= 0.02582644
Iteration 75 RMS(Cart)= 0.00010572 RMS(Int)= 0.02576650
Iteration 76 RMS(Cart)= 0.00010529 RMS(Int)= 0.02570674
Iteration 77 RMS(Cart)= 0.00010486 RMS(Int)= 0.02564714
Iteration 78 RMS(Cart)= 0.00010442 RMS(Int)= 0.02558768
Iteration 79 RMS(Cart)= 0.00010397 RMS(Int)= 0.02552832
Iteration 80 RMS(Cart)= 0.00010343 RMS(Int)= 0.02546896
Iteration 81 RMS(Cart)= 0.00010594 RMS(Int)= 0.02540713
Iteration 82 RMS(Cart)= 0.00010220 RMS(Int)= 0.48379006
Iteration 83 RMS(Cart)= 0.00002610 RMS(Int)= 0.02535062
Iteration 84 RMS(Cart)= 0.00010201 RMS(Int)= 0.02529265
Iteration 85 RMS(Cart)= 0.00010167 RMS(Int)= 0.02523484
Iteration 86 RMS(Cart)= 0.00010131 RMS(Int)= 0.02517719
Iteration 87 RMS(Cart)= 0.00010094 RMS(Int)= 0.02511971
Iteration 88 RMS(Cart)= 0.00010055 RMS(Int)= 0.02506239
Iteration 89 RMS(Cart)= 0.00010017 RMS(Int)= 0.02500522
Iteration 90 RMS(Cart)= 0.00009977 RMS(Int)= 0.02494819
Iteration 91 RMS(Cart)= 0.00009936 RMS(Int)= 0.02489127
Iteration 92 RMS(Cart)= 0.00009888 RMS(Int)= 0.02483440
Iteration 93 RMS(Cart)= 0.00009846 RMS(Int)= 0.02477713
Iteration 94 RMS(Cart)= 0.00009793 RMS(Int)= 0.02465734
Iteration 95 RMS(Cart)= 0.00000000 RMS(Int)= 0.02465631
ITry= 4 IFail=0 DXMaxC= 5.69D-01 DCOld= 1.00D+10 DXMaxT= 1.50D+00 DXLimC= 3.00D+00
Rises=F

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56643	-0.00082	0.00000	0.00125	0.00042	2.56685
R2	2.62276	-0.00047	0.00000	-0.00363	-0.00069	2.62207
R3	2.03393	0.00005	0.00000	-0.00012	0.00054	2.03447

R4	2.63061	-0.00014	0.00000	-0.00081	-0.00133	2.62928
R5	2.03108	-0.00008	0.00000	-0.00029	0.00044	2.03151
R6	2.54404	0.00004	0.00000	-0.00283	-0.00079	2.54325
R7	2.68747	0.00015	0.00000	0.00119	0.00155	2.68902
R8	2.51604	0.00122	0.00000	-0.00512	0.00526	2.52130
R9	2.11473	-0.00240	0.00000	-0.02741	-0.01692	2.09781
R10	2.79395	-0.00136	0.00000	-0.00002	0.00724	2.80119
R11	2.90997	-0.00190	0.00000	-0.00805	0.00168	2.91165
R12	2.06278	0.00012	0.00000	-0.00120	0.00177	2.06455
R13	2.06207	0.00013	0.00000	-0.00038	0.00215	2.06423
R14	2.07220	0.00024	0.00000	-0.00175	-0.00097	2.07124
R15	2.07027	-0.00023	0.00000	-0.00230	-0.00097	2.06930
R16	2.66683	-0.00261	0.00000	0.01319	0.01526	2.68208
R17	4.11038	-0.00083	0.00000	0.09772	0.06498	4.17536
R18	9.29620	-0.00176	0.00000	-0.93966	-0.34646	8.94975
R19	2.50703	-0.00019	0.00000	-0.00114	-0.00009	2.50693
R20	2.04715	-0.00015	0.00000	-0.00059	0.00019	2.04733
R21	2.04307	-0.00001	0.00000	-0.00014	0.00054	2.04362
R22	2.04629	-0.00011	0.00000	-0.00022	0.00053	2.04683
R23	1.84043	-0.00250	0.00000	-0.00288	-0.00070	1.83973
R24	3.68061	-0.00271	0.00000	-0.03978	-0.02512	3.65549
R25	2.77246	-0.00033	0.00000	0.00492	0.00821	2.78067
R26	2.73988	-0.00035	0.00000	0.00495	0.00674	2.74662
R27	2.05038	0.00195	0.00000	0.00185	0.00622	2.05660
R28	2.04728	0.00207	0.00000	0.00224	0.00331	2.05058
R29	2.73969	-0.00264	0.00000	-0.02055	-0.00759	2.73209
R30	2.05687	0.00013	0.00000	0.00011	0.00437	2.06124
R31	2.85849	-0.00325	0.00000	-0.00203	0.00292	2.86141
R32	2.06622	0.00001	0.00000	0.00192	0.00297	2.06919
R33	2.06932	-0.00082	0.00000	-0.00066	0.00096	2.07028
R34	2.06340	-0.00025	0.00000	-0.00070	0.00200	2.06540
A1	1.87254	0.00010	0.00000	-0.00035	0.00212	1.87466
A2	2.27706	-0.00010	0.00000	-0.00070	-0.00162	2.27544
A3	2.13345	0.00001	0.00000	0.00103	-0.00050	2.13295
A4	1.86194	0.00041	0.00000	0.00042	0.00042	1.86236
A5	2.27752	-0.00026	0.00000	-0.00058	-0.00046	2.27707
A6	2.14368	-0.00014	0.00000	0.00009	-0.00002	2.14366
A7	1.89762	0.00000	0.00000	-0.00362	-0.00074	1.89688
A8	2.25036	-0.00017	0.00000	0.00282	0.00099	2.25134
A9	2.13516	0.00017	0.00000	0.00080	-0.00025	2.13490
A10	1.88995	-0.00051	0.00000	0.00461	0.00190	1.89184
A11	2.24074	-0.00088	0.00000	-0.00088	-0.00832	2.23242
A12	2.15212	0.00139	0.00000	-0.00279	0.00680	2.15892
A13	1.90265	0.00001	0.00000	-0.00128	-0.00392	1.89872

A14	2.22505	-0.00166	0.00000	0.01409	-0.00125	2.22380
A15	2.15504	0.00165	0.00000	-0.01250	0.00537	2.16041
A16	1.95546	-0.00149	0.00000	-0.00694	-0.00499	1.95048
A17	1.86108	0.00058	0.00000	0.00367	0.00334	1.86442
A18	1.89091	0.00015	0.00000	-0.00052	-0.00093	1.88998
A19	1.93189	0.00012	0.00000	-0.00099	0.00264	1.93453
A20	1.91773	0.00055	0.00000	0.00689	0.00134	1.91907
A21	1.90514	0.00011	0.00000	-0.00221	-0.00141	1.90373
A22	1.90983	0.00121	0.00000	0.00462	-0.00102	1.90880
A23	1.91055	-0.00003	0.00000	0.00348	0.00317	1.91372
A24	1.92114	-0.00327	0.00000	-0.01091	-0.00070	1.92045
A25	1.88275	-0.00018	0.00000	0.01115	0.00805	1.89080
A26	1.88802	0.00075	0.00000	0.00057	-0.00288	1.88514
A27	1.95072	0.00161	0.00000	-0.00824	-0.00648	1.94424
A28	1.70738	-0.00159	0.00000	0.04591	0.00277	1.71016
A29	2.90978	-0.00140	0.00000	0.00319	0.00493	2.91471
A30	2.17589	-0.00004	0.00000	0.00088	0.00060	2.17649
A31	1.95399	0.00011	0.00000	-0.00028	-0.00017	1.95381
A32	2.15330	-0.00008	0.00000	-0.00059	-0.00042	2.15288
A33	2.07932	0.00003	0.00000	-0.00164	-0.00111	2.07821
A34	2.15762	-0.00003	0.00000	0.00295	0.00193	2.15955
A35	2.04624	0.00000	0.00000	-0.00130	-0.00082	2.04542
A36	1.91457	-0.00145	0.00000	-0.02872	-0.01261	1.90196
A37	3.14145	-0.00110	0.00000	0.00379	0.00014	3.14159
A38	2.09899	-0.00053	0.00000	-0.00069	0.00193	2.10092
A39	2.10191	-0.00020	0.00000	-0.01065	-0.00932	2.09259
A40	1.99600	0.00110	0.00000	0.00282	0.00426	2.00026
A41	1.98437	-0.00041	0.00000	-0.00566	-0.00714	1.97723
A42	2.01279	0.00058	0.00000	0.01320	0.00878	2.02157
A43	2.06153	-0.00063	0.00000	-0.00209	0.00261	2.06413
A44	2.13225	-0.00079	0.00000	0.00371	-0.00051	2.13174
A45	1.97224	-0.00153	0.00000	0.00373	0.00209	1.97433
A46	2.03267	0.00045	0.00000	0.00539	0.00514	2.03782
A47	2.00737	0.00137	0.00000	-0.00700	-0.00566	2.00170
A48	1.37769	0.00124	0.00000	0.07882	0.04110	1.41878
A49	1.01720	-0.00229	0.00000	-0.10180	-0.05482	0.96238
A50	2.39154	-0.00102	0.00000	-0.00906	-0.01090	2.38064
A51	2.22337	-0.00064	0.00000	-0.02220	-0.01267	2.21070
A52	1.91860	0.00159	0.00000	-0.00094	-0.00113	1.91747
A53	1.92079	-0.00036	0.00000	0.00006	0.00129	1.92208
A54	1.92076	0.00188	0.00000	0.01080	0.00691	1.92767
A55	1.89577	-0.00085	0.00000	-0.00316	-0.00331	1.89246
A56	1.91045	-0.00154	0.00000	-0.00131	0.00033	1.91077
A57	1.89714	-0.00078	0.00000	-0.00571	-0.00428	1.89286

A58	3.60106	0.00060	0.00000	0.05662	0.02843	3.62949
A59	4.70094	0.00112	0.00000	0.21578	0.14182	4.84276
D1	0.01171	-0.00042	0.00000	0.01433	0.00873	0.02044
D2	-3.13947	-0.00018	0.00000	0.00598	0.00360	-3.13587
D3	3.13565	-0.00004	0.00000	0.01304	0.00868	-3.13886
D4	-0.01552	0.00020	0.00000	0.00469	0.00354	-0.01198
D5	-0.01107	0.00038	0.00000	-0.02159	-0.01301	-0.02409
D6	-3.12113	0.00038	0.00000	-0.03223	-0.02077	3.14129
D7	-3.13679	0.00004	0.00000	-0.02041	-0.01295	3.13345
D8	0.03634	0.00004	0.00000	-0.03105	-0.02070	0.01564
D9	-0.00848	0.00033	0.00000	-0.00241	-0.00152	-0.01000
D10	-3.13977	0.00019	0.00000	-0.00166	-0.00042	-3.14019
D11	-3.14140	0.00012	0.00000	0.00515	0.00313	-3.13827
D12	0.01050	-0.00002	0.00000	0.00590	0.00423	0.01473
D13	0.00165	-0.00010	0.00000	-0.01104	-0.00660	-0.00495
D14	3.11414	-0.00003	0.00000	0.02506	0.01888	3.13303
D15	3.13376	0.00002	0.00000	-0.01172	-0.00761	3.12615
D16	-0.03694	0.00010	0.00000	0.02438	0.01788	-0.01906
D17	0.08570	-0.00014	0.00000	-0.03786	-0.02550	0.06019
D18	-3.05989	-0.00008	0.00000	-0.03671	-0.02472	-3.08461
D19	-3.04434	-0.00030	0.00000	-0.03699	-0.02427	-3.06861
D20	0.09326	-0.00023	0.00000	-0.03584	-0.02348	0.06977
D21	0.00575	-0.00017	0.00000	0.02012	0.01208	0.01784
D22	3.11735	-0.00024	0.00000	0.03081	0.01936	3.13670
D23	-3.10854	-0.00019	0.00000	-0.01377	-0.01178	-3.12033
D24	0.00305	-0.00027	0.00000	-0.00308	-0.00451	-0.00146
D25	-2.91766	-0.00025	0.00000	-0.15920	-0.10907	-3.02673
D26	0.19086	-0.00021	0.00000	-0.11806	-0.08013	0.11073
D27	1.26532	0.00017	0.00000	0.11605	0.07140	1.33672
D28	-2.90170	-0.00018	0.00000	0.11311	0.07386	-2.82785
D29	-0.85310	0.00033	0.00000	0.11219	0.07350	-0.77960
D30	-1.84053	0.00022	0.00000	0.10371	0.06274	-1.77778
D31	0.27563	-0.00014	0.00000	0.10077	0.06520	0.34084
D32	2.32424	0.00037	0.00000	0.09985	0.06485	2.38909
D33	-0.92232	-0.00015	0.00000	-0.09772	-0.06230	-0.98463
D34	1.13756	0.00033	0.00000	-0.07944	-0.05126	1.08630
D35	-2.99493	0.00016	0.00000	-0.09467	-0.05774	-3.05267
D36	-2.99715	0.00001	0.00000	-0.09714	-0.06502	-3.06217
D37	-0.93727	0.00049	0.00000	-0.07886	-0.05398	-0.99124
D38	1.21342	0.00032	0.00000	-0.09409	-0.06045	1.15297
D39	1.18059	-0.00056	0.00000	-0.09824	-0.06584	1.11476
D40	-3.04270	-0.00009	0.00000	-0.07996	-0.05480	-3.09750
D41	-0.89201	-0.00025	0.00000	-0.09519	-0.06127	-0.95328
D42	-1.79340	0.00064	0.00000	0.00903	-0.00050	-1.79391

D43	2.40385	0.00062	0.00000	0.00944	0.00288	2.40674
D44	0.33360	-0.00058	0.00000	0.00025	-0.00134	0.33226
D45	0.29133	-0.00046	0.00000	0.17253	0.11126	0.40259
D46	-0.35287	0.00019	0.00000	-0.04208	-0.02415	-0.37702
D47	2.86262	-0.00010	0.00000	-0.19341	-0.12789	2.73473
D48	-3.13757	0.00003	0.00000	-0.00104	-0.00067	-3.13824
D49	0.00647	-0.00001	0.00000	-0.00445	-0.00296	0.00352
D50	0.00846	-0.00004	0.00000	-0.00232	-0.00154	0.00692
D51	-3.13068	-0.00008	0.00000	-0.00573	-0.00383	-3.13451
D52	-1.42703	-0.00003	0.00000	0.06856	0.06191	-1.36512
D53	2.09162	0.00056	0.00000	-0.05369	-0.05863	2.03300
D54	2.18388	-0.00003	0.00000	-0.24954	-0.18640	1.99748
D55	-2.60931	-0.00056	0.00000	-0.26947	-0.20045	-2.80976
D56	-2.72700	-0.00022	0.00000	0.00670	0.00390	-2.72311
D57	-0.03081	0.00002	0.00000	-0.00892	-0.00656	-0.03737
D58	0.00455	-0.00051	0.00000	0.01496	0.00983	0.01438
D59	2.70074	-0.00027	0.00000	-0.00066	-0.00063	2.70011
D60	0.15526	0.00049	0.00000	-0.23975	-0.16189	-0.00663
D61	0.04877	0.00100	0.00000	-0.02184	-0.01261	0.03616
D62	-2.20720	-0.00115	0.00000	-0.25699	-0.17227	-2.37948
D63	-2.31369	-0.00064	0.00000	-0.03909	-0.02299	-2.33669
D64	2.11119	0.00087	0.00000	0.00928	0.00767	2.11887
D65	-0.26981	-0.00004	0.00000	0.00995	0.00840	-0.26141
D66	2.51724	0.00043	0.00000	-0.04946	-0.03252	2.48471
D67	-1.67862	0.00014	0.00000	-0.05391	-0.03651	-1.71513
D68	0.41176	0.00013	0.00000	-0.05413	-0.03663	0.37513
D69	1.30884	-0.00012	0.00000	-0.05952	-0.03804	1.27080
D70	-2.88702	-0.00041	0.00000	-0.06397	-0.04203	-2.92905
D71	-0.79663	-0.00042	0.00000	-0.06419	-0.04215	-0.83878
D72	-1.05704	0.00021	0.00000	-0.06359	-0.04074	-1.09778
D73	1.03029	-0.00008	0.00000	-0.06803	-0.04473	0.98556
D74	3.12067	-0.00009	0.00000	-0.06825	-0.04484	3.07583

Item	Value	Threshold	Converged?
Maximum Force	0.003265	0.000450	NO
RMS Force	0.000902	0.000300	NO
Maximum Displacement	0.569139	0.001800	NO
RMS Displacement	0.144039	0.001200	NO

Predicted change in Energy=-7.893192D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-1.426066	-1.886717	-0.311282
2	6	0	-2.565519	-1.152008	-0.228326
3	7	0	-2.188748	0.126779	0.169947
4	6	0	-0.853153	0.151309	0.333800
5	7	0	-0.373083	-1.063202	0.060625
6	6	0	1.065237	-1.415299	0.128051
7	6	0	1.707459	-1.463965	-1.271660
8	1	0	-1.279210	-2.917231	-0.586113
9	1	0	-3.586650	-1.423386	-0.426660
10	1	0	1.547298	-0.658040	0.750754
11	1	0	1.157331	-2.388993	0.614516
12	1	0	1.155051	-2.171492	-1.900610
13	1	0	1.652444	-0.474079	-1.736617
14	35	0	1.418658	2.404163	1.144751
15	1	0	-0.218998	1.010090	0.638249
16	6	0	-3.004979	1.268783	0.403239
17	6	0	-4.329728	1.277292	0.333469
18	1	0	-2.415960	2.143636	0.651132
19	1	0	-4.860155	2.199901	0.525671
20	1	0	-4.924976	0.405066	0.092466
21	8	0	3.049057	-1.917053	-1.175557
22	1	0	3.647621	-1.153646	-1.257496
23	6	0	4.830436	1.755426	-1.002887
24	6	0	5.808099	0.807313	-0.445686
25	8	0	4.836954	0.363223	-1.420308
26	1	0	3.958005	2.050592	-0.423101
27	1	0	5.129162	2.440547	-1.789562
28	1	0	6.826916	0.827560	-0.834737
29	6	0	5.676482	0.243735	0.953539
30	1	0	5.991063	-0.805027	0.963316
31	1	0	6.314241	0.803104	1.646786
32	1	0	4.642177	0.317235	1.299046

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.358319	0.000000			
3	N	2.206225	1.391357	0.000000		
4	C	2.213121	2.224144	1.345832	0.000000	
5	N	1.387539	2.213177	2.173624	1.334214	0.000000
6	C	2.573293	3.657693	3.601136	2.485320	1.482324
7	C	3.304546	4.409559	4.448497	3.426857	2.502849
8	H	1.076596	2.213281	3.265713	3.231671	2.162582

9	H	2.212716	1.075031	2.170963	3.244991	3.270197
10	H	3.387987	4.256508	3.861517	2.567306	2.080456
11	H	2.789861	4.012497	4.209869	3.251766	2.099211
12	H	3.044540	4.204583	4.555243	3.797482	2.722121
13	H	3.674826	4.530534	4.330216	3.309948	2.771264
14	Br	5.350153	5.514106	4.376083	3.300624	4.050714
15	H	3.278736	3.306324	2.208949	1.110111	2.157760
16	C	3.600095	2.540124	1.422966	2.425680	3.533046
17	C	4.342569	3.054431	2.436025	3.654369	4.605148
18	H	4.260267	3.414248	2.085876	2.551947	3.847838
19	H	5.403139	4.131485	3.400117	4.504399	5.567578
20	H	4.202101	2.845070	2.751434	4.086854	4.782944
21	O	4.557917	5.745085	5.781196	4.667282	3.737412
22	H	5.212966	6.297802	6.143312	4.948950	4.232220
23	C	7.272368	7.984564	7.300477	6.055007	6.012681
24	C	7.720686	8.602538	8.049328	6.738711	6.477823
25	O	6.746672	7.649402	7.207309	5.958114	5.601101
26	H	6.671066	7.269866	6.468024	5.227563	5.356120
27	H	7.992592	8.634352	7.921174	6.748139	6.780424
28	H	8.703621	9.617914	9.098499	7.797837	7.497776
29	C	7.522286	8.442481	7.905032	6.559631	6.253209
30	H	7.603187	8.646127	8.270853	6.939321	6.433029
31	H	8.425052	9.283784	8.656748	7.315757	7.121749
32	H	6.653881	7.512817	6.926231	5.581925	5.347161

		6	7	8	9	10
6	C	0.000000				
7	C	1.540781	0.000000			
8	H	2.874415	3.391483	0.000000		
9	H	4.684850	5.361275	2.753411	0.000000	
10	H	1.092512	2.182962	3.857499	5.322544	0.000000
11	H	1.092341	2.171630	2.767179	4.951949	1.779560
12	H	2.166877	1.096051	2.865250	5.021545	3.078006
13	H	2.169722	1.095028	3.985881	5.483181	2.496379
14	Br	3.968234	4.569996	6.212215	6.494042	3.090124
15	H	2.791429	3.671503	4.248171	4.289162	2.432101
16	C	4.883307	5.699147	4.634631	2.876604	4.955465
17	C	6.033067	6.821918	5.267382	2.902348	6.201537
18	H	5.005834	5.806419	5.332481	3.905867	4.854557
19	H	6.952557	7.732262	6.343837	3.956888	7.019540
20	H	6.260803	7.024480	4.978929	2.324618	6.591954
21	O	2.426250	1.419298	4.481260	6.696055	2.747920
22	H	2.942263	1.964873	5.275856	7.286819	2.947890
23	C	5.050667	4.493295	7.702934	9.015776	4.436110
24	C	5.269148	4.759851	8.007615	9.655967	4.661883

25	O	4.448191	3.626906	6.990331	8.668127	4.071649
26	H	4.547997	4.258769	7.220406	8.306043	3.811316
27	H	5.921172	5.217421	8.439272	9.630829	5.374402
28	H	6.257342	5.625907	8.932780	10.661878	5.709217
29	C	4.969648	4.860133	7.793837	9.512616	4.231369
30	H	5.033276	4.876328	7.727808	9.697783	4.451274
31	H	5.897449	5.905875	8.745697	10.357802	5.065724
32	H	4.143357	4.288796	7.005599	8.586118	3.290906

		11	12	13	14	15
11	H	0.000000				
12	H	2.524514	0.000000			
13	H	3.072436	1.776374	0.000000		
14	Br	4.829471	5.502756	4.079364	0.000000	
15	H	3.667235	4.296076	3.368240	2.209503	0.000000
16	C	5.545159	5.869332	5.413699	4.626823	2.807817
17	C	6.605184	6.853322	6.568024	5.913709	4.130664
18	H	5.771870	6.154985	5.394969	3.875027	2.472193
19	H	7.568090	7.821676	7.394732	6.312565	4.792563
20	H	6.713700	6.897661	6.883378	6.733898	4.775998
21	O	2.646831	2.043942	2.085064	5.168649	4.747445
22	H	3.351426	2.768124	2.161505	4.837052	4.819372
23	C	5.769220	5.452985	3.950783	4.083312	5.361496
24	C	5.741955	5.713225	4.536292	4.934228	6.127147
25	O	5.025418	4.495762	3.307905	4.736002	5.497158
26	H	5.350732	5.278785	3.662636	3.005237	4.433561
27	H	6.699216	6.089072	4.537116	4.730682	6.045105
28	H	6.677630	6.503880	5.411360	5.971039	7.200550
29	C	5.241080	5.867097	4.893371	4.778396	5.953435
30	H	5.098586	5.784143	5.120819	5.589160	6.478054
31	H	6.152136	6.931773	5.900082	5.175148	6.613864
32	H	4.465020	5.347112	4.333582	3.843195	4.954566

		16	17	18	19	20
16	C	0.000000				
17	C	1.326613	0.000000			
18	H	1.083402	2.124610	0.000000		
19	H	2.079339	1.081435	2.448059	0.000000	
20	H	2.128139	1.083134	3.103206	1.847512	0.000000
21	O	7.020932	8.180920	7.049283	9.077396	8.401506
22	H	7.272090	8.489920	7.161142	9.317093	8.817109
23	C	7.975446	9.269469	7.442899	9.820469	9.909154
24	C	8.865888	10.178580	8.403804	10.802522	10.754083
25	O	8.101930	9.377597	7.750194	10.059530	9.878538
26	H	7.055296	8.358044	6.464524	8.870310	9.048807
27	H	8.505625	9.763761	7.935617	10.256933	10.429329

28	H	9.919346	11.226650	9.453604	11.845745	11.795981
29	C	8.759070	10.078540	8.317974	10.725222	10.637593
30	H	9.248954	10.547582	8.914602	11.268100	11.017378
31	H	9.413348	10.735163	8.888462	11.317025	11.353164
32	H	7.758022	9.074642	7.319347	9.717863	9.643338

		21	22	23	24	25
21	O	0.000000				
22	H	0.973542	0.000000			
23	C	4.085367	3.150647	0.000000		
24	C	3.945529	3.028541	1.471467	0.000000	
25	O	2.907944	1.934402	1.453448	1.445762	0.000000
26	H	4.139394	3.325612	1.088307	2.229148	2.148066
27	H	4.867496	3.923810	1.085121	2.221354	2.130026
28	H	4.682017	3.769857	2.207972	1.090761	2.125665
29	C	4.013156	3.310231	2.613160	1.514191	2.520761
30	H	3.803522	3.247347	3.430587	2.149047	2.894553
31	H	5.101598	4.401657	3.182666	2.152820	3.432628
32	H	3.695096	3.112642	2.720796	2.154911	2.726709

		26	27	28	29	30
26	H	0.000000				
27	H	1.841437	0.000000			
28	H	3.145776	2.528990	0.000000		
29	C	2.848338	3.556705	2.205058	0.000000	
30	H	3.769620	4.342231	2.568460	1.094970	0.000000
31	H	3.375279	3.986744	2.534047	1.095546	1.776981
32	H	2.537402	3.779565	3.096215	1.092961	1.786528

		31	32
31	H	0.000000	
32	H	1.775609	0.000000

Stoichiometry C10H17BrN2O2
Framework group C1[X(C10H17BrN2O2)]
Deg. of freedom 90
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.666920	2.219279	-0.318125
2	6	0	-3.761513	1.476173	-0.010407
3	7	0	-3.333685	0.155937	0.088661
4	6	0	-2.013217	0.110287	-0.167354

5	7	0	-1.592238	1.348775	-0.430131
6	6	0	-0.186386	1.690360	-0.752907
7	6	0	0.544360	2.304044	0.456808
8	1	0	-2.566209	3.278992	-0.479134
9	1	0	-4.781857	1.771978	0.154181
10	1	0	0.298771	0.764767	-1.071471
11	1	0	-0.187938	2.397474	-1.585492
12	1	0	-0.007338	3.184199	0.806498
13	1	0	0.582392	1.574750	1.272756
14	35	0	0.334419	-2.208887	-0.231841
15	1	0	-1.348867	-0.779087	-0.167636
16	6	0	-4.091230	-1.010614	0.388852
17	6	0	-5.405181	-1.031913	0.570462
18	1	0	-3.467021	-1.893966	0.450593
19	1	0	-5.888990	-1.971838	0.798433
20	1	0	-6.035894	-0.153871	0.503960
21	8	0	1.845690	2.724237	0.076826
22	1	0	2.494690	2.073034	0.397008
23	6	0	3.836146	-0.664720	1.191849
24	6	0	4.713264	0.018431	0.227908
25	8	0	3.784236	0.779111	1.033203
26	1	0	2.946685	-1.190436	0.849951
27	1	0	4.229157	-0.976715	2.153976
28	1	0	5.755251	0.183869	0.504773
29	6	0	4.452966	-0.016475	-1.263333
30	1	0	4.700399	0.953527	-1.706991
31	1	0	5.076119	-0.783020	-1.736945
32	1	0	3.404314	-0.251488	-1.462486

Rotational constants (GHZ): 0.5624593 0.2137250 0.1648352

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.

475 basis functions, 751 primitive gaussians, 492 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1285.8467458822 Hartrees.

NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 475 RedAO= T EigKep= 3.74D-06 NBF= 475

NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999933 0.001073 -0.000943 -0.011521 Ang= 1.33 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3225.52202099 A.U. after 13 cycles
NFock= 13 Conv=0.24D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000159636	-0.000824211	0.001953193
2	6	0.000761396	-0.000080760	-0.001710842
3	7	0.000238151	-0.000069529	0.000358376
4	6	0.002074530	-0.002044616	0.000358528
5	7	0.000786238	0.001318759	-0.000596851
6	6	0.001223963	-0.000126047	-0.001045397
7	6	0.005350954	-0.001159755	0.000111778
8	1	-0.000038593	0.000009315	0.000352352
9	1	0.000272018	0.000028292	-0.000072083
10	1	-0.000571401	0.000186948	-0.001202946
11	1	-0.000892285	0.000616303	-0.000425733
12	1	-0.000131254	0.000196674	-0.000506641
13	1	-0.000895468	-0.000006880	0.000547428
14	35	0.000120889	-0.001570618	-0.000917263
15	1	0.000418870	0.001910417	0.000828760
16	6	-0.000007303	0.000018706	0.000017880

17	6	-0.000042234	0.000028732	-0.000260126
18	1	-0.000159756	-0.000151905	0.000049537
19	1	0.000074927	-0.000187854	0.000024593
20	1	0.000322630	0.000174927	0.000064332
21	8	-0.006670928	0.002340344	0.000317307
22	1	0.000673058	0.001306931	0.001167807
23	6	-0.000700752	-0.002830084	-0.000697791
24	6	-0.001760053	0.000618696	0.005436064
25	8	0.000419148	-0.001630660	0.000698482
26	1	0.000903562	-0.000565585	0.001399788
27	1	0.001244732	0.000725410	-0.000249609
28	1	-0.001973032	0.000537787	-0.001824858
29	6	-0.001037233	0.001556611	-0.004793885
30	1	-0.000349395	0.000654450	0.001127099
31	1	-0.000581372	-0.000524779	-0.000933136
32	1	0.001085633	-0.000456019	0.000423856

Cartesian Forces: Max 0.006670928 RMS 0.001472355

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.006995827 RMS 0.001067583
Search for a local minimum.
Step number 18 out of a maximum of 177
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 17 18
DE= -9.37D-04 DEPred=-7.89D-04 R= 1.19D+00
TightC=F SS= 1.41D+00 RLast= 6.47D-01 DXNew= 2.5227D+00 1.9420D+00
Trust test= 1.19D+00 RLast= 6.47D-01 DXMaxT set to 1.94D+00
ITU= 1 -1 1 1 1 1 1 1 1 1 1 1 1 0 1 0 1 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00000	0.00123	0.00232	0.00279	0.00366
Eigenvalues ---	0.00454	0.00900	0.01229	0.01399	0.01511
Eigenvalues ---	0.01755	0.01885	0.02051	0.02160	0.02200
Eigenvalues ---	0.02260	0.02319	0.02383	0.02608	0.03055
Eigenvalues ---	0.03064	0.03149	0.03553	0.03707	0.03996
Eigenvalues ---	0.04593	0.05094	0.05257	0.05566	0.05632
Eigenvalues ---	0.05918	0.06246	0.07773	0.09387	0.09625
Eigenvalues ---	0.10357	0.11093	0.11652	0.11979	0.12848
Eigenvalues ---	0.13874	0.15135	0.15435	0.15990	0.15999
Eigenvalues ---	0.16000	0.16000	0.16004	0.16007	0.16079

Eigenvalues --- 0.16757 0.17659 0.19756 0.21845 0.22046
Eigenvalues --- 0.22845 0.23649 0.23722 0.25055 0.25263
Eigenvalues --- 0.27744 0.29931 0.31266 0.32908 0.33100
Eigenvalues --- 0.33260 0.34098 0.34490 0.34674 0.34888
Eigenvalues --- 0.35143 0.35555 0.35687 0.35712 0.35866
Eigenvalues --- 0.36439 0.36662 0.37225 0.37237 0.37763
Eigenvalues --- 0.37965 0.42190 0.42551 0.45449 0.48651
Eigenvalues --- 0.51158 0.52777 0.54574 0.56338 0.60367
RFO step: Lambda=-1.17899688D-03 EMin= 2.39906276D-06
Quartic linear search produced a step of 0.42586.
Iteration 1 RMS(Cart)= 0.00209032 RMS(Int)= 0.03246026
SLEqS3 Cycle: 90 Max:0.847797E-01 RMS: 2865.34 Conv:0.173959E-01
Iteration 2 RMS(Cart)= 0.05280305 RMS(Int)= 0.01634085
SLEqS3 Cycle: 22 Max:0.853184E-01 RMS: 10920.2 Conv:0.663278E-01
Iteration 3 RMS(Cart)= 0.05743977 RMS(Int)= 0.00931541
Iteration 4 RMS(Cart)= 0.00373514 RMS(Int)= 0.00866043
Iteration 5 RMS(Cart)= 0.00463149 RMS(Int)= 0.00751866
Iteration 6 RMS(Cart)= 0.00527858 RMS(Int)= 0.00619604
Iteration 7 RMS(Cart)= 0.00867142 RMS(Int)= 0.00450379
Iteration 8 RMS(Cart)= 0.00586445 RMS(Int)= 0.00149376
Iteration 9 RMS(Cart)= 0.00001114 RMS(Int)= 0.00062340
Iteration 10 RMS(Cart)= 0.00000228 RMS(Int)= 0.00062340
Iteration 11 RMS(Cart)= 0.00000000 RMS(Int)= 0.00062340

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56685	-0.00124	0.00018	-0.00064	-0.00048	2.56637
R2	2.62207	-0.00050	-0.00029	-0.00182	-0.00210	2.61997
R3	2.03447	-0.00010	0.00023	-0.00038	-0.00015	2.03432
R4	2.62928	0.00010	-0.00057	0.00095	0.00036	2.62964
R5	2.03151	-0.00025	0.00019	-0.00056	-0.00037	2.03114
R6	2.54325	-0.00015	-0.00034	-0.00117	-0.00150	2.54175
R7	2.68902	-0.00021	0.00066	-0.00031	0.00036	2.68937
R8	2.52130	-0.00135	0.00224	-0.00785	-0.00541	2.51589
R9	2.09781	0.00026	-0.00721	-0.00178	-0.00895	2.08886
R10	2.80119	-0.00320	0.00308	-0.00918	-0.00594	2.79524
R11	2.91165	-0.00255	0.00072	-0.00724	-0.00648	2.90518
R12	2.06455	-0.00081	0.00075	-0.00358	-0.00283	2.06172
R13	2.06423	-0.00081	0.00092	-0.00287	-0.00195	2.06228
R14	2.07124	0.00023	-0.00041	-0.00057	-0.00098	2.07026
R15	2.06930	-0.00019	-0.00041	-0.00077	-0.00118	2.06812
R16	2.68208	-0.00700	0.00650	-0.01029	-0.00363	2.67845
R17	4.17536	-0.00179	0.02767	-0.00323	0.02444	4.19980
R18	8.94975	-0.00182	-0.14754	-0.13381	-0.28150	8.66824
R19	2.50693	-0.00035	-0.00004	-0.00067	-0.00070	2.50623

R20	2.04733	-0.00020	0.00008	-0.00043	-0.00035	2.04698
R21	2.04362	-0.00019	0.00023	-0.00051	-0.00028	2.04334
R22	2.04683	-0.00033	0.00023	-0.00076	-0.00053	2.04630
R23	1.83973	-0.00130	-0.00030	0.00084	0.00050	1.84023
R24	3.65549	-0.00264	-0.01070	-0.09469	-0.10543	3.55006
R25	2.78067	-0.00286	0.00350	-0.00429	-0.00124	2.77943
R26	2.74662	-0.00081	0.00287	-0.00162	0.00149	2.74810
R27	2.05660	-0.00013	0.00265	-0.00272	-0.00007	2.05653
R28	2.05058	0.00098	0.00141	0.00018	0.00159	2.05217
R29	2.73209	-0.00146	-0.00323	-0.00293	-0.00595	2.72615
R30	2.06124	-0.00118	0.00186	-0.00396	-0.00210	2.05914
R31	2.86141	-0.00422	0.00124	-0.01094	-0.00969	2.85171
R32	2.06919	-0.00071	0.00127	-0.00053	0.00074	2.06993
R33	2.07028	-0.00120	0.00041	-0.00114	-0.00073	2.06955
R34	2.06540	-0.00092	0.00085	-0.00175	-0.00090	2.06449
A1	1.87466	-0.00031	0.00090	-0.00215	-0.00121	1.87345
A2	2.27544	0.00018	-0.00069	0.00107	0.00036	2.27580
A3	2.13295	0.00014	-0.00021	0.00114	0.00090	2.13385
A4	1.86236	-0.00009	0.00018	-0.00124	-0.00106	1.86130
A5	2.27707	-0.00002	-0.00019	0.00013	-0.00007	2.27700
A6	2.14366	0.00012	-0.00001	0.00110	0.00109	2.14475
A7	1.89688	0.00022	-0.00032	0.00054	0.00026	1.89714
A8	2.25134	-0.00030	0.00042	0.00021	0.00062	2.25196
A9	2.13490	0.00008	-0.00011	-0.00077	-0.00090	2.13400
A10	1.89184	-0.00078	0.00081	-0.00142	-0.00067	1.89117
A11	2.23242	-0.00061	-0.00354	0.00229	-0.00144	2.23098
A12	2.15892	0.00139	0.00289	-0.00087	0.00209	2.16100
A13	1.89872	0.00099	-0.00167	0.00437	0.00264	1.90136
A14	2.22380	-0.00196	-0.00053	0.00214	0.00142	2.22522
A15	2.16041	0.00098	0.00229	-0.00657	-0.00406	2.15635
A16	1.95048	-0.00067	-0.00212	-0.00354	-0.00591	1.94456
A17	1.86442	0.00044	0.00142	-0.00064	0.00092	1.86534
A18	1.88998	-0.00054	-0.00040	-0.00420	-0.00456	1.88542
A19	1.93453	-0.00018	0.00112	0.00014	0.00120	1.93573
A20	1.91907	0.00058	0.00057	0.00448	0.00520	1.92427
A21	1.90373	0.00037	-0.00060	0.00366	0.00302	1.90675
A22	1.90880	0.00126	-0.00044	0.00312	0.00273	1.91154
A23	1.91372	-0.00029	0.00135	-0.00020	0.00079	1.91450
A24	1.92045	-0.00318	-0.00030	-0.00975	-0.00944	1.91100
A25	1.89080	-0.00039	0.00343	0.00010	0.00357	1.89437
A26	1.88514	0.00060	-0.00123	0.00179	0.00032	1.88546
A27	1.94424	0.00206	-0.00276	0.00516	0.00224	1.94648
A28	1.71016	-0.00195	0.00118	0.00042	0.00067	1.71083
A29	2.91471	-0.00099	0.00210	-0.00344	-0.00152	2.91320

A30	2.17649	-0.00033	0.00025	-0.00098	-0.00073	2.17576
A31	1.95381	0.00022	-0.00007	0.00041	0.00034	1.95415
A32	2.15288	0.00011	-0.00018	0.00057	0.00039	2.15327
A33	2.07821	0.00014	-0.00047	0.00025	-0.00022	2.07799
A34	2.15955	-0.00024	0.00082	-0.00043	0.00039	2.15994
A35	2.04542	0.00010	-0.00035	0.00018	-0.00017	2.04525
A36	1.90196	-0.00026	-0.00537	-0.00590	-0.01174	1.89022
A37	3.14159	-0.00158	0.00006	-0.00476	-0.00419	3.13740
A38	2.10092	-0.00118	0.00082	-0.01188	-0.01214	2.08878
A39	2.09259	0.00005	-0.00397	-0.00302	-0.00600	2.08659
A40	2.00026	0.00042	0.00181	0.00369	0.00591	2.00616
A41	1.97723	-0.00032	-0.00304	0.00268	-0.00093	1.97629
A42	2.02157	0.00078	0.00374	0.00882	0.01247	2.03405
A43	2.06413	-0.00089	0.00111	-0.00821	-0.00583	2.05830
A44	2.13174	-0.00096	-0.00022	0.00017	-0.00145	2.13029
A45	1.97433	-0.00154	0.00089	-0.00664	-0.00615	1.96818
A46	2.03782	0.00005	0.00219	0.00212	0.00474	2.04255
A47	2.00170	0.00185	-0.00241	0.00764	0.00525	2.00695
A48	1.41878	0.00023	0.01750	0.01602	0.03496	1.45374
A49	0.96238	-0.00060	-0.02334	-0.02146	-0.04053	0.92185
A50	2.38064	-0.00038	-0.00464	-0.00722	-0.01425	2.36639
A51	2.21070	0.00004	-0.00540	0.00055	-0.00566	2.20505
A52	1.91747	0.00156	-0.00048	0.00789	0.00738	1.92485
A53	1.92208	-0.00084	0.00055	-0.00435	-0.00379	1.91829
A54	1.92767	0.00106	0.00294	0.00562	0.00853	1.93620
A55	1.89246	-0.00051	-0.00141	-0.00339	-0.00479	1.88766
A56	1.91077	-0.00106	0.00014	-0.00220	-0.00213	1.90864
A57	1.89286	-0.00027	-0.00182	-0.00390	-0.00571	1.88715
A58	3.62949	0.00026	0.01211	0.01657	0.02930	3.65879
A59	4.84276	0.00165	0.06040	0.06525	0.12348	4.96624
D1	0.02044	-0.00095	0.00372	-0.00010	0.00367	0.02411
D2	-3.13587	-0.00049	0.00153	-0.00077	0.00076	-3.13510
D3	-3.13886	-0.00018	0.00370	0.00356	0.00729	-3.13156
D4	-0.01198	0.00029	0.00151	0.00289	0.00439	-0.00759
D5	-0.02409	0.00110	-0.00554	0.00487	-0.00070	-0.02478
D6	3.14129	0.00101	-0.00884	0.00776	-0.00105	3.14024
D7	3.13345	0.00040	-0.00551	0.00157	-0.00396	3.12949
D8	0.01564	0.00030	-0.00882	0.00446	-0.00431	0.01132
D9	-0.01000	0.00046	-0.00065	-0.00477	-0.00546	-0.01546
D10	-3.14019	0.00035	-0.00018	-0.00281	-0.00304	3.13996
D11	-3.13827	0.00004	0.00133	-0.00416	-0.00282	-3.14109
D12	0.01473	-0.00007	0.00180	-0.00219	-0.00040	0.01433
D13	-0.00495	0.00023	-0.00281	0.00790	0.00510	0.00015
D14	3.13303	0.00003	0.00804	0.00864	0.01652	-3.13364

D15	3.12615	0.00033	-0.00324	0.00610	0.00289	3.12904
D16	-0.01906	0.00014	0.00761	0.00684	0.01431	-0.00475
D17	0.06019	-0.00010	-0.01086	-0.01419	-0.02504	0.03515
D18	-3.08461	-0.00007	-0.01053	-0.01443	-0.02494	-3.10955
D19	-3.06861	-0.00023	-0.01033	-0.01200	-0.02234	-3.09095
D20	0.06977	-0.00020	-0.01000	-0.01223	-0.02224	0.04753
D21	0.01784	-0.00082	0.00515	-0.00789	-0.00274	0.01509
D22	3.13670	-0.00078	0.00824	-0.01051	-0.00232	3.13438
D23	-3.12033	-0.00063	-0.00502	-0.00861	-0.01359	-3.13391
D24	-0.00146	-0.00058	-0.00192	-0.01123	-0.01317	-0.01462
D25	-3.02673	-0.00017	-0.04645	0.00851	-0.03810	-3.06483
D26	0.11073	-0.00040	-0.03413	0.00936	-0.02506	0.08567
D27	1.33672	0.00002	0.03041	0.01200	0.04257	1.37929
D28	-2.82785	-0.00031	0.03145	0.00964	0.04112	-2.78672
D29	-0.77960	0.00008	0.03130	0.01144	0.04280	-0.73679
D30	-1.77778	-0.00008	0.02672	0.01512	0.04207	-1.73571
D31	0.34084	-0.00041	0.02777	0.01277	0.04062	0.38146
D32	2.38909	-0.00002	0.02762	0.01457	0.04230	2.43139
D33	-0.98463	0.00030	-0.02653	0.01534	-0.01110	-0.99572
D34	1.08630	0.00041	-0.02183	0.01721	-0.00463	1.08168
D35	-3.05267	0.00070	-0.02459	0.01710	-0.00750	-3.06017
D36	-3.06217	0.00030	-0.02769	0.01837	-0.00918	-3.07135
D37	-0.99124	0.00041	-0.02299	0.02024	-0.00271	-0.99395
D38	1.15297	0.00070	-0.02574	0.02013	-0.00559	1.14739
D39	1.11476	-0.00043	-0.02804	0.01075	-0.01721	1.09755
D40	-3.09750	-0.00031	-0.02334	0.01262	-0.01073	-3.10824
D41	-0.95328	-0.00002	-0.02609	0.01251	-0.01361	-0.96690
D42	-1.79391	0.00054	-0.00021	0.01094	0.01118	-1.78273
D43	2.40674	0.00049	0.00123	0.01173	0.01311	2.41985
D44	0.33226	-0.00063	-0.00057	0.00745	0.00721	0.33947
D45	0.40259	-0.00042	0.04738	-0.01378	0.03307	0.43566
D46	-0.37702	0.00048	-0.01028	0.01478	0.00582	-0.37120
D47	2.73473	0.00021	-0.05446	-0.03613	-0.09169	2.64303
D48	-3.13824	-0.00004	-0.00029	-0.00217	-0.00246	-3.14070
D49	0.00352	0.00002	-0.00126	-0.00065	-0.00191	0.00160
D50	0.00692	-0.00007	-0.00066	-0.00191	-0.00257	0.00435
D51	-3.13451	-0.00002	-0.00163	-0.00039	-0.00202	-3.13654
D52	-1.36512	0.00043	0.02636	-0.06304	-0.03562	-1.40074
D53	2.03300	0.00079	-0.02497	0.05033	0.02346	2.05646
D54	1.99748	0.00050	-0.07938	-0.00944	-0.08612	1.91136
D55	-2.80976	-0.00086	-0.08536	-0.01491	-0.10002	-2.90978
D56	-2.72311	-0.00006	0.00166	0.00650	0.00822	-2.71488
D57	-0.03737	0.00041	-0.00279	0.00735	0.00445	-0.03292
D58	0.01438	-0.00088	0.00418	-0.00872	-0.00451	0.00987

D59	2.70011	-0.00041	-0.00027	-0.00788	-0.00828	2.69183
D60	-0.00663	0.00064	-0.06894	-0.05590	-0.12631	-0.13294
D61	0.03616	0.00101	-0.00537	0.01687	0.01214	0.04830
D62	-2.37948	-0.00068	-0.07336	-0.07657	-0.15140	-2.53088
D63	-2.33669	-0.00031	-0.00979	-0.00379	-0.01295	-2.34964
D64	2.11887	0.00104	0.00327	0.01596	0.02043	2.13929
D65	-0.26141	-0.00016	0.00358	0.00910	0.01383	-0.24758
D66	2.48471	0.00040	-0.01385	0.00318	-0.01072	2.47400
D67	-1.71513	0.00022	-0.01555	0.00122	-0.01439	-1.72952
D68	0.37513	0.00002	-0.01560	-0.00283	-0.01851	0.35662
D69	1.27080	-0.00002	-0.01620	0.00109	-0.01511	1.25569
D70	-2.92905	-0.00020	-0.01790	-0.00087	-0.01878	-2.94783
D71	-0.83878	-0.00040	-0.01795	-0.00492	-0.02290	-0.86169
D72	-1.09778	0.00022	-0.01735	0.00025	-0.01700	-1.11477
D73	0.98556	0.00004	-0.01905	-0.00170	-0.02067	0.96489
D74	3.07583	-0.00016	-0.01910	-0.00575	-0.02479	3.05103

Item	Value	Threshold	Converged?
Maximum Force	0.006996	0.000450	NO
RMS Force	0.001068	0.000300	NO
Maximum Displacement	0.584263	0.001800	NO
RMS Displacement	0.121382	0.001200	NO

Predicted change in Energy=-7.700962D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.382622	-1.900376	-0.293280
2	6	0	-2.506864	-1.146206	-0.185372
3	7	0	-2.096699	0.129120	0.191068
4	6	0	-0.758251	0.129888	0.324054
5	7	0	-0.308659	-1.092183	0.046728
6	6	0	1.122571	-1.464126	0.081505
7	6	0	1.735436	-1.470001	-1.328395
8	1	0	-1.259571	-2.933779	-0.568635
9	1	0	-3.537018	-1.401518	-0.355259
10	1	0	1.623652	-0.735791	0.720853
11	1	0	1.203255	-2.454551	0.532620
12	1	0	1.170786	-2.155172	-1.970191
13	1	0	1.680368	-0.465229	-1.758650
14	35	0	1.575396	2.337698	1.115524
15	1	0	-0.106704	0.973098	0.617894

16	6	0	-2.885070	1.288779	0.434030
17	6	0	-4.209243	1.327449	0.370942
18	1	0	-2.275022	2.148577	0.682916
19	1	0	-4.717633	2.260259	0.572401
20	1	0	-4.825272	0.470892	0.127240
21	8	0	3.072940	-1.934185	-1.260770
22	1	0	3.666938	-1.164567	-1.316942
23	6	0	4.732635	1.724524	-1.063654
24	6	0	5.674713	0.818155	-0.389661
25	8	0	4.811930	0.320246	-1.433131
26	1	0	3.812166	2.015693	-0.561373
27	1	0	5.094354	2.392714	-1.839537
28	1	0	6.721584	0.854836	-0.689754
29	6	0	5.429635	0.302417	1.007200
30	1	0	5.749226	-0.742175	1.087865
31	1	0	6.005062	0.892014	1.728749
32	1	0	4.372450	0.379112	1.271769

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.358063	0.000000			
3	N	2.205301	1.391546	0.000000		
4	C	2.211993	2.223865	1.345039	0.000000	
5	N	1.386426	2.211084	2.170140	1.331354	0.000000
6	C	2.570364	3.653094	3.593625	2.477338	1.479179
7	C	3.313453	4.405502	4.421676	3.392449	2.492395
8	H	1.076515	2.213153	3.264856	3.230212	2.162031
9	H	2.212266	1.074832	2.171600	3.244721	3.267964
10	H	3.379705	4.248628	3.856132	2.565212	2.077326
11	H	2.770556	3.999032	4.204963	3.251204	2.092371
12	H	3.065427	4.210546	4.534919	3.769117	2.717842
13	H	3.686308	4.524582	4.291956	3.261700	2.758385
14	Br	5.356853	5.522206	4.383688	3.308589	4.056609
15	H	3.273386	3.301129	2.203306	1.105377	2.152302
16	C	3.599588	2.540837	1.423154	2.424558	3.529430
17	C	4.341640	3.053940	2.435403	3.653177	4.601554
18	H	4.259502	3.415153	2.086126	2.550389	3.843677
19	H	5.402091	4.131068	3.399480	4.502984	5.563655
20	H	4.201379	2.843897	2.750635	4.086035	4.780114
21	O	4.559519	5.736863	5.752411	4.631425	3.722060
22	H	5.204551	6.276672	6.096493	4.893953	4.203594
23	C	7.150506	7.837270	7.124566	5.883742	5.880597
24	C	7.563443	8.416569	7.823481	6.508926	6.296075

25	O	6.678539	7.567834	7.099556	5.843873	5.514106
26	H	6.511013	7.075953	6.248200	5.022843	5.197103
27	H	7.922926	8.546270	7.807590	6.637357	6.700378
28	H	8.568929	9.456364	8.891829	7.582961	7.331958
29	C	7.276702	8.155290	7.572438	6.227872	5.982929
30	H	7.356103	8.363456	7.944932	6.609929	6.156658
31	H	8.152541	8.959413	8.281607	6.949562	6.828565
32	H	6.384849	7.195472	6.563559	5.223444	5.057491

		6	7	8	9	10
6	C	0.000000				
7	C	1.537353	0.000000			
8	H	2.873528	3.419056	0.000000		
9	H	4.680433	5.361945	2.753202	0.000000	
10	H	1.091017	2.179673	3.847973	5.313541	0.000000
11	H	1.091310	2.171619	2.740061	4.936334	1.779409
12	H	2.165485	1.095532	2.911567	5.033827	3.075946
13	H	2.166818	1.094404	4.019094	5.483362	2.494865
14	Br	3.965868	4.527353	6.217869	6.502439	3.099102
15	H	2.781886	3.626328	4.242716	4.284026	2.434140
16	C	4.874827	5.662692	4.634391	2.878491	4.950729
17	C	6.025356	6.786213	5.267014	2.902846	6.196940
18	H	4.995694	5.763962	5.331779	3.908147	4.849813
19	H	6.944063	7.692202	6.343358	3.957653	7.015002
20	H	6.254856	6.994915	4.978981	2.323429	6.587646
21	O	2.413834	1.417377	4.499877	6.692924	2.731925
22	H	2.918765	1.955536	5.287774	7.271723	2.917443
23	C	4.950902	4.388426	7.606008	8.869110	4.347803
24	C	5.113980	4.651320	7.886274	9.475448	4.478737
25	O	4.369150	3.561007	6.942560	8.592509	3.989985
26	H	4.444811	4.129309	7.086595	8.107423	3.742240
27	H	5.860092	5.144334	8.388033	9.544625	5.328126
28	H	6.109122	5.538448	8.835559	10.509136	5.523479
29	C	4.746408	4.716310	7.596163	9.228248	3.955425
30	H	4.789563	4.741155	7.527972	9.420811	4.141872
31	H	5.665997	5.758034	8.525817	10.032680	4.781461
32	H	3.921220	4.139314	6.788372	8.269072	3.017021

		11	12	13	14	15
11	H	0.000000				
12	H	2.520862	0.000000			
13	H	3.071637	1.777732	0.000000		
14	Br	4.841892	5.465458	4.016005	0.000000	
15	H	3.670428	4.256317	3.303085	2.222438	0.000000
16	C	5.544063	5.838753	5.359815	4.632539	2.802280
17	C	6.604907	6.823069	6.514321	5.919211	4.125212

18	H	5.771463	6.118401	5.332761	3.879257	2.467303
19	H	7.568879	7.786802	7.334610	6.316897	4.787433
20	H	6.713098	6.873729	6.837855	6.740195	4.770518
21	O	2.642490	2.042132	2.084460	5.112573	4.700193
22	H	3.339861	2.763839	2.151892	4.749453	4.749061
23	C	5.698182	5.344213	3.820258	3.884965	5.177977
24	C	5.617396	5.623531	4.413161	4.623742	5.870601
25	O	4.958448	4.435544	3.244936	4.587037	5.368974
26	H	5.290209	5.133981	3.483247	2.814038	4.223176
27	H	6.653102	6.007889	4.453054	4.595485	5.924972
28	H	6.549671	6.442905	5.319677	5.651651	6.953377
29	C	5.068371	5.748251	4.721886	4.359962	5.590387
30	H	4.889415	5.684222	4.973424	5.187219	6.120045
31	H	5.973908	6.807182	5.719007	4.699786	6.212428
32	H	4.315065	5.213785	4.140490	3.418184	4.565435

		16	17	18	19	20
16	C	0.000000				
17	C	1.326240	0.000000			
18	H	1.083215	2.124333	0.000000		
19	H	2.078752	1.081286	2.447659	0.000000	
20	H	2.127780	1.082854	3.102770	1.847049	0.000000
21	O	6.982673	8.144381	7.003397	9.035868	8.372140
22	H	7.212046	8.431686	7.091068	9.252031	8.768011
23	C	7.775754	9.064928	7.234472	9.605793	9.713054
24	C	8.612191	9.926252	8.131342	10.535942	10.518435
25	O	7.979232	9.254766	7.618749	9.929671	9.763868
26	H	6.809713	8.104684	6.214481	8.608294	8.801474
27	H	8.370125	9.621743	7.792951	10.104954	10.293717
28	H	9.681890	10.992335	9.192221	11.594134	11.582089
29	C	8.392601	9.714088	7.929390	10.343561	10.293972
30	H	8.894006	10.196491	8.538676	10.901168	10.687111
31	H	8.992673	10.313355	8.439936	10.871312	10.956200
32	H	7.362125	8.680800	6.904103	9.308998	9.269114

		21	22	23	24	25
21	O	0.000000				
22	H	0.973807	0.000000			
23	C	4.022386	3.089775	0.000000		
24	C	3.886313	2.970219	1.470810	0.000000	
25	O	2.852412	1.878610	1.454234	1.442615	0.000000
26	H	4.078866	3.272007	1.088269	2.220960	2.152680
27	H	4.810733	3.868447	1.085963	2.217700	2.130741
28	H	4.627883	3.715134	2.202743	1.089652	2.117824
29	C	3.962334	3.265085	2.607035	1.509062	2.517358
30	H	3.754927	3.208962	3.427403	2.150177	2.891830

31	H	5.051927	4.355753	3.179569	2.145285	3.427531
32	H	3.667946	3.095500	2.719203	2.156153	2.741002

		26	27	28	29	30
26	H	0.000000				
27	H	1.849286	0.000000			
28	H	3.135089	2.516932	0.000000		
29	C	2.830537	3.547628	2.203168	0.000000	
30	H	3.752068	4.338901	2.579894	1.095361	0.000000
31	H	3.363942	3.976701	2.522686	1.095160	1.773911
32	H	2.520461	3.775707	3.097147	1.092484	1.785110

		31	32
31	H	0.000000	
32	H	1.771249	0.000000

Stoichiometry C10H17BrN2O2

Framework group C1[X(C10H17BrN2O2)]

Deg. of freedom 90

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.689416	2.179398	-0.347816
2	6	0	-3.761744	1.403699	-0.043288
3	7	0	-3.288674	0.101035	0.081891
4	6	0	-1.966011	0.097280	-0.162394
5	7	0	-1.586646	1.343758	-0.436030
6	6	0	-0.191455	1.723965	-0.747244
7	6	0	0.515568	2.318999	0.481376
8	1	0	-2.621648	3.240173	-0.518253
9	1	0	-4.793250	1.666778	0.105201
10	1	0	0.314848	0.819528	-1.087787
11	1	0	-0.213075	2.451882	-1.560034
12	1	0	-0.050740	3.182535	0.847151
13	1	0	0.562257	1.570537	1.278460
14	35	0	0.458814	-2.152907	-0.222724
15	1	0	-1.277869	-0.767748	-0.155670
16	6	0	-4.007213	-1.087285	0.393284
17	6	0	-5.317698	-1.147165	0.588101
18	1	0	-3.356069	-1.950987	0.451463
19	1	0	-5.770957	-2.100716	0.821507
20	1	0	-5.974922	-0.288737	0.527027

21	8	0	1.808642	2.766872	0.112149
22	1	0	2.458501	2.107665	0.414520
23	6	0	3.707532	-0.597305	1.232917
24	6	0	4.533605	-0.003430	0.170751
25	8	0	3.711813	0.838969	1.005113
26	1	0	2.777625	-1.100205	0.974667
27	1	0	4.168856	-0.883234	2.173523
28	1	0	5.598683	0.123019	0.362999
29	6	0	4.156230	-0.102140	-1.287026
30	1	0	4.394116	0.833200	-1.805067
31	1	0	4.720920	-0.909877	-1.764582
32	1	0	3.091438	-0.318432	-1.400849

Rotational constants (GHZ): 0.5690779 0.2234424 0.1713774

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.

475 basis functions, 751 primitive gaussians, 492 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1300.5523443860 Hartrees.

NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 475 RedAO= T EigKep= 3.71D-06 NBF= 475

NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999967 0.002268 -0.001058 -0.007765 Ang= 0.93 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3225.52286184 A.U. after 12 cycles
NFock= 12 Conv=0.58D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000461782	-0.000955463	0.001782253
2	6	0.000676890	0.000525026	-0.002259226
3	7	-0.001154950	0.000393493	0.000914708
4	6	-0.000086457	-0.001950795	0.000228354
5	7	0.001104319	0.000297650	0.000014497
6	6	-0.000372795	-0.000631109	-0.001367369
7	6	0.006523426	-0.002966091	0.000709604
8	1	0.000077003	-0.000076800	0.000538313
9	1	0.000136493	0.000117217	-0.000108164
10	1	0.000031367	0.000588033	-0.000785299
11	1	-0.000061180	0.000132919	-0.000314225
12	1	-0.000725559	0.000282259	-0.000712206
13	1	-0.000885170	0.000380878	0.000229128
14	35	-0.001042124	-0.001531113	-0.000441746
15	1	0.001571883	0.003364073	0.000940331
16	6	0.000071614	-0.000407479	0.000059132
17	6	-0.000299710	0.000265184	-0.000131691
18	1	-0.000086722	-0.000050395	0.000026430
19	1	-0.000007666	-0.000088725	-0.000012184
20	1	0.000236693	0.000015883	0.000026802
21	8	-0.006496298	0.002225818	-0.000487152
22	1	0.002261979	0.001230511	0.000991747
23	6	0.000867377	-0.001865513	-0.000545589
24	6	-0.000830022	0.001862890	0.004208680
25	8	-0.001404945	-0.001794109	-0.000641066
26	1	0.000871956	-0.000458456	0.000730858
27	1	0.000465545	0.000440247	0.000038631
28	1	-0.000834874	0.000140481	-0.001579920
29	6	-0.000270361	-0.000141200	-0.001819514
30	1	-0.000083632	0.000697616	0.000386635
31	1	-0.000411732	-0.000273759	-0.000662294
32	1	0.000619433	0.000230828	0.000041542

Cartesian Forces: Max 0.006523426 RMS 0.001412238

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.005551445 RMS 0.000734119

Search for a local minimum.

Step number 19 out of a maximum of 177

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 18 19

DE= -8.41D-04 DEPred=-7.70D-04 R= 1.09D+00

TightC=F SS= 1.41D+00 RLast= 4.48D-01 DXNew= 3.2661D+00 1.3440D+00

Trust test= 1.09D+00 RLast= 4.48D-01 DXMaxT set to 1.94D+00

ITU= 1 1 -1 1 1 1 1 1 1 1 1 1 1 0 1 0 1 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00000	0.00178	0.00231	0.00288	0.00436
Eigenvalues ---	0.00450	0.00918	0.01073	0.01399	0.01511
Eigenvalues ---	0.01609	0.01869	0.02044	0.02139	0.02190
Eigenvalues ---	0.02270	0.02322	0.02384	0.02493	0.03058
Eigenvalues ---	0.03062	0.03244	0.03426	0.03698	0.04034
Eigenvalues ---	0.04643	0.05155	0.05195	0.05476	0.05630
Eigenvalues ---	0.05881	0.06254	0.07959	0.09369	0.09537
Eigenvalues ---	0.10400	0.10966	0.11562	0.11782	0.12931
Eigenvalues ---	0.13843	0.14673	0.15243	0.15991	0.16000
Eigenvalues ---	0.16000	0.16001	0.16004	0.16033	0.16073
Eigenvalues ---	0.16448	0.17488	0.19710	0.21975	0.22097
Eigenvalues ---	0.22867	0.23521	0.23783	0.25047	0.25274
Eigenvalues ---	0.27785	0.28034	0.31384	0.32934	0.33053
Eigenvalues ---	0.33211	0.34071	0.34110	0.34508	0.34779
Eigenvalues ---	0.35022	0.35686	0.35693	0.35859	0.35999
Eigenvalues ---	0.36436	0.36658	0.37202	0.37228	0.37754
Eigenvalues ---	0.38007	0.42152	0.42389	0.44287	0.46008
Eigenvalues ---	0.49365	0.52987	0.54675	0.56435	0.60368

RFO step: Lambda=-9.05216088D-04 EMin= 2.69463700D-06

Quartic linear search produced a step of 0.17451.

Iteration 1 RMS(Cart)= 0.04142387 RMS(Int)= 0.00514656

Iteration 2 RMS(Cart)= 0.00278257 RMS(Int)= 0.00025981

Iteration 3 RMS(Cart)= 0.00001071 RMS(Int)= 0.00012002

Iteration 4 RMS(Cart)= 0.00000023 RMS(Int)= 0.00012002

Variable	Old X	-DE/DX	Delta X	Delta X	Delta X	New X

			(Linear)	(Quad)	(Total)	
R1	2.56637	-0.00020	-0.00008	-0.00021	-0.00030	2.56606
R2	2.61997	0.00003	-0.00037	-0.00059	-0.00095	2.61902
R3	2.03432	-0.00006	-0.00003	-0.00014	-0.00017	2.03415
R4	2.62964	0.00003	0.00006	0.00029	0.00034	2.62998
R5	2.03114	-0.00014	-0.00007	-0.00037	-0.00043	2.03070
R6	2.54175	0.00088	-0.00026	0.00189	0.00163	2.54339
R7	2.68937	-0.00016	0.00006	-0.00025	-0.00019	2.68918
R8	2.51589	0.00069	-0.00094	-0.00243	-0.00322	2.51268
R9	2.08886	0.00205	-0.00156	0.00344	0.00196	2.09082
R10	2.79524	-0.00067	-0.00104	-0.00474	-0.00570	2.78954
R11	2.90518	-0.00086	-0.00113	-0.00515	-0.00623	2.89895
R12	2.06172	-0.00005	-0.00049	-0.00110	-0.00160	2.06013
R13	2.06228	-0.00025	-0.00034	-0.00100	-0.00134	2.06093
R14	2.07026	0.00061	-0.00017	0.00163	0.00146	2.07172
R15	2.06812	0.00030	-0.00021	0.00071	0.00051	2.06863
R16	2.67845	-0.00555	-0.00063	-0.01482	-0.01537	2.66308
R17	4.19980	-0.00167	0.00427	-0.03984	-0.03553	4.16427
R18	8.66824	-0.00018	-0.04912	0.12552	0.07629	8.74453
R19	2.50623	0.00008	-0.00012	0.00013	0.00001	2.50624
R20	2.04698	-0.00008	-0.00006	-0.00031	-0.00037	2.04661
R21	2.04334	-0.00007	-0.00005	-0.00015	-0.00020	2.04313
R22	2.04630	-0.00016	-0.00009	-0.00038	-0.00047	2.04583
R23	1.84023	0.00055	0.00009	0.00173	0.00176	1.84198
R24	3.55006	-0.00174	-0.01840	-0.15808	-0.17654	3.37351
R25	2.77943	-0.00228	-0.00022	-0.00215	-0.00240	2.77703
R26	2.74810	-0.00040	0.00026	-0.00442	-0.00417	2.74393
R27	2.05653	-0.00053	-0.00001	-0.00020	-0.00022	2.05631
R28	2.05217	0.00040	0.00028	0.00238	0.00266	2.05483
R29	2.72615	0.00102	-0.00104	0.00145	0.00046	2.72660
R30	2.05914	-0.00036	-0.00037	-0.00122	-0.00158	2.05756
R31	2.85171	-0.00205	-0.00169	-0.01258	-0.01428	2.83744
R32	2.06993	-0.00066	0.00013	-0.00070	-0.00058	2.06936
R33	2.06955	-0.00080	-0.00013	-0.00115	-0.00128	2.06827
R34	2.06449	-0.00057	-0.00016	-0.00111	-0.00127	2.06323
A1	1.87345	0.00004	-0.00021	-0.00033	-0.00054	1.87291
A2	2.27580	0.00012	0.00006	0.00104	0.00108	2.27688
A3	2.13385	-0.00016	0.00016	-0.00061	-0.00047	2.13338
A4	1.86130	0.00044	-0.00019	0.00075	0.00054	1.86184
A5	2.27700	-0.00016	-0.00001	-0.00007	-0.00010	2.27689
A6	2.14475	-0.00027	0.00019	-0.00049	-0.00032	2.14443
A7	1.89714	-0.00028	0.00004	-0.00142	-0.00138	1.89576
A8	2.25196	-0.00021	0.00011	-0.00008	0.00001	2.25197
A9	2.13400	0.00049	-0.00016	0.00162	0.00145	2.13545

A10	1.89117	-0.00019	-0.00012	0.00044	0.00030	1.89147
A11	2.23098	-0.00013	-0.00025	-0.00134	-0.00166	2.22932
A12	2.16100	0.00032	0.00036	0.00089	0.00134	2.16234
A13	1.90136	0.00003	0.00046	0.00091	0.00131	1.90267
A14	2.22522	-0.00096	0.00025	-0.00414	-0.00400	2.22122
A15	2.15635	0.00094	-0.00071	0.00289	0.00222	2.15858
A16	1.94456	0.00085	-0.00103	-0.00089	-0.00180	1.94277
A17	1.86534	-0.00014	0.00016	0.00037	0.00046	1.86580
A18	1.88542	-0.00024	-0.00080	0.00108	0.00027	1.88569
A19	1.93573	-0.00079	0.00021	-0.00379	-0.00361	1.93212
A20	1.92427	-0.00015	0.00091	-0.00161	-0.00074	1.92353
A21	1.90675	0.00049	0.00053	0.00516	0.00570	1.91245
A22	1.91154	0.00068	0.00048	0.00151	0.00205	1.91359
A23	1.91450	-0.00073	0.00014	-0.00469	-0.00460	1.90990
A24	1.91100	-0.00124	-0.00165	-0.00745	-0.00907	1.90193
A25	1.89437	-0.00033	0.00062	-0.00390	-0.00330	1.89107
A26	1.88546	0.00058	0.00006	0.00560	0.00567	1.89113
A27	1.94648	0.00108	0.00039	0.00907	0.00941	1.95589
A28	1.71083	0.00014	0.00012	-0.00570	-0.00615	1.70467
A29	2.91320	-0.00133	-0.00026	-0.01670	-0.01703	2.89616
A30	2.17576	-0.00006	-0.00013	0.00051	0.00038	2.17614
A31	1.95415	0.00008	0.00006	0.00012	0.00018	1.95433
A32	2.15327	-0.00002	0.00007	-0.00062	-0.00055	2.15272
A33	2.07799	0.00019	-0.00004	0.00104	0.00100	2.07899
A34	2.15994	-0.00028	0.00007	-0.00127	-0.00120	2.15874
A35	2.04525	0.00009	-0.00003	0.00023	0.00020	2.04546
A36	1.89022	0.00083	-0.00205	0.01293	0.01036	1.90058
A37	3.13740	-0.00157	-0.00073	-0.02815	-0.02863	3.10877
A38	2.08878	-0.00066	-0.00212	-0.01311	-0.01529	2.07349
A39	2.08659	-0.00022	-0.00105	-0.00406	-0.00522	2.08137
A40	2.00616	0.00006	0.00103	0.00548	0.00651	2.01268
A41	1.97629	-0.00042	-0.00016	0.00624	0.00598	1.98227
A42	2.03405	0.00051	0.00218	0.00731	0.00918	2.04323
A43	2.05830	-0.00086	-0.00102	-0.01211	-0.01299	2.04531
A44	2.13029	-0.00021	-0.00025	0.00158	0.00116	2.13145
A45	1.96818	-0.00108	-0.00107	-0.01471	-0.01583	1.95235
A46	2.04255	0.00023	0.00083	0.00559	0.00641	2.04897
A47	2.00695	0.00112	0.00092	0.01233	0.01325	2.02021
A48	1.45374	-0.00060	0.00610	-0.01413	-0.00817	1.44557
A49	0.92185	0.00115	-0.00707	0.02154	0.01537	0.93722
A50	2.36639	0.00054	-0.00249	0.00642	0.00344	2.36983
A51	2.20505	0.00072	-0.00099	0.01828	0.01724	2.22228
A52	1.92485	0.00068	0.00129	0.01114	0.01237	1.93722
A53	1.91829	-0.00048	-0.00066	-0.00402	-0.00466	1.91363

A54	1.93620	0.00007	0.00149	0.00705	0.00848	1.94469
A55	1.88766	-0.00014	-0.00084	-0.00566	-0.00647	1.88119
A56	1.90864	-0.00010	-0.00037	-0.00296	-0.00345	1.90519
A57	1.88715	-0.00003	-0.00100	-0.00622	-0.00719	1.87995
A58	3.65879	0.00011	0.00511	0.00414	0.00907	3.66786
A59	4.96624	0.00085	0.02155	-0.01135	0.01009	4.97633
D1	0.02411	-0.00110	0.00064	-0.01439	-0.01375	0.01036
D2	-3.13510	-0.00048	0.00013	-0.00212	-0.00198	-3.13708
D3	-3.13156	-0.00034	0.00127	-0.00611	-0.00486	-3.13642
D4	-0.00759	0.00029	0.00077	0.00616	0.00692	-0.00067
D5	-0.02478	0.00113	-0.00012	0.00949	0.00936	-0.01542
D6	3.14024	0.00111	-0.00018	0.02603	0.02579	-3.11716
D7	3.12949	0.00044	-0.00069	0.00203	0.00135	3.13084
D8	0.01132	0.00042	-0.00075	0.01857	0.01778	0.02910
D9	-0.01546	0.00071	-0.00095	0.01446	0.01351	-0.00195
D10	3.13996	0.00045	-0.00053	0.00506	0.00454	-3.13869
D11	-3.14109	0.00015	-0.00049	0.00334	0.00285	-3.13824
D12	0.01433	-0.00011	-0.00007	-0.00606	-0.00613	0.00820
D13	0.00015	-0.00002	0.00089	-0.00869	-0.00781	-0.00766
D14	-3.13364	-0.00027	0.00288	-0.00748	-0.00461	-3.13824
D15	3.12904	0.00022	0.00050	-0.00007	0.00042	3.12947
D16	-0.00475	-0.00003	0.00250	0.00114	0.00363	-0.00112
D17	0.03515	0.00001	-0.00437	-0.00823	-0.01259	0.02256
D18	-3.10955	0.00007	-0.00435	-0.00482	-0.00916	-3.11871
D19	-3.09095	-0.00028	-0.00390	-0.01873	-0.02263	-3.11358
D20	0.04753	-0.00022	-0.00388	-0.01532	-0.01921	0.02832
D21	0.01509	-0.00068	-0.00048	-0.00040	-0.00086	0.01423
D22	3.13438	-0.00069	-0.00040	-0.01626	-0.01667	3.11771
D23	-3.13391	-0.00045	-0.00237	-0.00157	-0.00394	-3.13785
D24	-0.01462	-0.00046	-0.00230	-0.01743	-0.01975	-0.03437
D25	-3.06483	-0.00014	-0.00665	0.03405	0.02747	-3.03736
D26	0.08567	-0.00042	-0.00437	0.03544	0.03115	0.11682
D27	1.37929	0.00023	0.00743	-0.00813	-0.00069	1.37860
D28	-2.78672	-0.00033	0.00718	-0.01308	-0.00589	-2.79261
D29	-0.73679	0.00005	0.00747	-0.00630	0.00116	-0.73563
D30	-1.73571	0.00022	0.00734	0.01069	0.01800	-1.71771
D31	0.38146	-0.00033	0.00709	0.00574	0.01281	0.39427
D32	2.43139	0.00005	0.00738	0.01252	0.01986	2.45125
D33	-0.99572	0.00024	-0.00194	0.03946	0.03752	-0.95821
D34	1.08168	-0.00019	-0.00081	0.03278	0.03196	1.11363
D35	-3.06017	-0.00013	-0.00131	0.03617	0.03480	-3.02537
D36	-3.07135	0.00038	-0.00160	0.04208	0.04047	-3.03088
D37	-0.99395	-0.00005	-0.00047	0.03540	0.03492	-0.95903
D38	1.14739	0.00001	-0.00097	0.03879	0.03776	1.18515

D39	1.09755	0.00039	-0.00300	0.03917	0.03619	1.13374
D40	-3.10824	-0.00004	-0.00187	0.03249	0.03063	-3.07761
D41	-0.96690	0.00002	-0.00238	0.03588	0.03348	-0.93342
D42	-1.78273	0.00069	0.00195	0.00705	0.00915	-1.77358
D43	2.41985	0.00024	0.00229	0.00619	0.00856	2.42840
D44	0.33947	-0.00037	0.00126	0.00204	0.00331	0.34278
D45	0.43566	-0.00039	0.00577	-0.04892	-0.04301	0.39265
D46	-0.37120	0.00014	0.00102	0.01543	0.01664	-0.35456
D47	2.64303	0.00018	-0.01600	0.00996	-0.00600	2.63704
D48	-3.14070	0.00003	-0.00043	0.00215	0.00173	-3.13897
D49	0.00160	0.00004	-0.00033	0.00134	0.00100	0.00260
D50	0.00435	-0.00004	-0.00045	-0.00163	-0.00208	0.00227
D51	-3.13654	-0.00003	-0.00035	-0.00245	-0.00280	-3.13934
D52	-1.40074	0.00024	-0.00622	-0.01974	-0.02601	-1.42674
D53	2.05646	0.00042	0.00409	-0.00424	-0.00030	2.05616
D54	1.91136	0.00025	-0.01503	-0.01383	-0.02875	1.88261
D55	-2.90978	-0.00044	-0.01745	0.00711	-0.01039	-2.92017
D56	-2.71488	-0.00004	0.00143	0.00108	0.00245	-2.71243
D57	-0.03292	0.00038	0.00078	0.00854	0.00919	-0.02373
D58	0.00987	-0.00089	-0.00079	-0.02370	-0.02443	-0.01456
D59	2.69183	-0.00047	-0.00145	-0.01625	-0.01768	2.67414
D60	-0.13294	0.00051	-0.02204	0.03402	0.01203	-0.12091
D61	0.04830	0.00054	0.00212	0.04274	0.04502	0.09332
D62	-2.53088	0.00013	-0.02642	0.00899	-0.01754	-2.54842
D63	-2.34964	0.00015	-0.00226	0.01771	0.01545	-2.33419
D64	2.13929	0.00046	0.00356	0.00244	0.00612	2.14542
D65	-0.24758	-0.00034	0.00241	-0.00634	-0.00372	-0.25130
D66	2.47400	0.00023	-0.00187	0.00043	-0.00144	2.47256
D67	-1.72952	0.00016	-0.00251	-0.00216	-0.00470	-1.73422
D68	0.35662	-0.00014	-0.00323	-0.00802	-0.01132	0.34530
D69	1.25569	0.00004	-0.00264	-0.00069	-0.00326	1.25243
D70	-2.94783	-0.00002	-0.00328	-0.00327	-0.00652	-2.95435
D71	-0.86169	-0.00033	-0.00400	-0.00914	-0.01314	-0.87483
D72	-1.11477	0.00016	-0.00297	0.00182	-0.00111	-1.11588
D73	0.96489	0.00010	-0.00361	-0.00077	-0.00437	0.96052
D74	3.05103	-0.00021	-0.00433	-0.00663	-0.01099	3.04004

Item	Value	Threshold	Converged?
Maximum Force	0.005551	0.000450	NO
RMS Force	0.000734	0.000300	NO
Maximum Displacement	0.191120	0.001800	NO
RMS Displacement	0.044043	0.001200	NO

Predicted change in Energy=-5.057007D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.354288	-1.896055	-0.279948
2	6	0	-2.488300	-1.155274	-0.184251
3	7	0	-2.098769	0.122770	0.205330
4	6	0	-0.759861	0.141227	0.341118
5	7	0	-0.293607	-1.072504	0.062844
6	6	0	1.140466	-1.422094	0.079234
7	6	0	1.736269	-1.398581	-1.334199
8	1	0	-1.214813	-2.927282	-0.555287
9	1	0	-3.513618	-1.423832	-0.361371
10	1	0	1.637266	-0.692522	0.719069
11	1	0	1.240568	-2.417359	0.513785
12	1	0	1.152535	-2.054035	-1.991102
13	1	0	1.688351	-0.380135	-1.732669
14	35	0	1.549327	2.347217	1.123138
15	1	0	-0.121419	0.993649	0.640975
16	6	0	-2.904674	1.270273	0.447888
17	6	0	-4.227613	1.296099	0.357907
18	1	0	-2.309442	2.133796	0.717989
19	1	0	-4.750731	2.220475	0.559955
20	1	0	-4.828175	0.435980	0.090414
21	8	0	3.057831	-1.885170	-1.282479
22	1	0	3.673595	-1.130153	-1.312368
23	6	0	4.742587	1.666134	-1.091495
24	6	0	5.665771	0.761299	-0.392530
25	8	0	4.795309	0.253999	-1.425380
26	1	0	3.838291	1.989954	-0.580155
27	1	0	5.125672	2.313316	-1.876847
28	1	0	6.707484	0.771596	-0.709141
29	6	0	5.415647	0.294824	1.012591
30	1	0	5.708265	-0.753169	1.136016
31	1	0	6.010814	0.892456	1.710091
32	1	0	4.365728	0.408716	1.289633

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357902	0.000000			
3	N	2.205765	1.391727	0.000000		
4	C	2.211240	2.223607	1.345902	0.000000	

5	N	1.385924	2.210109	2.169698	1.329651	0.000000
6	C	2.564653	3.648090	3.590981	2.474631	1.476160
7	C	3.303100	4.385039	4.403655	3.377627	2.485650
8	H	1.076426	2.213470	3.265384	3.228973	2.161228
9	H	2.211862	1.074603	2.171387	3.244391	3.266781
10	H	3.375784	4.248579	3.858314	2.565970	2.074437
11	H	2.763159	3.998071	4.206967	3.252367	2.089421
12	H	3.039271	4.162711	4.487067	3.730374	2.696930
13	H	3.696764	4.521378	4.283810	3.250562	2.762499
14	Br	5.329633	5.502649	4.370257	3.287902	4.026800
15	H	3.273905	3.301666	2.204117	1.106412	2.152411
16	C	3.599872	2.540915	1.423054	2.426184	3.529098
17	C	4.341970	3.054239	2.435561	3.655039	4.601493
18	H	4.260035	3.415262	2.086008	2.552169	3.843587
19	H	5.402507	4.131358	3.399858	4.505353	5.563882
20	H	4.200410	2.842982	2.749720	4.086674	4.778973
21	O	4.524597	5.700738	5.730263	4.617047	3.701683
22	H	5.189615	6.264362	6.098640	4.899588	4.199194
23	C	7.107720	7.814676	7.132172	5.886821	5.847725
24	C	7.507025	8.378873	7.813657	6.497036	6.251751
25	O	6.614552	7.521796	7.085531	5.830365	5.465482
26	H	6.492616	7.076366	6.273121	5.040788	5.183115
27	H	7.890423	8.536309	7.831124	6.654085	6.677931
28	H	8.502513	9.410143	8.877349	7.567143	7.280930
29	C	7.232055	8.124506	7.559611	6.213804	5.947032
30	H	7.293202	8.311948	7.910956	6.577877	6.105419
31	H	8.122855	8.945204	8.283844	6.948416	6.805896
32	H	6.363500	7.183043	6.561036	5.219473	5.040677

		6	7	8	9	10
6	C	0.000000				
7	C	1.534056	0.000000			
8	H	2.866278	3.413579	0.000000		
9	H	4.674894	5.339321	2.753629	0.000000	
10	H	1.090171	2.173530	3.840897	5.313546	0.000000
11	H	1.090600	2.167643	2.726139	4.935107	1.781733
12	H	2.164669	1.096306	2.903182	4.982587	3.071435
13	H	2.160752	1.094672	4.037642	5.479986	2.472087
14	Br	3.932506	4.483800	6.186915	6.485213	3.067739
15	H	2.782754	3.615949	4.242671	4.284382	2.437672
16	C	4.873182	5.642427	4.634810	2.878179	4.955333
17	C	6.023495	6.759616	5.267621	2.902615	6.203374
18	H	4.995421	5.749518	5.332350	3.907912	4.854337
19	H	6.943026	7.665936	6.343964	3.957305	7.022633
20	H	6.251179	6.963265	4.978438	2.321868	6.593227

21	O	2.396871	1.409244	4.457610	6.651707	2.728847
22	H	2.904915	1.955955	5.263020	7.255803	2.909449
23	C	4.887027	4.299922	7.541724	8.845671	4.299351
24	C	5.046598	4.581791	7.808621	9.435939	4.424715
25	O	4.293138	3.478083	6.855595	8.543156	3.932913
26	H	4.399446	4.058232	7.050794	8.108783	3.705155
27	H	5.801845	5.055759	8.331395	9.534164	5.286097
28	H	6.035354	5.460159	8.744607	10.460008	5.467224
29	C	4.700652	4.681118	7.536790	9.196375	3.916270
30	H	4.735930	4.721787	7.450925	9.366701	4.092744
31	H	5.633571	5.726106	8.481275	10.018530	4.756281
32	H	3.901185	4.130965	6.758332	8.256400	2.997127

		11	12	13	14	15
11	H	0.000000				
12	H	2.532630	0.000000			
13	H	3.065510	1.776466	0.000000		
14	Br	4.813297	5.406197	3.951381	0.000000	
15	H	3.675073	4.223644	3.285838	2.203638	0.000000
16	C	5.548514	5.784518	5.345518	4.631836	2.803626
17	C	6.611737	6.759234	6.494528	5.921441	4.127037
18	H	5.775577	6.071442	5.320520	3.885846	2.468464
19	H	7.576761	7.721910	7.313076	6.326450	4.789802
20	H	6.719407	6.804541	6.815775	6.737349	4.771548
21	O	2.610025	2.039807	2.084053	5.096634	4.700521
22	H	3.303234	2.769473	2.163417	4.747242	4.767412
23	C	5.613909	5.247611	3.731846	3.945299	5.206942
24	C	5.523377	5.554353	4.349564	4.664493	5.883339
25	O	4.851051	4.349353	3.185866	4.627408	5.384340
26	H	5.231566	5.055483	3.401154	2.875448	4.261817
27	H	6.571791	5.905305	4.369283	4.668116	5.967655
28	H	6.446096	6.362788	5.250313	5.696175	6.964627
29	C	5.003601	5.719566	4.678114	4.378694	5.593348
30	H	4.808016	5.676777	4.952597	5.187420	6.105870
31	H	5.928007	6.781115	5.670606	4.729240	6.225555
32	H	4.284304	5.210852	4.113993	3.423101	4.571366

		16	17	18	19	20
16	C	0.000000				
17	C	1.326246	0.000000			
18	H	1.083018	2.123858	0.000000		
19	H	2.079271	1.081179	2.447934	0.000000	
20	H	2.126896	1.082604	3.101684	1.846859	0.000000
21	O	6.964370	8.117205	6.997255	9.012465	8.334366
22	H	7.220400	8.432414	7.111431	9.257515	8.757891
23	C	7.810699	9.094074	7.295483	9.651823	9.721608

24	C	8.626580	9.936206	8.168294	10.561247	10.510088
25	O	7.989474	9.256306	7.655401	9.946631	9.743829
26	H	6.858746	8.149859	6.284942	8.667427	8.830183
27	H	8.424892	9.670201	7.876950	10.173002	10.318603
28	H	9.694379	10.999547	9.230236	11.618974	11.568204
29	C	8.396317	9.717181	7.946421	10.357039	10.286215
30	H	8.874152	10.174803	8.531878	10.888756	10.654761
31	H	9.012316	10.335217	8.470647	10.904004	10.968838
32	H	7.369503	8.689135	6.918134	9.323343	9.271824

		21	22	23	24	25
21	O	0.000000				
22	H	0.974736	0.000000			
23	C	3.935307	3.001791	0.000000		
24	C	3.820623	2.896974	1.469539	0.000000	
25	O	2.759583	1.785187	1.452027	1.442856	0.000000
26	H	4.014843	3.209101	1.088154	2.210085	2.154954
27	H	4.717682	3.779503	1.087371	2.214421	2.133951
28	H	4.550504	3.631117	2.192535	1.088814	2.106493
29	C	3.947026	3.235852	2.600130	1.501508	2.515986
30	H	3.762359	3.205711	3.427443	2.152178	2.899762
31	H	5.038928	4.323054	3.171098	2.134777	3.422902
32	H	3.686227	3.101222	2.718988	2.155017	2.753139

		26	27	28	29	30
26	H	0.000000				
27	H	1.855619	0.000000			
28	H	3.119824	2.498512	0.000000		
29	C	2.810401	3.536558	2.204658	0.000000	
30	H	3.737214	4.338212	2.593829	1.095057	0.000000
31	H	3.342093	3.958339	2.520445	1.094484	1.768949
32	H	2.504918	3.772482	3.100097	1.091812	1.782128

		31	32
31	H	0.000000	
32	H	1.765531	0.000000

Stoichiometry C10H17BrN2O2
Framework group C1[X(C10H17BrN2O2)]
Deg. of freedom 90
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-2.638115	2.189730	-0.378035
2	6	0	-3.726050	1.441958	-0.060019
3	7	0	-3.284353	0.128362	0.067541
4	6	0	-1.960412	0.094982	-0.172289
5	7	0	-1.554288	1.329317	-0.454157
6	6	0	-0.150658	1.683216	-0.743339
7	6	0	0.546346	2.257632	0.496646
8	1	0	-2.545698	3.246906	-0.558399
9	1	0	-4.750977	1.729473	0.087055
10	1	0	0.344358	0.770498	-1.075571
11	1	0	-0.146590	2.415905	-1.551149
12	1	0	-0.029186	3.107212	0.882476
13	1	0	0.593092	1.490556	1.276208
14	35	0	0.423161	-2.169512	-0.203128
15	1	0	-1.291862	-0.786495	-0.158616
16	6	0	-4.030201	-1.040861	0.386464
17	6	0	-5.338720	-1.066147	0.601099
18	1	0	-3.401786	-1.921542	0.435693
19	1	0	-5.814535	-2.007067	0.840297
20	1	0	-5.972410	-0.189793	0.551370
21	8	0	1.826615	2.718726	0.130217
22	1	0	2.490237	2.060376	0.406425
23	6	0	3.718137	-0.548918	1.239852
24	6	0	4.528054	0.017076	0.152088
25	8	0	3.703941	0.877058	0.966400
26	1	0	2.801861	-1.079864	0.989620
27	1	0	4.198017	-0.806515	2.180987
28	1	0	5.588481	0.167633	0.347900
29	6	0	4.147196	-0.139905	-1.291806
30	1	0	4.362040	0.773819	-1.855810
31	1	0	4.727443	-0.953036	-1.739050
32	1	0	3.089464	-0.387759	-1.400545

Rotational constants (GHZ): 0.5737082 0.2241041 0.1721234

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.

475 basis functions, 751 primitive gaussians, 492 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1303.7934528933 Hartrees.

NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 475 RedAO= T EigKep= 3.69D-06 NBF= 475
NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999982 0.004440 0.000083 0.003912 Ang= 0.68 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3225.52327474 A.U. after 11 cycles
NFock= 11 Conv=0.56D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000770187	-0.000463846	0.000416965
2	6	0.000206397	0.000271245	-0.000689616
3	7	-0.000853171	0.000148818	-0.000296733
4	6	-0.001473525	-0.000441588	0.001249015
5	7	0.000350101	-0.000332378	0.000290009
6	6	-0.001376629	-0.000582112	-0.000625460
7	6	0.004063439	-0.002452063	0.000282472
8	1	0.000044097	-0.000088573	0.000371665
9	1	-0.000048861	-0.000010750	0.000023981
10	1	0.000295024	0.000501629	0.000033779
11	1	0.000177667	-0.000170105	-0.000075039
12	1	-0.000583052	0.000206380	-0.000482225

13	1	-0.000292757	0.000498707	-0.000175527
14	35	0.000185553	-0.000837335	-0.000360852
15	1	0.001444741	0.002735474	0.000550579
16	6	0.000304137	-0.000503385	-0.000234833
17	6	-0.000266816	0.000168397	-0.000065170
18	1	-0.000007495	0.000013077	0.000061856
19	1	0.000006450	-0.000032868	0.000050844
20	1	0.000083836	-0.000080837	-0.000008543
21	8	-0.003318466	-0.000944982	-0.001054575
22	1	0.001559653	0.001544122	0.000431699
23	6	0.001850277	0.000125593	0.000849845
24	6	0.001282496	0.002286305	0.000053739
25	8	-0.001756247	-0.000235069	-0.001224450
26	1	-0.000219181	-0.000444015	-0.000830968
27	1	-0.000899378	-0.000359348	0.000339022
28	1	0.000089966	-0.000207129	-0.000028993
29	6	-0.000064020	-0.001184471	0.002428791
30	1	0.000118867	0.000455466	-0.000495673
31	1	0.000009158	0.000113600	-0.000223912
32	1	-0.000142074	0.000302040	-0.000561692

Cartesian Forces: Max 0.004063439 RMS 0.000961156

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.002957519 RMS 0.000572143
Search for a local minimum.
Step number 20 out of a maximum of 177
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 18 19 20
DE= -4.13D-04 DEPred=-5.06D-04 R= 8.16D-01
TightC=F SS= 1.41D+00 RLast= 2.61D-01 DXNew= 3.2661D+00 7.8394D-01
Trust test= 8.16D-01 RLast= 2.61D-01 DXMaxT set to 1.94D+00
ITU= 1 1 1 -1 1 1 1 1 1 1 1 1 1 1 0 1 0 1 0

Eigenvalues ---	0.00001	0.00172	0.00237	0.00284	0.00429
Eigenvalues ---	0.00461	0.00914	0.01203	0.01399	0.01497
Eigenvalues ---	0.01748	0.01865	0.02030	0.02100	0.02166
Eigenvalues ---	0.02253	0.02322	0.02388	0.02507	0.03058
Eigenvalues ---	0.03059	0.03172	0.03385	0.03753	0.04082
Eigenvalues ---	0.04657	0.05114	0.05190	0.05367	0.05623

Eigenvalues --- 0.05916 0.06254 0.07820 0.09305 0.09460
Eigenvalues --- 0.10194 0.11069 0.11597 0.11651 0.12890
Eigenvalues --- 0.13889 0.14721 0.15271 0.15993 0.15999
Eigenvalues --- 0.16001 0.16002 0.16003 0.16014 0.16065
Eigenvalues --- 0.16390 0.17408 0.19630 0.22033 0.22669
Eigenvalues --- 0.22858 0.23413 0.23788 0.25042 0.25178
Eigenvalues --- 0.27551 0.28286 0.31449 0.32637 0.33099
Eigenvalues --- 0.33288 0.33982 0.34140 0.34510 0.34781
Eigenvalues --- 0.35053 0.35686 0.35691 0.35858 0.36321
Eigenvalues --- 0.36435 0.36667 0.37212 0.37247 0.37755
Eigenvalues --- 0.39600 0.42013 0.42602 0.43383 0.45766
Eigenvalues --- 0.49287 0.53893 0.55187 0.56859 0.60384
Eigenvalue 1 is 1.26D-05 Eigenvector:

	D54	D52	D55	D53	D47
1	0.50076	-0.50063	0.50014	0.49763	0.01138
	R18	D46	D42	D35	D38
1	-0.00922	0.00842	0.00765	-0.00665	-0.00621

En-DIIS/RFO-DIIS IScMMF= 0 using points: 20 19
RFO step: Lambda=-1.07952897D-04.
DidBck=F Rises=F RFO-DIIS coefs: 0.85731 0.14269
Iteration 1 RMS(Cart)= 0.04854799 RMS(Int)= 0.00559110
Iteration 2 RMS(Cart)= 0.00873699 RMS(Int)= 0.00007239
Iteration 3 RMS(Cart)= 0.00002426 RMS(Int)= 0.00007026
Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00007026

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56606	-0.00005	0.00004	-0.00005	0.00000	2.56606
R2	2.61902	0.00056	0.00014	0.00007	0.00020	2.61921
R3	2.03415	-0.00001	0.00002	-0.00012	-0.00010	2.03405
R4	2.62998	0.00001	-0.00005	-0.00002	-0.00006	2.62992
R5	2.03070	0.00005	0.00006	-0.00015	-0.00009	2.03061
R6	2.54339	0.00080	-0.00023	0.00154	0.00131	2.54470
R7	2.68918	-0.00045	0.00003	-0.00088	-0.00085	2.68833
R8	2.51268	0.00180	0.00046	0.00048	0.00099	2.51366
R9	2.09082	0.00254	-0.00028	0.00487	0.00464	2.09546
R10	2.78954	0.00116	0.00081	0.00048	0.00129	2.79083
R11	2.89895	0.00154	0.00089	0.00234	0.00320	2.90214
R12	2.06013	0.00049	0.00023	0.00016	0.00039	2.06051
R13	2.06093	0.00014	0.00019	-0.00075	-0.00055	2.06038
R14	2.07172	0.00048	-0.00021	0.00130	0.00109	2.07281
R15	2.06863	0.00054	-0.00007	0.00150	0.00143	2.07006
R16	2.66308	-0.00162	0.00219	-0.00945	-0.00725	2.65583
R17	4.16427	-0.00045	0.00507	-0.02484	-0.01973	4.14454
R18	8.74453	-0.00036	-0.01089	-0.26004	-0.27092	8.47361

R19	2.50624	0.00018	0.00000	0.00013	0.00013	2.50637
R20	2.04661	0.00002	0.00005	-0.00018	-0.00013	2.04648
R21	2.04313	-0.00002	0.00003	-0.00019	-0.00016	2.04297
R22	2.04583	0.00002	0.00007	-0.00022	-0.00016	2.04567
R23	1.84198	0.00296	-0.00025	0.00482	0.00451	1.84649
R24	3.37351	0.00079	0.02519	-0.01377	0.01136	3.38487
R25	2.77703	-0.00060	0.00034	-0.00473	-0.00433	2.77269
R26	2.74393	-0.00006	0.00060	-0.00193	-0.00134	2.74259
R27	2.05631	-0.00034	0.00003	-0.00131	-0.00128	2.05503
R28	2.05483	-0.00078	-0.00038	-0.00070	-0.00108	2.05375
R29	2.72660	0.00230	-0.00007	0.00544	0.00533	2.73193
R30	2.05756	0.00009	0.00023	-0.00091	-0.00069	2.05687
R31	2.83744	0.00119	0.00204	-0.00265	-0.00061	2.83683
R32	2.06936	-0.00046	0.00008	-0.00105	-0.00097	2.06839
R33	2.06827	-0.00008	0.00018	-0.00066	-0.00047	2.06780
R34	2.06323	0.00003	0.00018	-0.00042	-0.00024	2.06299
A1	1.87291	0.00018	0.00008	-0.00008	-0.00002	1.87289
A2	2.27688	-0.00001	-0.00015	0.00098	0.00084	2.27772
A3	2.13338	-0.00017	0.00007	-0.00089	-0.00081	2.13257
A4	1.86184	0.00034	-0.00008	0.00083	0.00075	1.86259
A5	2.27689	-0.00016	0.00001	-0.00028	-0.00026	2.27663
A6	2.14443	-0.00018	0.00005	-0.00052	-0.00047	2.14396
A7	1.89576	0.00019	0.00020	-0.00075	-0.00056	1.89520
A8	2.25197	-0.00039	0.00000	-0.00075	-0.00074	2.25122
A9	2.13545	0.00020	-0.00021	0.00149	0.00128	2.13673
A10	1.89147	-0.00046	-0.00004	0.00008	-0.00002	1.89144
A11	2.22932	0.00049	0.00024	0.00316	0.00334	2.23266
A12	2.16234	-0.00003	-0.00019	-0.00312	-0.00327	2.15908
A13	1.90267	-0.00025	-0.00019	0.00015	-0.00006	1.90261
A14	2.22122	-0.00021	0.00057	-0.00042	0.00017	2.22138
A15	2.15858	0.00046	-0.00032	0.00001	-0.00028	2.15830
A16	1.94277	0.00190	0.00026	0.00849	0.00885	1.95161
A17	1.86580	-0.00067	-0.00007	-0.00169	-0.00176	1.86404
A18	1.88569	-0.00031	-0.00004	0.00059	0.00050	1.88619
A19	1.93212	-0.00079	0.00051	-0.00835	-0.00790	1.92422
A20	1.92353	-0.00048	0.00011	-0.00021	-0.00011	1.92342
A21	1.91245	0.00036	-0.00081	0.00131	0.00050	1.91294
A22	1.91359	0.00003	-0.00029	0.00265	0.00246	1.91605
A23	1.90990	-0.00064	0.00066	-0.00530	-0.00473	1.90517
A24	1.90193	0.00095	0.00129	0.00025	0.00148	1.90341
A25	1.89107	-0.00011	0.00047	-0.00440	-0.00393	1.88714
A26	1.89113	0.00012	-0.00081	0.00507	0.00427	1.89540
A27	1.95589	-0.00033	-0.00134	0.00188	0.00056	1.95646
A28	1.70467	0.00117	0.00088	0.03110	0.03187	1.73654

A29	2.89616	-0.00073	0.00243	-0.01325	-0.01078	2.88538
A30	2.17614	-0.00008	-0.00005	0.00010	0.00005	2.17619
A31	1.95433	0.00006	-0.00003	0.00028	0.00026	1.95458
A32	2.15272	0.00002	0.00008	-0.00038	-0.00030	2.15241
A33	2.07899	0.00008	-0.00014	0.00071	0.00057	2.07956
A34	2.15874	-0.00015	0.00017	-0.00113	-0.00095	2.15778
A35	2.04546	0.00008	-0.00003	0.00041	0.00038	2.04584
A36	1.90058	-0.00009	-0.00148	0.00414	0.00235	1.90293
A37	3.10877	-0.00062	0.00409	-0.01570	-0.01127	3.09750
A38	2.07349	0.00010	0.00218	-0.00465	-0.00244	2.07105
A39	2.08137	0.00006	0.00075	0.00232	0.00307	2.08444
A40	2.01268	-0.00066	-0.00093	-0.00380	-0.00468	2.00800
A41	1.98227	-0.00016	-0.00085	0.00044	-0.00045	1.98182
A42	2.04323	-0.00009	-0.00131	0.00208	0.00080	2.04403
A43	2.04531	0.00023	0.00185	-0.00285	-0.00089	2.04442
A44	2.13145	-0.00003	-0.00017	-0.00050	-0.00076	2.13069
A45	1.95235	0.00027	0.00226	-0.00566	-0.00340	1.94895
A46	2.04897	-0.00006	-0.00092	0.00124	0.00034	2.04931
A47	2.02021	-0.00012	-0.00189	0.00473	0.00283	2.02303
A48	1.44557	0.00005	0.00117	0.00715	0.00828	1.45386
A49	0.93722	0.00011	-0.00219	0.00224	0.00052	0.93774
A50	2.36983	0.00017	-0.00049	0.00292	0.00226	2.37209
A51	2.22228	0.00060	-0.00246	0.00719	0.00472	2.22700
A52	1.93722	-0.00048	-0.00177	0.00268	0.00092	1.93814
A53	1.91363	-0.00009	0.00067	-0.00330	-0.00265	1.91098
A54	1.94469	-0.00077	-0.00121	-0.00078	-0.00198	1.94270
A55	1.88119	0.00034	0.00092	-0.00030	0.00062	1.88181
A56	1.90519	0.00066	0.00049	0.00306	0.00357	1.90876
A57	1.87995	0.00041	0.00103	-0.00146	-0.00044	1.87951
A58	3.66786	0.00064	-0.00129	0.01434	0.01300	3.68086
A59	4.97633	0.00045	-0.00144	0.03900	0.03759	5.01393
D1	0.01036	-0.00036	0.00196	-0.00422	-0.00224	0.00812
D2	-3.13708	-0.00018	0.00028	-0.00019	0.00010	-3.13698
D3	-3.13642	-0.00012	0.00069	-0.00148	-0.00079	-3.13721
D4	-0.00067	0.00006	-0.00099	0.00255	0.00155	0.00087
D5	-0.01542	0.00052	-0.00134	0.01235	0.01098	-0.00444
D6	-3.11716	0.00049	-0.00368	0.01929	0.01557	-3.10159
D7	3.13084	0.00031	-0.00019	0.00988	0.00968	3.14051
D8	0.02910	0.00028	-0.00254	0.01682	0.01426	0.04336
D9	-0.00195	0.00008	-0.00193	-0.00518	-0.00711	-0.00905
D10	-3.13869	0.00007	-0.00065	-0.00297	-0.00365	3.14085
D11	-3.13824	-0.00008	-0.00041	-0.00883	-0.00923	3.13571
D12	0.00820	-0.00010	0.00087	-0.00663	-0.00577	0.00244
D13	-0.00766	0.00024	0.00111	0.01295	0.01404	0.00638

D14	-3.13824	-0.00016	0.00066	0.00081	0.00140	-3.13685
D15	3.12947	0.00026	-0.00006	0.01091	0.01085	3.14032
D16	-0.00112	-0.00014	-0.00052	-0.00122	-0.00180	-0.00292
D17	0.02256	-0.00002	0.00180	-0.01465	-0.01284	0.00972
D18	-3.11871	-0.00005	0.00131	-0.01481	-0.01350	-3.13221
D19	-3.11358	-0.00004	0.00323	-0.01217	-0.00895	-3.12253
D20	0.02832	-0.00007	0.00274	-0.01233	-0.00960	0.01872
D21	0.01423	-0.00047	0.00012	-0.01564	-0.01549	-0.00126
D22	3.11771	-0.00046	0.00238	-0.02230	-0.01986	3.09785
D23	-3.13785	-0.00009	0.00056	-0.00403	-0.00345	-3.14130
D24	-0.03437	-0.00008	0.00282	-0.01068	-0.00782	-0.04219
D25	-3.03736	0.00014	-0.00392	-0.01258	-0.01638	-3.05375
D26	0.11682	-0.00031	-0.00444	-0.02648	-0.03084	0.08598
D27	1.37860	0.00031	0.00010	0.02425	0.02445	1.40304
D28	-2.79261	0.00003	0.00084	0.01795	0.01884	-2.77377
D29	-0.73563	-0.00006	-0.00017	0.01889	0.01874	-0.71688
D30	-1.71771	0.00029	-0.00257	0.03214	0.02965	-1.68806
D31	0.39427	0.00002	-0.00183	0.02584	0.02404	0.41830
D32	2.45125	-0.00007	-0.00283	0.02678	0.02395	2.47520
D33	-0.95821	0.00010	-0.00535	-0.02270	-0.02807	-0.98627
D34	1.11363	-0.00040	-0.00456	-0.02966	-0.03422	1.07941
D35	-3.02537	-0.00062	-0.00497	-0.03055	-0.03558	-3.06095
D36	-3.03088	0.00023	-0.00578	-0.02061	-0.02636	-3.05724
D37	-0.95903	-0.00027	-0.00498	-0.02757	-0.03251	-0.99155
D38	1.18515	-0.00049	-0.00539	-0.02846	-0.03388	1.15127
D39	1.13374	0.00062	-0.00516	-0.01659	-0.02172	1.11202
D40	-3.07761	0.00012	-0.00437	-0.02355	-0.02787	-3.10548
D41	-0.93342	-0.00010	-0.00478	-0.02444	-0.02924	-0.96266
D42	-1.77358	0.00052	-0.00131	0.01549	0.01442	-1.75916
D43	2.42840	-0.00012	-0.00122	0.00922	0.00810	2.43651
D44	0.34278	0.00015	-0.00047	0.01021	0.00984	0.35262
D45	0.39265	-0.00009	0.00614	0.04372	0.05001	0.44266
D46	-0.35456	-0.00020	-0.00237	-0.01714	-0.01959	-0.37415
D47	2.63704	-0.00015	0.00086	-0.05397	-0.05304	2.58400
D48	-3.13897	-0.00006	-0.00025	-0.00181	-0.00205	-3.14102
D49	0.00260	-0.00001	-0.00014	-0.00070	-0.00085	0.00176
D50	0.00227	-0.00003	0.00030	-0.00162	-0.00133	0.00095
D51	-3.13934	0.00002	0.00040	-0.00052	-0.00012	-3.13946
D52	-1.42674	-0.00012	0.00371	-0.03197	-0.02815	-1.45489
D53	2.05616	0.00010	0.00004	0.03348	0.03355	2.08972
D54	1.88261	0.00012	0.00410	-0.01005	-0.00587	1.87674
D55	-2.92017	-0.00035	0.00148	-0.00551	-0.00404	-2.92421
D56	-2.71243	-0.00033	-0.00035	-0.00686	-0.00723	-2.71966
D57	-0.02373	-0.00016	-0.00131	-0.00228	-0.00360	-0.02733

D58	-0.01456	-0.00020	0.00349	-0.00696	-0.00350	-0.01806
D59	2.67414	-0.00002	0.00252	-0.00237	0.00012	2.67427
D60	-0.12091	-0.00050	-0.00172	-0.04352	-0.04524	-0.16615
D61	0.09332	-0.00054	-0.00642	0.01034	0.00394	0.09727
D62	-2.54842	0.00064	0.00250	-0.04287	-0.04037	-2.58879
D63	-2.33419	0.00060	-0.00220	0.01099	0.00882	-2.32537
D64	2.14542	0.00019	-0.00087	-0.00053	-0.00129	2.14413
D65	-0.25130	0.00012	0.00053	-0.00279	-0.00216	-0.25347
D66	2.47256	-0.00026	0.00020	0.00290	0.00308	2.47564
D67	-1.73422	-0.00020	0.00067	0.00208	0.00273	-1.73149
D68	0.34530	-0.00023	0.00161	-0.00236	-0.00075	0.34455
D69	1.25243	0.00023	0.00046	0.00356	0.00404	1.25647
D70	-2.95435	0.00029	0.00093	0.00275	0.00370	-2.95066
D71	-0.87483	0.00026	0.00188	-0.00169	0.00021	-0.87462
D72	-1.11588	0.00000	0.00016	0.00562	0.00578	-1.11011
D73	0.96052	0.00006	0.00062	0.00481	0.00543	0.96595
D74	3.04004	0.00003	0.00157	0.00037	0.00194	3.04199

Item	Value	Threshold	Converged?
Maximum Force	0.002958	0.000450	NO
RMS Force	0.000572	0.000300	NO
Maximum Displacement	0.203127	0.001800	NO
RMS Displacement	0.054986	0.001200	NO

Predicted change in Energy=-2.174936D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.365287	-1.913349	-0.262637
2	6	0	-2.483052	-1.148542	-0.164834
3	7	0	-2.065652	0.123836	0.214163
4	6	0	-0.726025	0.113205	0.350586
5	7	0	-0.285279	-1.109046	0.065625
6	6	0	1.143486	-1.482706	0.057095
7	6	0	1.737828	-1.433851	-1.358141
8	1	0	-1.248144	-2.949011	-0.531449
9	1	0	-3.514862	-1.397565	-0.332237
10	1	0	1.658297	-0.774769	0.707262
11	1	0	1.232476	-2.488546	0.468355
12	1	0	1.159861	-2.084133	-2.026149
13	1	0	1.673115	-0.409197	-1.740054
14	35	0	1.647427	2.239727	1.118375

15	1	0	-0.064313	0.952828	0.645138
16	6	0	-2.847184	1.288945	0.449818
17	6	0	-4.168505	1.344581	0.349191
18	1	0	-2.235167	2.138909	0.725092
19	1	0	-4.672899	2.279795	0.548502
20	1	0	-4.785206	0.497775	0.076327
21	8	0	3.063177	-1.899474	-1.315579
22	1	0	3.670278	-1.133894	-1.324488
23	6	0	4.698207	1.683816	-1.094427
24	6	0	5.621827	0.801091	-0.372947
25	8	0	4.776664	0.271550	-1.419497
26	1	0	3.779391	1.992450	-0.601346
27	1	0	5.081460	2.331764	-1.878270
28	1	0	6.667573	0.824060	-0.673962
29	6	0	5.353242	0.342305	1.030952
30	1	0	5.662613	-0.698306	1.170407
31	1	0	5.924582	0.958329	1.731974
32	1	0	4.296535	0.443041	1.285912

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357900	0.000000			
3	N	2.206348	1.391693	0.000000		
4	C	2.211700	2.223692	1.346597	0.000000	
5	N	1.386029	2.210176	2.170666	1.330172	0.000000
6	C	2.565467	3.648656	3.592244	2.475508	1.476843
7	C	3.325564	4.395590	4.400567	3.373975	2.495109
8	H	1.076374	2.213841	3.265983	3.229205	2.160805
9	H	2.211685	1.074555	2.171042	3.244423	3.266763
10	H	3.373296	4.248650	3.862439	2.569184	2.073867
11	H	2.759270	4.000211	4.215068	3.258636	2.090166
12	H	3.084723	4.196503	4.505337	3.746163	2.723003
13	H	3.698259	4.505738	4.252231	3.224834	2.754192
14	Br	5.313349	5.494347	4.368243	3.277937	4.007233
15	H	3.275905	3.304861	2.208693	1.108869	2.153134
16	C	3.599763	2.540026	1.422605	2.427246	3.530060
17	C	4.341252	3.052972	2.435250	3.656085	4.602189
18	H	4.260644	3.414784	2.085738	2.553671	3.845279
19	H	5.401916	4.130106	3.399658	4.506783	5.564946
20	H	4.198125	2.840498	2.748600	4.086570	4.778214
21	O	4.551942	5.713910	5.721782	4.602721	3.707379
22	H	5.204997	6.261668	6.070439	4.867095	4.192787
23	C	7.099114	7.775402	7.063691	5.828994	5.829316

24	C	7.496673	8.338671	7.739554	6.425878	6.223734
25	O	6.620851	7.502954	7.036188	5.782547	5.452971
26	H	6.468207	7.019585	6.190420	4.973582	5.156130
27	H	7.886178	8.501190	7.767524	6.604293	6.664817
28	H	8.496437	9.374664	8.806151	7.498021	7.254381
29	C	7.204163	8.065980	7.466917	6.121509	5.901796
30	H	7.274704	8.266646	7.830479	6.491946	6.063553
31	H	8.084998	8.872716	8.175816	6.844928	6.753749
32	H	6.325093	7.113410	6.459718	5.119545	4.989097

		6	7	8	9	10
6	C	0.000000				
7	C	1.535748	0.000000			
8	H	2.866414	3.448937	0.000000		
9	H	4.675364	5.352060	2.754029	0.000000	
10	H	1.090377	2.169471	3.835249	5.313191	0.000000
11	H	1.090307	2.168837	2.713875	4.936436	1.781974
12	H	2.168384	1.096881	2.963213	5.019337	3.071548
13	H	2.159322	1.095427	4.055261	5.465705	2.474514
14	Br	3.903432	4.431306	6.166787	6.479459	3.042420
15	H	2.781438	3.599594	4.243838	4.287878	2.440458
16	C	4.874600	5.630690	4.634661	2.876585	4.962313
17	C	6.024626	6.746810	5.266780	2.900165	6.210595
18	H	4.997760	5.734907	5.332920	3.906688	4.863013
19	H	6.944654	7.650090	6.343158	3.954709	7.031330
20	H	6.250765	6.952615	4.975995	2.317976	6.598194
21	O	2.396486	1.405406	4.505983	6.670043	2.707496
22	H	2.900883	1.955881	5.302306	7.258121	2.881848
23	C	4.897847	4.307346	7.559042	8.805131	4.304855
24	C	5.045414	4.588138	7.828467	9.397597	4.399973
25	O	4.296245	3.485208	6.889046	8.527454	3.916899
26	H	4.411151	4.059588	7.049755	8.048028	3.724111
27	H	5.814074	5.062634	8.352509	9.497097	5.296562
28	H	6.030850	5.465222	8.770118	10.427578	5.436625
29	C	4.690534	4.683344	7.540037	9.139403	3.873661
30	H	4.719879	4.726364	7.464621	9.325929	4.031737
31	H	5.623411	5.727149	8.475753	9.945567	4.717505
32	H	3.893612	4.130462	6.749244	8.186828	2.962803

		11	12	13	14	15
11	H	0.000000				
12	H	2.528117	0.000000			
13	H	3.065115	1.775019	0.000000		
14	Br	4.790749	5.368568	3.897188	0.000000	
15	H	3.681843	4.225815	3.250063	2.193198	0.000000
16	C	5.559982	5.793486	5.302106	4.642465	2.809892

17	C	6.624022	6.766817	6.447109	5.934476	4.133455
18	H	5.788246	6.076975	5.276785	3.903763	2.475032
19	H	7.590583	7.726175	7.262235	6.346092	4.796795
20	H	6.729360	6.813991	6.769915	6.745296	4.776761
21	O	2.623146	2.040005	2.081677	5.006143	4.664894
22	H	3.315456	2.774433	2.164842	4.630424	4.709672
23	C	5.644660	5.252184	3.734798	3.809565	5.122697
24	C	5.549405	5.564776	4.350413	4.482139	5.778556
25	O	4.872718	4.358731	3.193460	4.484042	5.306780
26	H	5.264063	5.050795	3.391307	2.750247	4.172362
27	H	6.599751	5.907703	4.375932	4.558610	5.894746
28	H	6.466725	6.373452	5.253769	5.515293	6.861115
29	C	5.030998	5.728692	4.667607	4.164243	5.465482
30	H	4.829488	5.693265	4.946763	4.975587	5.983297
31	H	5.957645	6.788419	5.656860	4.506944	6.086716
32	H	4.318687	5.214890	4.094522	3.205296	4.437057

		16	17	18	19	20
16	C	0.000000				
17	C	1.326315	0.000000			
18	H	1.082949	2.123690	0.000000		
19	H	2.079605	1.081093	2.448177	0.000000	
20	H	2.126352	1.082522	3.101115	1.846932	0.000000
21	O	6.943703	8.098925	6.967447	8.988212	8.323540
22	H	7.176045	8.389909	7.055941	9.207061	8.724668
23	C	7.711908	8.989866	7.182578	9.532682	9.628731
24	C	8.522856	9.831962	8.045358	10.441121	10.421141
25	O	7.915332	9.181269	7.566509	9.859021	9.680806
26	H	6.746211	8.030711	6.160828	8.534983	8.720414
27	H	8.328916	9.565457	7.768379	10.051837	10.224238
28	H	9.592163	10.896715	9.107412	11.498691	11.481966
29	C	8.275314	9.598595	7.804183	10.223019	10.184478
30	H	8.768413	10.074655	8.403750	10.773981	10.572821
31	H	8.871139	10.194690	8.305966	10.744928	10.846789
32	H	7.242052	8.564294	6.771529	9.185215	9.162101

		21	22	23	24	25
21	O	0.000000				
22	H	0.977121	0.000000			
23	C	3.944895	3.008165	0.000000		
24	C	3.837746	2.908288	1.467246	0.000000	
25	O	2.767703	1.791198	1.451317	1.445676	0.000000
26	H	4.021215	3.210742	1.087477	2.205917	2.150679
27	H	4.721596	3.782710	1.086798	2.213810	2.132570
28	H	4.563002	3.638756	2.189606	1.088450	2.106331
29	C	3.971924	3.249558	2.597298	1.501185	2.518362

30	H	3.792097	3.222365	3.425501	2.152161	2.903985
31	H	5.063818	4.336039	3.165259	2.132388	3.423616
32	H	3.711644	3.113376	2.714198	2.153233	2.753029

		26	27	28	29	30
26	H	0.000000				
27	H	1.855007	0.000000			
28	H	3.116409	2.497856	0.000000		
29	C	2.804351	3.534882	2.205967	0.000000	
30	H	3.731729	4.337453	2.594078	1.094545	0.000000
31	H	3.334011	3.953611	2.521624	1.094233	1.768735
32	H	2.495966	3.767682	3.099694	1.091687	1.783868

		31	32
31	H	0.000000	
32	H	1.764945	0.000000

Stoichiometry C10H17BrN2O2
Framework group C1[X(C10H17BrN2O2)]
Deg. of freedom 90
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.696962	2.143077	-0.399847
2	6	0	-3.759025	1.364119	-0.069489
3	7	0	-3.275599	0.066668	0.070973
4	6	0	-1.953069	0.071611	-0.182430
5	7	0	-1.585537	1.317735	-0.467833
6	6	0	-0.191237	1.716266	-0.747407
7	6	0	0.501362	2.283693	0.500333
8	1	0	-2.638650	3.200391	-0.592897
9	1	0	-4.792434	1.619924	0.076445
10	1	0	0.328532	0.822612	-1.094023
11	1	0	-0.205666	2.462486	-1.542213
12	1	0	-0.075732	3.129936	0.892741
13	1	0	0.539313	1.509115	1.273993
14	35	0	0.512836	-2.087615	-0.226307
15	1	0	-1.252844	-0.788046	-0.166193
16	6	0	-3.982996	-1.120266	0.409471
17	6	0	-5.286450	-1.180278	0.647209
18	1	0	-3.330113	-1.983230	0.452090
19	1	0	-5.732670	-2.132460	0.898207

20	1	0	-5.943925	-0.321369	0.604140
21	8	0	1.782434	2.740506	0.146294
22	1	0	2.443787	2.072235	0.412358
23	6	0	3.659453	-0.543537	1.266143
24	6	0	4.463074	-0.005800	0.162583
25	8	0	3.655240	0.877835	0.972875
26	1	0	2.734209	-1.064751	1.031907
27	1	0	4.142881	-0.791263	2.207450
28	1	0	5.525922	0.139171	0.347134
29	6	0	4.064947	-0.183420	-1.273906
30	1	0	4.285949	0.716019	-1.857170
31	1	0	4.630630	-1.012528	-1.709715
32	1	0	3.003545	-0.422051	-1.364807

Rotational constants (GHZ): 0.5865619 0.2269697 0.1753397

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.

475 basis functions, 751 primitive gaussians, 492 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1311.5117449600 Hartrees.

NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 475 RedAO= T EigKep= 3.74D-06 NBF= 475

NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999971 -0.001607 0.000007 -0.007482 Ang= -0.88 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3225.52341648 A.U. after 11 cycles
NFock= 11 Conv=0.65D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000530610	0.000002587	-0.000215381
2	6	0.000013488	0.000145749	-0.000874230
3	7	-0.000210505	-0.000585486	0.000840699
4	6	-0.000760412	0.000579686	-0.000581158
5	7	0.000371865	-0.000824393	0.000666447
6	6	-0.000662692	-0.000388264	0.000268603
7	6	0.001094236	-0.000458954	-0.000259036
8	1	0.000012469	-0.000086653	0.000197727
9	1	-0.000070161	-0.000014559	-0.000015490
10	1	0.000267874	0.000247005	0.000073598
11	1	0.000073357	-0.000288468	0.000167816
12	1	-0.000273213	-0.000002786	-0.000089647
13	1	-0.000118679	0.000300302	-0.000054699
14	35	-0.000492177	-0.000022355	0.000356365
15	1	0.000423613	0.001702556	0.000130970
16	6	0.000202443	-0.000414277	0.000148145
17	6	-0.000135718	0.000090218	0.000003097
18	1	0.000004452	0.000042285	0.000011727
19	1	0.000000920	0.000028948	-0.000023658
20	1	-0.000013394	-0.000073967	-0.000029535
21	8	-0.000609868	-0.000443478	-0.000935351
22	1	0.000350125	0.000318827	0.000426317
23	6	0.000741031	0.000727030	-0.000079942
24	6	0.001403952	0.001179196	-0.000375712
25	8	-0.001138942	-0.000999647	-0.000650774
26	1	-0.000141543	-0.000082526	-0.000566560
27	1	-0.000379328	-0.000065452	0.000050982
28	1	0.000384629	-0.000246692	0.000109615
29	6	-0.000071049	-0.000906174	0.002144314
30	1	0.000248123	0.000106245	-0.000475221
31	1	0.000088180	0.000142073	0.000053997

```
      32        1             -0.000072466       0.000291424      -0.000424027
 ----------------------------------------------------------------------
 Cartesian Forces:  Max         0.002144314 RMS         0.000530245

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 GSVD:  received Info=                 1 from GESDD.
 Internal  Forces:  Max         0.001749612 RMS         0.000374759
 Search for a local minimum.
 Step number   21 out of a maximum of   177
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swapping is turned off.
 Update second derivatives using D2CorX and points     19     20     21
 DE= -1.42D-04 DEPred=-2.17D-04 R= 6.52D-01
 TightC=F SS=  1.41D+00  RLast= 3.23D-01 DXNew= 3.2661D+00 9.6998D-01
 Trust test= 6.52D-01 RLast= 3.23D-01 DXMaxT set to 1.94D+00
 ITU=  1  1  1  1 -1  1  1  1  1  1  1  1  1  1  1  0  1  0  1
 ITU=  0
      Eigenvalues ---     0.00002     0.00222     0.00240     0.00325     0.00462
      Eigenvalues ---     0.00519     0.00916     0.01108     0.01396     0.01443
      Eigenvalues ---     0.01699     0.01857     0.02030     0.02057     0.02167
      Eigenvalues ---     0.02242     0.02319     0.02385     0.02640     0.03045
      Eigenvalues ---     0.03061     0.03151     0.03513     0.03791     0.04203
      Eigenvalues ---     0.04675     0.04880     0.05192     0.05358     0.05647
      Eigenvalues ---     0.05935     0.06261     0.07320     0.09345     0.09633
      Eigenvalues ---     0.09968     0.11074     0.11596     0.11881     0.12930
      Eigenvalues ---     0.13879     0.14862     0.15278     0.15959     0.15995
      Eigenvalues ---     0.16000     0.16001     0.16003     0.16006     0.16062
      Eigenvalues ---     0.16576     0.17399     0.19587     0.22022     0.22282
      Eigenvalues ---     0.22921     0.23347     0.23797     0.24526     0.25056
      Eigenvalues ---     0.27554     0.28357     0.31048     0.32174     0.33101
      Eigenvalues ---     0.33273     0.33980     0.34157     0.34515     0.34808
      Eigenvalues ---     0.35079     0.35681     0.35689     0.35852     0.35922
      Eigenvalues ---     0.36436     0.36663     0.37217     0.37243     0.37743
      Eigenvalues ---     0.38743     0.42022     0.42631     0.43810     0.45686
      Eigenvalues ---     0.49162     0.53414     0.54846     0.56153     0.60374
 Eigenvalue     1 is      1.94D-05 Eigenvector:
                              D54         D52         D55         D53         D47
   1                      -0.50094     0.50072    -0.50042    -0.49634    -0.01597
                              R18         D46         D42         D35         D43
   1                       0.01323    -0.01150    -0.01014     0.00876    -0.00823
```

En-DIIS/RFO-DIIS IScMMF= 0 using points: 21 20 19
RFO step: Lambda=-5.99163982D-05.
DidBck=T Rises=F RFO-DIIS coefs: 0.73119 0.35985 -0.09103
Iteration 1 RMS(Cart)= 0.03398486 RMS(Int)= 0.00075236
Iteration 2 RMS(Cart)= 0.00039482 RMS(Int)= 0.00002787
Iteration 3 RMS(Cart)= 0.00000064 RMS(Int)= 0.00002786

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56606	-0.00017	-0.00003	-0.00083	-0.00086	2.56520
R2	2.61921	0.00046	-0.00014	0.00106	0.00092	2.62013
R3	2.03405	0.00003	0.00001	0.00004	0.00005	2.03410
R4	2.62992	0.00004	0.00005	-0.00015	-0.00009	2.62982
R5	2.03061	0.00007	-0.00002	0.00014	0.00012	2.03074
R6	2.54470	0.00030	-0.00020	0.00117	0.00097	2.54567
R7	2.68833	-0.00028	0.00021	-0.00104	-0.00083	2.68750
R8	2.51366	0.00125	-0.00056	0.00266	0.00210	2.51576
R9	2.09546	0.00154	-0.00107	0.00654	0.00548	2.10094
R10	2.79083	0.00041	-0.00087	0.00082	-0.00005	2.79078
R11	2.90214	0.00086	-0.00143	0.00316	0.00174	2.90388
R12	2.06051	0.00033	-0.00025	0.00106	0.00081	2.06132
R13	2.06038	0.00034	0.00003	0.00051	0.00054	2.06092
R14	2.07281	0.00020	-0.00016	0.00102	0.00086	2.07367
R15	2.07006	0.00031	-0.00034	0.00121	0.00087	2.07093
R16	2.65583	-0.00014	0.00055	-0.00417	-0.00363	2.65221
R17	4.14454	0.00009	0.00207	-0.01488	-0.01280	4.13174
R18	8.47361	0.00097	0.07977	0.00862	0.08839	8.56200
R19	2.50637	0.00015	-0.00003	0.00026	0.00023	2.50660
R20	2.04648	0.00004	0.00000	0.00002	0.00002	2.04649
R21	2.04297	0.00002	0.00002	-0.00003	-0.00001	2.04296
R22	2.04567	0.00007	0.00000	0.00008	0.00008	2.04575
R23	1.84649	0.00091	-0.00105	0.00237	0.00131	1.84780
R24	3.38487	0.00043	-0.01912	0.01448	-0.00465	3.38022
R25	2.77269	0.00041	0.00095	-0.00024	0.00061	2.77330
R26	2.74259	0.00036	-0.00002	-0.00155	-0.00153	2.74106
R27	2.05503	-0.00016	0.00032	-0.00001	0.00032	2.05535
R28	2.05375	-0.00021	0.00053	-0.00059	-0.00006	2.05369
R29	2.73193	0.00175	-0.00139	0.00494	0.00361	2.73555
R30	2.05687	0.00033	0.00004	0.00034	0.00038	2.05725
R31	2.83683	0.00130	-0.00114	0.00251	0.00138	2.83821
R32	2.06839	-0.00009	0.00021	-0.00080	-0.00059	2.06780
R33	2.06780	0.00016	0.00001	-0.00001	0.00000	2.06780
R34	2.06299	0.00000	-0.00005	0.00002	-0.00004	2.06295
A1	1.87289	0.00016	-0.00004	0.00041	0.00036	1.87325
A2	2.27772	-0.00005	-0.00013	0.00022	0.00009	2.27781

A3	2.13257	-0.00011	0.00018	-0.00063	-0.00045	2.13212
A4	1.86259	0.00005	-0.00015	-0.00013	-0.00029	1.86230
A5	2.27663	-0.00002	0.00006	0.00007	0.00012	2.27675
A6	2.14396	-0.00003	0.00010	0.00008	0.00016	2.14413
A7	1.89520	0.00042	0.00002	0.00157	0.00159	1.89679
A8	2.25122	-0.00033	0.00020	-0.00174	-0.00154	2.24969
A9	2.13673	-0.00008	-0.00021	0.00019	-0.00002	2.13671
A10	1.89144	-0.00051	0.00003	-0.00205	-0.00201	1.88944
A11	2.23266	0.00049	-0.00105	0.00153	0.00051	2.23317
A12	2.15908	0.00002	0.00100	0.00051	0.00149	2.16057
A13	1.90261	-0.00012	0.00013	0.00025	0.00039	1.90300
A14	2.22138	-0.00018	-0.00041	-0.00305	-0.00345	2.21794
A15	2.15830	0.00029	0.00028	0.00248	0.00271	2.16100
A16	1.95161	0.00015	-0.00254	0.00371	0.00113	1.95275
A17	1.86404	0.00006	0.00052	-0.00046	0.00004	1.86408
A18	1.88619	-0.00005	-0.00011	0.00015	0.00007	1.88627
A19	1.92422	-0.00032	0.00180	-0.00431	-0.00249	1.92173
A20	1.92342	0.00013	-0.00004	-0.00013	-0.00016	1.92326
A21	1.91294	0.00003	0.00039	0.00110	0.00149	1.91443
A22	1.91605	-0.00007	-0.00047	0.00095	0.00047	1.91652
A23	1.90517	-0.00027	0.00085	-0.00331	-0.00245	1.90272
A24	1.90341	0.00030	-0.00122	0.00070	-0.00051	1.90290
A25	1.88714	0.00002	0.00076	-0.00242	-0.00167	1.88546
A26	1.89540	0.00004	-0.00063	0.00247	0.00185	1.89725
A27	1.95646	-0.00002	0.00071	0.00164	0.00231	1.95877
A28	1.73654	0.00085	-0.00913	0.01182	0.00268	1.73922
A29	2.88538	-0.00096	0.00135	-0.00900	-0.00769	2.87769
A30	2.17619	0.00001	0.00002	-0.00008	-0.00006	2.17613
A31	1.95458	0.00002	-0.00005	0.00036	0.00030	1.95489
A32	2.15241	-0.00003	0.00003	-0.00028	-0.00025	2.15216
A33	2.07956	0.00001	-0.00006	0.00034	0.00028	2.07984
A34	2.15778	-0.00004	0.00015	-0.00072	-0.00057	2.15721
A35	2.04584	0.00003	-0.00008	0.00038	0.00030	2.04614
A36	1.90293	0.00035	0.00031	0.00341	0.00358	1.90652
A37	3.09750	-0.00071	0.00042	-0.01268	-0.01231	3.08519
A38	2.07105	0.00053	-0.00074	0.00341	0.00266	2.07371
A39	2.08444	-0.00037	-0.00130	0.00286	0.00155	2.08598
A40	2.00800	-0.00036	0.00185	-0.00560	-0.00377	2.00422
A41	1.98182	-0.00001	0.00066	0.00073	0.00139	1.98321
A42	2.04403	-0.00013	0.00062	-0.00317	-0.00257	2.04146
A43	2.04442	-0.00004	-0.00094	0.00005	-0.00092	2.04350
A44	2.13069	0.00052	0.00031	0.00166	0.00197	2.13266
A45	1.94895	0.00033	-0.00053	-0.00167	-0.00220	1.94675
A46	2.04931	-0.00002	0.00049	-0.00140	-0.00092	2.04839

A47	2.02303	-0.00040	0.00045	0.00065	0.00110	2.02413
A48	1.45386	-0.00044	-0.00297	-0.01038	-0.01342	1.44044
A49	0.93774	0.00098	0.00126	0.01641	0.01763	0.95536
A50	2.37209	0.00053	-0.00029	0.00637	0.00598	2.37807
A51	2.22700	0.00074	0.00030	0.01258	0.01285	2.23985
A52	1.93814	-0.00061	0.00088	-0.00171	-0.00084	1.93730
A53	1.91098	0.00012	0.00029	-0.00048	-0.00019	1.91079
A54	1.94270	-0.00058	0.00131	-0.00281	-0.00151	1.94119
A55	1.88181	0.00026	-0.00076	0.00124	0.00049	1.88230
A56	1.90876	0.00062	-0.00127	0.00220	0.00091	1.90967
A57	1.87951	0.00024	-0.00054	0.00181	0.00127	1.88078
A58	3.68086	0.00030	-0.00267	0.00220	-0.00057	3.68028
A59	5.01393	-0.00046	-0.00919	-0.01490	-0.02420	4.98973
D1	0.00812	-0.00020	-0.00065	-0.00597	-0.00662	0.00150
D2	-3.13698	0.00006	-0.00021	0.00149	0.00129	-3.13569
D3	-3.13721	-0.00025	-0.00023	-0.00693	-0.00716	3.13881
D4	0.00087	0.00001	0.00021	0.00052	0.00074	0.00161
D5	-0.00444	-0.00006	-0.00210	0.00354	0.00145	-0.00299
D6	-3.10159	0.00005	-0.00184	0.01128	0.00944	-3.09215
D7	3.14051	-0.00001	-0.00248	0.00441	0.00194	-3.14073
D8	0.04336	0.00010	-0.00222	0.01215	0.00992	0.05329
D9	-0.00905	0.00038	0.00314	0.00637	0.00952	0.00046
D10	3.14085	0.00018	0.00139	0.00264	0.00405	-3.13828
D11	3.13571	0.00015	0.00274	-0.00038	0.00236	3.13807
D12	0.00244	-0.00006	0.00099	-0.00411	-0.00311	-0.00067
D13	0.00638	-0.00043	-0.00449	-0.00423	-0.00871	-0.00233
D14	-3.13685	-0.00036	-0.00079	-0.00894	-0.00972	3.13662
D15	3.14032	-0.00024	-0.00288	-0.00081	-0.00368	3.13664
D16	-0.00292	-0.00018	0.00081	-0.00552	-0.00469	-0.00760
D17	0.00972	0.00006	0.00231	-0.00070	0.00160	0.01133
D18	-3.13221	0.00010	0.00279	-0.00027	0.00252	-3.12969
D19	-3.12253	-0.00017	0.00034	-0.00489	-0.00454	-3.12707
D20	0.01872	-0.00013	0.00083	-0.00446	-0.00362	0.01510
D21	-0.00126	0.00030	0.00409	0.00047	0.00454	0.00328
D22	3.09785	0.00018	0.00382	-0.00710	-0.00331	3.09453
D23	-3.14130	0.00024	0.00057	0.00494	0.00550	-3.13580
D24	-0.04219	0.00012	0.00030	-0.00263	-0.00236	-0.04455
D25	-3.05375	-0.00004	0.00690	0.00663	0.01351	-3.04023
D26	0.08598	0.00003	0.01113	0.00126	0.01236	0.09833
D27	1.40304	0.00021	-0.00663	-0.00067	-0.00732	1.39572
D28	-2.77377	-0.00006	-0.00560	-0.00407	-0.00969	-2.78346
D29	-0.71688	-0.00002	-0.00493	-0.00294	-0.00789	-0.72477
D30	-1.68806	0.00035	-0.00633	0.00820	0.00185	-1.68621
D31	0.41830	0.00008	-0.00530	0.00480	-0.00051	0.41779

D32	2.47520	0.00013	-0.00463	0.00593	0.00129	2.47649
D33	-0.98627	0.00008	0.01096	0.00792	0.01886	-0.96741
D34	1.07941	-0.00010	0.01211	0.00356	0.01565	1.09507
D35	-3.06095	-0.00010	0.01273	0.00393	0.01663	-3.04432
D36	-3.05724	0.00012	0.01077	0.00895	0.01972	-3.03751
D37	-0.99155	-0.00006	0.01192	0.00460	0.01651	-0.97504
D38	1.15127	-0.00007	0.01255	0.00496	0.01749	1.16876
D39	1.11202	0.00020	0.00913	0.01047	0.01959	1.13161
D40	-3.10548	0.00003	0.01028	0.00611	0.01638	-3.08909
D41	-0.96266	0.00002	0.01091	0.00648	0.01736	-0.94530
D42	-1.75916	0.00023	-0.00304	0.00554	0.00247	-1.75669
D43	2.43651	0.00011	-0.00140	0.00252	0.00111	2.43761
D44	0.35262	0.00008	-0.00234	0.00291	0.00054	0.35316
D45	0.44266	-0.00003	-0.01736	-0.00341	-0.02080	0.42186
D46	-0.37415	-0.00027	0.00678	0.00193	0.00883	-0.36532
D47	2.58400	-0.00019	0.01371	0.00513	0.01881	2.60281
D48	-3.14102	0.00005	0.00071	0.00011	0.00081	-3.14021
D49	0.00176	0.00001	0.00032	0.00018	0.00050	0.00225
D50	0.00095	0.00001	0.00017	-0.00037	-0.00021	0.00074
D51	-3.13946	-0.00003	-0.00022	-0.00030	-0.00052	-3.13998
D52	-1.45489	-0.00023	0.00520	-0.03335	-0.02819	-1.48308
D53	2.08972	-0.00017	-0.00905	0.02416	0.01505	2.10477
D54	1.87674	-0.00034	-0.00104	0.02386	0.02279	1.89953
D55	-2.92421	0.00029	0.00014	0.03906	0.03925	-2.88496
D56	-2.71966	-0.00016	0.00217	-0.01026	-0.00808	-2.72774
D57	-0.02733	-0.00007	0.00181	-0.00425	-0.00245	-0.02978
D58	-0.01806	-0.00013	-0.00128	-0.00335	-0.00463	-0.02269
D59	2.67427	-0.00004	-0.00164	0.00265	0.00100	2.67527
D60	-0.16615	-0.00021	0.01326	0.01247	0.02568	-0.14047
D61	0.09727	-0.00020	0.00304	0.00927	0.01234	0.10961
D62	-2.58879	0.00045	0.00925	0.02344	0.03265	-2.55614
D63	-2.32537	0.00046	-0.00096	0.02024	0.01931	-2.30606
D64	2.14413	-0.00016	0.00090	-0.00672	-0.00584	2.13829
D65	-0.25347	0.00011	0.00024	-0.00415	-0.00392	-0.25739
D66	2.47564	-0.00013	-0.00096	0.00757	0.00663	2.48227
D67	-1.73149	-0.00011	-0.00116	0.00775	0.00659	-1.72490
D68	0.34455	-0.00010	-0.00083	0.00793	0.00711	0.35166
D69	1.25647	0.00007	-0.00138	0.00968	0.00829	1.26476
D70	-2.95066	0.00009	-0.00159	0.00985	0.00825	-2.94241
D71	-0.87462	0.00010	-0.00125	0.01003	0.00877	-0.86585
D72	-1.11011	0.00003	-0.00165	0.01336	0.01171	-1.09839
D73	0.96595	0.00006	-0.00186	0.01353	0.01168	0.97763
D74	3.04199	0.00007	-0.00152	0.01372	0.01219	3.05418

Item	Value	Threshold	Converged?

Maximum Force	0.001750	0.000450	NO
RMS Force	0.000375	0.000300	NO
Maximum Displacement	0.145162	0.001800	NO
RMS Displacement	0.034021	0.001200	NO

Predicted change in Energy=-1.215930D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.372328	-1.908953	-0.264743
2	6	0	-2.496020	-1.152511	-0.176569
3	7	0	-2.091673	0.120211	0.215034
4	6	0	-0.752075	0.122631	0.357067
5	7	0	-0.300395	-1.097136	0.073391
6	6	0	1.130521	-1.462368	0.065069
7	6	0	1.727006	-1.409178	-1.350108
8	1	0	-1.245302	-2.943764	-0.532457
9	1	0	-3.524693	-1.409050	-0.352146
10	1	0	1.641521	-0.750257	0.714399
11	1	0	1.225439	-2.468080	0.476076
12	1	0	1.142167	-2.047497	-2.024392
13	1	0	1.670399	-0.380261	-1.723064
14	35	0	1.605987	2.259639	1.120282
15	1	0	-0.097541	0.970790	0.654125
16	6	0	-2.885651	1.276178	0.451451
17	6	0	-4.206729	1.320048	0.340713
18	1	0	-2.283975	2.130541	0.735789
19	1	0	-4.721644	2.249328	0.540850
20	1	0	-4.812821	0.468679	0.058278
21	8	0	3.045922	-1.887244	-1.309032
22	1	0	3.663516	-1.129155	-1.309431
23	6	0	4.736230	1.673516	-1.093790
24	6	0	5.661552	0.783211	-0.383234
25	8	0	4.787050	0.258996	-1.410832
26	1	0	3.828183	1.996295	-0.589572
27	1	0	5.111906	2.311932	-1.889000
28	1	0	6.700908	0.787950	-0.707084
29	6	0	5.414509	0.334218	1.028545
30	1	0	5.720564	-0.707027	1.168108
31	1	0	6.001398	0.951263	1.715685
32	1	0	4.362538	0.442669	1.299349

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357447	0.000000			
3	N	2.205708	1.391643	0.000000		
4	C	2.213300	2.225331	1.347109	0.000000	
5	N	1.386514	2.210501	2.170409	1.331285	0.000000
6	C	2.563682	3.647766	3.592990	2.478236	1.476815
7	C	3.321696	4.390560	4.401251	3.377385	2.496813
8	H	1.076402	2.213490	3.265430	3.230682	2.161003
9	H	2.211384	1.074620	2.171147	3.245988	3.267181
10	H	3.374105	4.251456	3.865724	2.572727	2.074188
11	H	2.758592	4.000740	4.215522	3.261366	2.090409
12	H	3.072173	4.177542	4.491293	3.737507	2.717511
13	H	3.704293	4.510772	4.261441	3.232371	2.761374
14	Br	5.307147	5.490997	4.366843	3.272577	3.999777
15	H	3.280598	3.309254	2.211979	1.111770	2.157480
16	C	3.598352	2.538651	1.422165	2.427287	3.529745
17	C	4.338993	3.050845	2.434926	3.656324	4.601488
18	H	4.260244	3.414058	2.085568	2.553791	3.845941
19	H	5.399834	4.128027	3.399418	4.507116	5.564601
20	H	4.194577	2.837425	2.747845	4.086402	4.776400
21	O	4.540038	5.703983	5.722546	4.608716	3.705833
22	H	5.201844	6.262891	6.083347	4.882789	4.198310
23	C	7.129929	7.818770	7.123625	5.884872	5.865698
24	C	7.532413	8.386639	7.804485	6.489917	6.268096
25	O	6.629589	7.520562	7.069620	5.816009	5.470293
26	H	6.511666	7.076800	6.261931	5.038403	5.201345
27	H	7.905654	8.533189	7.818066	6.650122	6.690719
28	H	8.523268	9.414368	8.865984	7.557911	7.292526
29	C	7.263991	8.138742	7.553169	6.206642	5.968351
30	H	7.335312	8.337797	7.913515	6.575802	6.132090
31	H	8.153206	8.956149	8.272872	6.938435	6.826835
32	H	6.392589	7.194633	6.552599	5.210526	5.061315

		6	7	8	9	10
6	C	0.000000				
7	C	1.536668	0.000000			
8	H	2.862885	3.443562	0.000000		
9	H	4.674177	5.345678	2.753812	0.000000	
10	H	1.090804	2.168796	3.834041	5.316136	0.000000
11	H	1.090593	2.169744	2.710715	4.936724	1.783490
12	H	2.169876	1.097336	2.954517	4.998360	3.071346
13	H	2.158667	1.095888	4.060837	5.470539	2.465554

14	Br	3.897804	4.424668	6.159286	6.476975	3.037347
15	H	2.788437	3.606961	4.248420	4.292038	2.447442
16	C	4.876327	5.633236	4.633220	2.874820	4.966978
17	C	6.025285	6.746611	5.264274	2.897103	6.215130
18	H	5.001764	5.741824	5.332529	3.905341	4.869186
19	H	6.946286	7.651502	6.340754	3.951439	7.036867
20	H	6.249185	6.948326	4.972015	2.313783	6.601124
21	O	2.395294	1.403486	4.487082	6.657123	2.712813
22	H	2.901093	1.957074	5.290840	7.257071	2.885813
23	C	4.917099	4.315568	7.577143	8.848452	4.326829
24	C	5.076794	4.606741	7.849665	9.444261	4.440379
25	O	4.302508	3.485736	6.886108	8.543317	3.928046
26	H	4.434894	4.073157	7.081504	8.106635	3.745047
27	H	5.823671	5.059111	8.359224	9.528823	5.310203
28	H	6.057174	5.475450	8.780571	10.464975	5.475773
29	C	4.744318	4.721768	7.585181	9.211657	3.938300
30	H	4.780766	4.773147	7.511205	9.395679	4.104425
31	H	5.681161	5.765518	8.528778	10.029627	4.786050
32	H	3.949499	4.170729	6.802302	8.268295	3.028063

		11	12	13	14	15
11	H	0.000000				
12	H	2.536960	0.000000			
13	H	3.064831	1.774684	0.000000		
14	Br	4.786558	5.353086	3.880443	0.000000	
15	H	3.688875	4.221539	3.256068	2.186422	0.000000
16	C	5.560677	5.779268	5.313181	4.646433	2.812098
17	C	6.623948	6.748687	6.456846	5.939547	4.135896
18	H	5.790574	6.067376	5.290289	3.911049	2.476325
19	H	7.591174	7.708921	7.273119	6.354114	4.798940
20	H	6.727533	6.791948	6.776874	6.748073	4.779228
21	O	2.614984	2.040025	2.081942	5.017132	4.680139
22	H	3.305295	2.776998	2.168974	4.649823	4.734012
23	C	5.651809	5.256353	3.743435	3.878670	5.187906
24	C	5.566723	5.579529	4.367850	4.570340	5.854780
25	O	4.866460	4.356780	3.196819	4.530813	5.350694
26	H	5.276412	5.062178	3.404241	2.816222	4.243790
27	H	6.598994	5.897607	4.372574	4.620604	5.950166
28	H	6.479380	6.377669	5.263360	5.609221	6.935793
29	C	5.070148	5.765925	4.701084	4.268548	5.561304
30	H	4.877126	5.740264	4.986931	5.072784	6.076972
31	H	6.003193	6.825897	5.688190	4.624499	6.190667
32	H	4.357938	5.255375	4.130351	3.306360	4.537348

		16	17	18	19	20
16	C	0.000000				

17	C	1.326437	0.000000			
18	H	1.082958	2.123668	0.000000		
19	H	2.079876	1.081089	2.448334	0.000000	
20	H	2.126176	1.082565	3.100946	1.847133	0.000000
21	O	6.949107	8.099959	6.980809	8.992685	8.317437
22	H	7.195687	8.406089	7.083868	9.227600	8.733384
23	C	7.787086	9.064174	7.269079	9.615352	9.693465
24	C	8.601999	9.909352	8.136271	10.526832	10.488391
25	O	7.960722	9.223979	7.622995	9.908872	9.713896
26	H	6.832120	8.116806	6.255644	8.627944	8.798879
27	H	8.397107	9.632882	7.849935	10.129501	10.280549
28	H	9.668644	10.970759	9.198509	11.583077	11.543556
29	C	8.373349	9.696040	7.910697	10.327008	10.274131
30	H	8.860792	10.165862	8.503607	10.870749	10.656745
31	H	8.982400	10.306911	8.426049	10.865029	10.951129
32	H	7.345060	8.667244	6.880599	9.293100	9.258950

		21	22	23	24	25
21	O	0.000000				
22	H	0.977814	0.000000			
23	C	3.947465	3.008684	0.000000		
24	C	3.850967	2.916699	1.467567	0.000000	
25	O	2.765544	1.788735	1.450505	1.447589	0.000000
26	H	4.026342	3.211503	1.087645	2.208029	2.147581
27	H	4.715689	3.778202	1.086768	2.215046	2.132773
28	H	4.569237	3.641959	2.189459	1.088652	2.106634
29	C	4.001170	3.267042	2.599632	1.501914	2.519905
30	H	3.831819	3.247743	3.428131	2.151965	2.907848
31	H	5.093218	4.352604	3.164720	2.132885	3.424761
32	H	3.737060	3.124899	2.716936	2.152787	2.749368

		26	27	28	29	30
26	H	0.000000				
27	H	1.853668	0.000000			
28	H	3.118727	2.498875	0.000000		
29	C	2.810202	3.537653	2.207511	0.000000	
30	H	3.738783	4.339411	2.590826	1.094230	0.000000
31	H	3.336041	3.954285	2.527014	1.094233	1.768795
32	H	2.503460	3.771109	3.100479	1.091668	1.784169

		31	32
31	H	0.000000	
32	H	1.765749	0.000000

Stoichiometry C10H17BrN2O2

Framework group C1[X(C10H17BrN2O2)]

Deg. of freedom 90

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.685086	2.152235	-0.400280
2	6	0	-3.755515	1.387642	-0.065254
3	7	0	-3.289716	0.082817	0.065642
4	6	0	-1.966388	0.069865	-0.186027
5	7	0	-1.584087	1.312559	-0.472170
6	6	0	-0.185644	1.699518	-0.747133
7	6	0	0.509608	2.261109	0.502903
8	1	0	-2.613783	3.208508	-0.594816
9	1	0	-4.785211	1.656682	0.083580
10	1	0	0.328563	0.800830	-1.090359
11	1	0	-0.191187	2.445982	-1.542213
12	1	0	-0.071097	3.100452	0.905932
13	1	0	0.552290	1.479117	1.269478
14	35	0	0.479256	-2.104441	-0.217336
15	1	0	-1.275299	-0.800808	-0.167128
16	6	0	-4.013892	-1.094591	0.400054
17	6	0	-5.317664	-1.136051	0.640668
18	1	0	-3.374079	-1.967519	0.437927
19	1	0	-5.777772	-2.082311	0.888952
20	1	0	-5.961790	-0.266794	0.602710
21	8	0	1.785158	2.726027	0.147099
22	1	0	2.453664	2.059553	0.402114
23	6	0	3.705555	-0.538341	1.259959
24	6	0	4.513799	0.008641	0.163917
25	8	0	3.677427	0.880753	0.961047
26	1	0	2.790064	-1.074057	1.019426
27	1	0	4.179823	-0.774309	2.208881
28	1	0	5.570771	0.176467	0.363437
29	6	0	4.138339	-0.179253	-1.278120
30	1	0	4.359146	0.719980	-1.861184
31	1	0	4.718681	-1.004534	-1.701746
32	1	0	3.080538	-0.428337	-1.381820

Rotational constants (GHZ): 0.5864757 0.2241664 0.1735551

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.

475 basis functions, 751 primitive gaussians, 492 cartesian basis functions
71 alpha electrons 71 beta electrons
nuclear repulsion energy 1307.7672443807 Hartrees.
NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 475 RedAO= T EigKep= 3.74D-06 NBF= 475
NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999997 0.001088 0.000214 0.002213 Ang= 0.28 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3225.52354660 A.U. after 11 cycles
NFock= 11 Conv=0.30D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Atomic Forces (Hartrees/Bohr)
Number Number X Y Z
---
1 6 -0.000003133 0.000158622 -0.000424600
2 6 -0.000120540 0.000045593 0.000158442
3 7 0.000010527 -0.000100707 -0.000051013
4 6 -0.000532678 0.000060176 -0.000006147
5 7 0.000187336 -0.000310279 0.000273090

6	6	-0.000478158	-0.000030823	0.000366524
7	6	-0.000389857	0.000182468	-0.000112535
8	1	0.000038590	-0.000025540	0.000039000
9	1	-0.000023292	-0.000009914	0.000058676
10	1	0.000103387	-0.000050995	0.000146003
11	1	0.000055566	-0.000108216	0.000061869
12	1	-0.000038280	-0.000055622	0.000129826
13	1	0.000059645	0.000053704	-0.000064724
14	35	0.000245409	-0.000045954	0.000088614
15	1	-0.000151333	0.000514316	-0.000118929
16	6	0.000080093	-0.000156342	-0.000005853
17	6	-0.000067584	0.000055750	0.000020933
18	1	-0.000017943	0.000031846	0.000019540
19	1	-0.000001517	0.000012551	0.000001694
20	1	-0.000029571	-0.000013878	-0.000015398
21	8	0.000954041	-0.000374796	-0.000894391
22	1	-0.000361924	-0.000163115	0.000241552
23	6	0.000003603	0.000556230	0.000230898
24	6	0.000796243	0.000630497	-0.000959350
25	8	-0.000279103	-0.000707124	-0.000180191
26	1	-0.000019411	0.000107541	-0.000301588
27	1	-0.000286336	-0.000074560	0.000085316
28	1	0.000237580	-0.000133632	0.000333172
29	6	-0.000035146	-0.000272346	0.001488457
30	1	0.000118685	-0.000010284	-0.000374452
31	1	0.000092079	0.000101844	0.000084963
32	1	-0.000146980	0.000132987	-0.000319397

Cartesian Forces: Max 0.001488457 RMS 0.000319659

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000925890 RMS 0.000212294
Search for a local minimum.
Step number 22 out of a maximum of 177
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 19 20 21 22
DE= -1.30D-04 DEPred=-1.22D-04 R= 1.07D+00
TightC=F SS= 1.41D+00 RLast= 1.45D-01 DXNew= 3.2661D+00 4.3362D-01

Trust test= 1.07D+00 RLast= 1.45D-01 DXMaxT set to 1.94D+00

ITU= 1 1 1 1 1 -1 1 1 1 1 1 1 1 1 1 1 0 1 0

ITU= 1 0

Eigenvalues ---	0.00003	0.00227	0.00237	0.00318	0.00446
Eigenvalues ---	0.00526	0.00915	0.01200	0.01396	0.01412
Eigenvalues ---	0.01712	0.01835	0.01939	0.02052	0.02175
Eigenvalues ---	0.02220	0.02316	0.02381	0.02594	0.03053
Eigenvalues ---	0.03062	0.03233	0.03382	0.03741	0.04168
Eigenvalues ---	0.04644	0.04968	0.05197	0.05403	0.05654
Eigenvalues ---	0.05948	0.06316	0.07278	0.09396	0.09604
Eigenvalues ---	0.10335	0.11176	0.11494	0.11770	0.13006
Eigenvalues ---	0.13903	0.14958	0.15024	0.15937	0.15994
Eigenvalues ---	0.16000	0.16002	0.16003	0.16008	0.16062
Eigenvalues ---	0.16569	0.17401	0.19564	0.21336	0.22044
Eigenvalues ---	0.22915	0.23426	0.23846	0.24265	0.25067
Eigenvalues ---	0.27717	0.28661	0.30751	0.32153	0.33099
Eigenvalues ---	0.33195	0.34010	0.34141	0.34519	0.34792
Eigenvalues ---	0.35053	0.35678	0.35688	0.35777	0.35861
Eigenvalues ---	0.36437	0.36663	0.37208	0.37226	0.37495
Eigenvalues ---	0.37835	0.42134	0.42485	0.44530	0.45865
Eigenvalues ---	0.49265	0.53352	0.54690	0.56025	0.60363

Eigenvalue 1 is 2.93D-05 Eigenvector:

	D54	D55	D52	D53	D47
1	-0.50142	-0.50105	0.50009	-0.49481	-0.02066
	R18	D46	D42	D35	D38
1	0.01672	-0.01439	-0.01269	0.01114	0.01043

En-DIIS/RFO-DIIS IScMMF= 0 using points: 22 21 20 19

RFO step: Lambda=-1.91965987D-05.

DidBck=F Rises=F RFO-DIIS coefs: 1.37635 -0.22305 -0.25880 0.10550

Iteration 1 RMS(Cart)= 0.01554553 RMS(Int)= 0.00148786

Iteration 2 RMS(Cart)= 0.00018994 RMS(Int)= 0.00005535

Iteration 3 RMS(Cart)= 0.00000206 RMS(Int)= 0.00005535

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00005535

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56520	0.00011	-0.00029	0.00015	-0.00014	2.56506
R2	2.62013	0.00006	0.00048	-0.00014	0.00033	2.62046
R3	2.03410	0.00002	0.00002	0.00009	0.00012	2.03422
R4	2.62982	-0.00006	-0.00008	-0.00027	-0.00035	2.62948
R5	2.03074	0.00002	0.00008	0.00000	0.00007	2.03081
R6	2.54567	0.00004	0.00039	0.00015	0.00055	2.54621
R7	2.68750	-0.00003	-0.00042	0.00012	-0.00031	2.68720
R8	2.51576	0.00046	0.00128	0.00095	0.00227	2.51804
R9	2.10094	0.00045	0.00257	-0.00013	0.00250	2.10344

R10	2.79078	0.00028	0.00078	0.00038	0.00114	2.79192
R11	2.90388	0.00068	0.00180	0.00103	0.00282	2.90670
R12	2.06132	0.00010	0.00053	0.00007	0.00060	2.06192
R13	2.06092	0.00013	0.00026	0.00027	0.00053	2.06145
R14	2.07367	-0.00003	0.00034	-0.00008	0.00026	2.07392
R15	2.07093	0.00007	0.00049	-0.00005	0.00045	2.07137
R16	2.65221	0.00093	-0.00086	0.00149	0.00063	2.65283
R17	4.13174	0.00027	-0.00409	0.00627	0.00223	4.13397
R18	8.56200	0.00016	-0.01632	-0.02608	-0.04240	8.51960
R19	2.50660	0.00010	0.00011	0.00019	0.00029	2.50690
R20	2.04649	0.00002	0.00003	0.00003	0.00005	2.04655
R21	2.04296	0.00001	-0.00001	0.00007	0.00007	2.04303
R22	2.04575	0.00003	0.00006	0.00004	0.00010	2.04585
R23	1.84780	0.00012	0.00100	-0.00064	0.00029	1.84809
R24	3.38022	0.00046	0.01862	-0.00312	0.01543	3.39565
R25	2.77330	0.00019	-0.00018	0.00064	0.00042	2.77372
R26	2.74106	0.00051	-0.00034	0.00131	0.00099	2.74205
R27	2.05535	-0.00009	-0.00005	0.00027	0.00022	2.05557
R28	2.05369	-0.00021	-0.00047	0.00024	-0.00023	2.05347
R29	2.73555	0.00088	0.00213	0.00127	0.00341	2.73896
R30	2.05725	0.00013	0.00021	0.00050	0.00071	2.05796
R31	2.83821	0.00085	0.00193	0.00101	0.00294	2.84115
R32	2.06780	0.00000	-0.00031	0.00018	-0.00013	2.06767
R33	2.06780	0.00016	0.00006	0.00035	0.00041	2.06821
R34	2.06295	0.00008	0.00008	0.00029	0.00037	2.06332
A1	1.87325	0.00010	0.00019	0.00061	0.00080	1.87405
A2	2.27781	-0.00001	0.00005	0.00010	0.00015	2.27796
A3	2.13212	-0.00009	-0.00025	-0.00071	-0.00096	2.13116
A4	1.86230	0.00001	-0.00005	-0.00006	-0.00010	1.86220
A5	2.27675	0.00001	0.00002	0.00014	0.00015	2.27690
A6	2.14413	-0.00002	0.00002	-0.00008	-0.00006	2.14406
A7	1.89679	0.00006	0.00066	-0.00010	0.00057	1.89735
A8	2.24969	-0.00005	-0.00069	-0.00012	-0.00082	2.24887
A9	2.13671	-0.00001	0.00004	0.00022	0.00025	2.13696
A10	1.88944	-0.00001	-0.00079	0.00035	-0.00047	1.88897
A11	2.23317	0.00017	0.00088	-0.00023	0.00064	2.23381
A12	2.16057	-0.00016	-0.00008	-0.00012	-0.00018	2.16039
A13	1.90300	-0.00017	0.00000	-0.00081	-0.00080	1.90220
A14	2.21794	-0.00003	-0.00085	-0.00166	-0.00247	2.21547
A15	2.16100	0.00019	0.00074	0.00228	0.00297	2.16397
A16	1.95275	0.00006	0.00197	-0.00181	0.00016	1.95290
A17	1.86408	0.00001	-0.00030	0.00165	0.00133	1.86540
A18	1.88627	-0.00001	0.00008	-0.00056	-0.00045	1.88582
A19	1.92173	-0.00006	-0.00177	-0.00016	-0.00192	1.91981

A20	1.92326	0.00003	0.00000	0.00047	0.00047	1.92372
A21	1.91443	-0.00005	0.00003	0.00045	0.00048	1.91491
A22	1.91652	-0.00019	0.00034	-0.00155	-0.00117	1.91535
A23	1.90272	-0.00013	-0.00116	-0.00097	-0.00218	1.90054
A24	1.90290	0.00057	0.00099	0.00191	0.00291	1.90581
A25	1.88546	0.00010	-0.00088	0.00088	0.00000	1.88546
A26	1.89725	-0.00012	0.00075	-0.00058	0.00021	1.89746
A27	1.95877	-0.00024	-0.00004	0.00023	0.00017	1.95894
A28	1.73922	0.00059	0.00654	0.00774	0.01426	1.75348
A29	2.87769	-0.00047	-0.00275	-0.00744	-0.01017	2.86752
A30	2.17613	0.00010	-0.00005	0.00065	0.00060	2.17673
A31	1.95489	-0.00002	0.00014	0.00008	0.00022	1.95511
A32	2.15216	-0.00009	-0.00008	-0.00073	-0.00081	2.15135
A33	2.07984	-0.00002	0.00009	-0.00006	0.00003	2.07987
A34	2.15721	0.00003	-0.00024	0.00015	-0.00009	2.15712
A35	2.04614	-0.00001	0.00015	-0.00009	0.00006	2.04620
A36	1.90652	-0.00002	0.00062	0.00060	0.00072	1.90724
A37	3.08519	-0.00019	-0.00334	-0.01196	-0.01514	3.07005
A38	2.07371	0.00029	0.00224	-0.00093	0.00137	2.07508
A39	2.08598	-0.00013	0.00160	-0.00020	0.00135	2.08733
A40	2.00422	-0.00006	-0.00282	0.00208	-0.00075	2.00347
A41	1.98321	-0.00001	-0.00018	0.00015	-0.00004	1.98317
A42	2.04146	-0.00015	-0.00181	-0.00020	-0.00202	2.03945
A43	2.04350	0.00031	0.00089	0.00142	0.00233	2.04583
A44	2.13266	-0.00010	0.00050	-0.00113	-0.00065	2.13201
A45	1.94675	0.00027	0.00032	-0.00018	0.00016	1.94691
A46	2.04839	-0.00010	-0.00097	0.00050	-0.00049	2.04790
A47	2.02413	-0.00023	-0.00055	-0.00040	-0.00096	2.02317
A48	1.44044	-0.00009	-0.00292	-0.00318	-0.00629	1.43414
A49	0.95536	0.00014	0.00509	0.00923	0.01450	0.96986
A50	2.37807	0.00005	0.00223	0.00276	0.00487	2.38293
A51	2.23985	0.00038	0.00374	0.00861	0.01236	2.25220
A52	1.93730	-0.00048	-0.00148	-0.00202	-0.00350	1.93380
A53	1.91079	0.00016	0.00001	0.00097	0.00099	1.91177
A54	1.94119	-0.00044	-0.00177	-0.00162	-0.00338	1.93781
A55	1.88230	0.00020	0.00096	0.00072	0.00168	1.88398
A56	1.90967	0.00041	0.00125	0.00121	0.00246	1.91213
A57	1.88078	0.00019	0.00117	0.00089	0.00206	1.88285
A58	3.68028	0.00029	0.00082	0.00543	0.00606	3.68635
A59	4.98973	0.00001	-0.00441	0.00995	0.00557	4.99531
D1	0.00150	0.00014	-0.00138	0.00058	-0.00080	0.00070
D2	-3.13569	0.00011	0.00071	0.00218	0.00289	-3.13281
D3	3.13881	-0.00003	-0.00231	-0.00145	-0.00377	3.13504
D4	0.00161	-0.00006	-0.00021	0.00014	-0.00008	0.00154

D5	-0.00299	-0.00018	0.00124	-0.00241	-0.00117	-0.00416
D6	-3.09215	-0.00014	0.00322	0.00149	0.00469	-3.08746
D7	-3.14073	-0.00003	0.00207	-0.00059	0.00149	-3.13925
D8	0.05329	0.00001	0.00405	0.00332	0.00735	0.06064
D9	0.00046	-0.00005	0.00107	0.00142	0.00249	0.00295
D10	-3.13828	-0.00006	0.00049	0.00006	0.00055	-3.13774
D11	3.13807	-0.00002	-0.00083	-0.00003	-0.00085	3.13722
D12	-0.00067	-0.00003	-0.00141	-0.00138	-0.00279	-0.00347
D13	-0.00233	-0.00006	-0.00030	-0.00293	-0.00324	-0.00557
D14	3.13662	-0.00011	-0.00296	-0.00243	-0.00539	3.13123
D15	3.13664	-0.00006	0.00023	-0.00168	-0.00145	3.13518
D16	-0.00760	-0.00010	-0.00242	-0.00118	-0.00360	-0.01120
D17	0.01133	-0.00001	-0.00004	-0.00432	-0.00435	0.00697
D18	-3.12969	-0.00001	-0.00015	-0.00363	-0.00379	-3.13348
D19	-3.12707	-0.00002	-0.00069	-0.00584	-0.00653	-3.13361
D20	0.01510	-0.00002	-0.00081	-0.00516	-0.00597	0.00913
D21	0.00328	0.00015	-0.00057	0.00330	0.00273	0.00602
D22	3.09453	0.00010	-0.00253	-0.00058	-0.00311	3.09142
D23	-3.13580	0.00019	0.00196	0.00282	0.00477	-3.13103
D24	-0.04455	0.00015	0.00000	-0.00106	-0.00108	-0.04563
D25	-3.04023	0.00010	-0.00033	-0.01366	-0.01395	-3.05419
D26	0.09833	0.00004	-0.00336	-0.01307	-0.01640	0.08193
D27	1.39572	0.00009	0.00106	0.01013	0.01120	1.40692
D28	-2.78346	0.00007	-0.00014	0.00993	0.00979	-2.77367
D29	-0.72477	0.00001	-0.00022	0.01105	0.01082	-0.71395
D30	-1.68621	0.00015	0.00334	0.01467	0.01803	-1.66818
D31	0.41779	0.00013	0.00214	0.01448	0.01661	0.43440
D32	2.47649	0.00007	0.00206	0.01560	0.01765	2.49413
D33	-0.96741	0.00003	-0.00116	0.00363	0.00243	-0.96499
D34	1.09507	-0.00004	-0.00273	0.00321	0.00045	1.09552
D35	-3.04432	-0.00005	-0.00287	0.00410	0.00112	-3.04320
D36	-3.03751	0.00001	-0.00089	0.00281	0.00194	-3.03558
D37	-0.97504	-0.00006	-0.00245	0.00240	-0.00004	-0.97507
D38	1.16876	-0.00007	-0.00260	0.00328	0.00063	1.16939
D39	1.13161	0.00009	0.00023	0.00205	0.00228	1.13390
D40	-3.08909	0.00002	-0.00134	0.00164	0.00031	-3.08878
D41	-0.94530	0.00000	-0.00148	0.00252	0.00098	-0.94432
D42	-1.75669	0.00014	0.00218	0.00773	0.01002	-1.74667
D43	2.43761	0.00011	0.00076	0.00883	0.00961	2.44722
D44	0.35316	0.00021	0.00136	0.00797	0.00937	0.36253
D45	0.42186	0.00009	0.00438	0.01215	0.01660	0.43847
D46	-0.36532	-0.00024	-0.00144	0.00350	0.00214	-0.36318
D47	2.60281	-0.00027	-0.00042	-0.01168	-0.01200	2.59081
D48	-3.14021	0.00000	-0.00019	0.00041	0.00022	-3.13999

D49	0.00225	-0.00001	-0.00005	-0.00032	-0.00037	0.00188
D50	0.00074	0.00000	-0.00006	-0.00035	-0.00041	0.00033
D51	-3.13998	-0.00001	0.00008	-0.00108	-0.00100	-3.14098
D52	-1.48308	-0.00036	-0.01218	-0.04712	-0.05928	-1.54236
D53	2.10477	-0.00009	0.01084	0.03158	0.04248	2.14725
D54	1.89953	-0.00016	0.01071	0.01159	0.02221	1.92174
D55	-2.88496	-0.00010	0.01525	0.02163	0.03690	-2.84806
D56	-2.72774	0.00005	-0.00441	0.00220	-0.00222	-2.72996
D57	-0.02978	-0.00003	-0.00244	0.00187	-0.00058	-0.03036
D58	-0.02269	0.00002	0.00030	-0.00121	-0.00094	-0.02362
D59	2.67527	-0.00006	0.00226	-0.00155	0.00070	2.67597
D60	-0.14047	-0.00013	0.00146	-0.00879	-0.00731	-0.14778
D61	0.10961	-0.00008	0.00050	0.01397	0.01452	0.12412
D62	-2.55614	0.00020	0.00795	-0.01109	-0.00312	-2.55926
D63	-2.30606	0.00025	0.00699	0.01167	0.01870	-2.28736
D64	2.13829	-0.00014	-0.00304	-0.00436	-0.00737	2.13092
D65	-0.25739	0.00002	-0.00141	-0.00408	-0.00547	-0.26286
D66	2.48227	-0.00009	0.00312	-0.00107	0.00205	2.48431
D67	-1.72490	-0.00005	0.00340	-0.00081	0.00259	-1.72231
D68	0.35166	0.00002	0.00375	-0.00008	0.00367	0.35533
D69	1.26476	-0.00001	0.00408	-0.00114	0.00294	1.26770
D70	-2.94241	0.00004	0.00436	-0.00088	0.00348	-2.93892
D71	-0.86585	0.00011	0.00472	-0.00015	0.00457	-0.86128
D72	-1.09839	-0.00005	0.00541	-0.00096	0.00444	-1.09395
D73	0.97763	0.00000	0.00569	-0.00070	0.00499	0.98262
D74	3.05418	0.00006	0.00605	0.00003	0.00607	3.06025

Item	Value	Threshold	Converged?
Maximum Force	0.000926	0.000450	NO
RMS Force	0.000212	0.000300	YES
Maximum Displacement	0.053466	0.001800	NO
RMS Displacement	0.015524	0.001200	NO

Predicted change in Energy=-3.740747D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.381379	-1.913158	-0.262557
2	6	0	-2.503550	-1.154650	-0.173923
3	7	0	-2.096730	0.116681	0.218979
4	6	0	-0.756575	0.117784	0.358493
5	7	0	-0.307013	-1.104235	0.075501

6	6	0	1.123020	-1.475099	0.060045
7	6	0	1.718971	-1.402965	-1.356137
8	1	0	-1.256452	-2.948799	-0.528291
9	1	0	-3.533058	-1.409647	-0.347078
10	1	0	1.639171	-0.774412	0.718204
11	1	0	1.213977	-2.487386	0.456290
12	1	0	1.128637	-2.027204	-2.038981
13	1	0	1.665514	-0.367382	-1.711382
14	35	0	1.622606	2.235351	1.112304
15	1	0	-0.098967	0.966720	0.651467
16	6	0	-2.889310	1.273149	0.456657
17	6	0	-4.210057	1.320619	0.341682
18	1	0	-2.287183	2.125700	0.745552
19	1	0	-4.723417	2.250497	0.543220
20	1	0	-4.817177	0.471719	0.053867
21	8	0	3.036170	-1.887622	-1.327837
22	1	0	3.657612	-1.132724	-1.308844
23	6	0	4.755544	1.672726	-1.101625
24	6	0	5.674162	0.785231	-0.378503
25	8	0	4.796727	0.253820	-1.402443
26	1	0	3.847758	2.007407	-0.604498
27	1	0	5.135148	2.299273	-1.904212
28	1	0	6.714733	0.776878	-0.699633
29	6	0	5.420550	0.354740	1.039517
30	1	0	5.722655	-0.686141	1.189486
31	1	0	6.007339	0.977783	1.721658
32	1	0	4.367042	0.470962	1.301779

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357372	0.000000			
3	N	2.205414	1.391459	0.000000		
4	C	2.213777	2.225866	1.347398	0.000000	
5	N	1.386688	2.211228	2.171246	1.332487	0.000000
6	C	2.562807	3.648211	3.595249	2.481779	1.477421
7	C	3.326918	4.391922	4.398851	3.373568	2.498687
8	H	1.076464	2.213550	3.265218	3.231130	2.160652
9	H	2.211423	1.074659	2.170975	3.246495	3.267907
10	H	3.373775	4.254717	3.873014	2.581668	2.075929
11	H	2.753607	3.999170	4.218799	3.267958	2.090817
12	H	3.077152	4.175234	4.483037	3.728657	2.717352
13	H	3.711074	4.512723	4.256183	3.222775	2.761660
14	Br	5.303234	5.492873	4.372671	3.273045	3.993898

15	H	3.282334	3.311118	2.213746	1.113092	2.159601
16	C	3.597732	2.537844	1.422002	2.427562	3.530650
17	C	4.338645	3.050405	2.435297	3.656998	4.602665
18	H	4.260181	3.413641	2.085595	2.554271	3.847404
19	H	5.399492	4.127605	3.399674	4.507596	5.565753
20	H	4.194338	2.837223	2.748481	4.087365	4.777623
21	O	4.544250	5.705897	5.723332	4.609802	3.709437
22	H	5.205307	6.264858	6.083396	4.881478	4.199461
23	C	7.157123	7.845326	7.149750	5.910435	5.892930
24	C	7.554827	8.407138	7.822449	6.507152	6.288931
25	O	6.645610	7.535722	7.082907	5.827398	5.484232
26	H	6.544587	7.107961	6.292050	5.069310	5.235154
27	H	7.931250	8.559977	7.846764	6.677659	6.717161
28	H	8.542503	9.433129	8.883783	7.574594	7.310563
29	C	7.287317	8.157332	7.565676	6.219069	5.988565
30	H	7.353999	8.351577	7.920176	6.581586	6.145947
31	H	8.178496	8.976398	8.287066	6.953297	6.849501
32	H	6.416816	7.212860	6.563408	5.221684	5.082499

		6	7	8	9	10
6	C	0.000000				
7	C	1.538159	0.000000			
8	H	2.860038	3.453705	0.000000		
9	H	4.674302	5.348089	2.754045	0.000000	
10	H	1.091122	2.168949	3.829666	5.318863	0.000000
11	H	1.090875	2.171608	2.699134	4.933686	1.784283
12	H	2.170429	1.097472	2.969877	4.997531	3.071190
13	H	2.158538	1.096124	4.074470	5.474741	2.463586
14	Br	3.888994	4.397707	6.152718	6.480484	3.035500
15	H	2.793835	3.598719	4.250046	4.293855	2.461122
16	C	4.879443	5.628859	4.632623	2.873638	4.976751
17	C	6.028024	6.741949	5.263893	2.896043	6.224500
18	H	5.006512	5.737407	5.332507	3.904449	4.881358
19	H	6.949413	7.645894	6.340399	3.950473	7.047214
20	H	6.251087	6.944335	4.971682	2.312846	6.608981
21	O	2.399277	1.403819	4.493548	6.659212	2.716087
22	H	2.900902	1.957957	5.296737	7.259987	2.882953
23	C	4.945049	4.329599	7.604689	8.875319	4.360280
24	C	5.100423	4.624663	7.873934	9.465272	4.462780
25	O	4.315571	3.495664	6.903759	8.559570	3.940123
26	H	4.471427	4.089906	7.114967	8.137504	3.790240
27	H	5.848193	5.067269	8.383792	9.556074	5.342889
28	H	6.075834	5.490023	8.800558	10.484389	5.493459
29	C	4.772467	4.746617	7.612736	9.230536	3.959426
30	H	4.801535	4.798283	7.535139	9.410245	4.111537

31	H	5.712631	5.790585	8.558211	10.049809	4.812275
32	H	3.981550	4.193853	6.831370	8.286556	3.054963

		11	12	13	14	15
11	H	0.000000				
12	H	2.538785	0.000000			
13	H	3.065469	1.774984	0.000000		
14	Br	4.785559	5.323906	3.840476	0.000000	
15	H	3.700373	4.208219	3.236707	2.187603	0.000000
16	C	5.565841	5.767533	5.304541	4.659731	2.813870
17	C	6.628287	6.736255	6.448779	5.954037	4.137907
18	H	5.798479	6.055416	5.279753	3.928483	2.477978
19	H	7.596561	7.695000	7.263260	6.371506	4.800556
20	H	6.730012	6.780659	6.770929	6.760288	4.781596
21	O	2.619773	2.040561	2.082531	4.995133	4.679102
22	H	3.304869	2.780092	2.171691	4.620296	4.728887
23	C	5.681226	5.265223	3.752616	3.877283	5.209419
24	C	5.594654	5.597212	4.378852	4.554169	5.867094
25	O	4.879057	4.366136	3.207153	4.508376	5.356734
26	H	5.316506	5.072421	3.409839	2.819692	4.270493
27	H	6.622662	5.898195	4.380250	4.630486	5.975212
28	H	6.499992	6.392277	5.275185	5.598215	6.948958
29	C	5.110097	5.794077	4.710541	4.238675	5.566881
30	H	4.910218	5.772907	4.997703	5.035024	6.075582
31	H	6.048542	6.853764	5.696198	4.602029	6.199387
32	H	4.405507	5.280983	4.132822	3.268164	4.540256

		16	17	18	19	20
16	C	0.000000				
17	C	1.326593	0.000000			
18	H	1.082987	2.123373	0.000000		
19	H	2.080060	1.081124	2.447805	0.000000	
20	H	2.126312	1.082618	3.100799	1.847243	0.000000
21	O	6.948827	8.098636	6.981674	8.990888	8.315687
22	H	7.194957	8.404960	7.083675	9.225940	8.732312
23	C	7.812278	9.087855	7.295015	9.637947	9.716716
24	C	8.617924	9.924873	8.151280	10.540694	10.504924
25	O	7.973108	9.235919	7.635417	9.919953	9.726021
26	H	6.859538	8.142194	6.282843	8.651091	8.824561
27	H	8.427251	9.660987	7.883043	10.157933	10.306445
28	H	9.686120	10.987768	9.216418	11.599461	11.560529
29	C	8.380750	9.704045	7.914029	10.331518	10.285730
30	H	8.862381	10.168807	8.500649	10.870231	10.663880
31	H	8.990985	10.315864	8.430278	10.870033	10.963930
32	H	7.349311	8.672390	6.879408	9.294009	9.268612

		21	22	23	24	25

21	O	0.000000				
22	H	0.977969	0.000000			
23	C	3.960240	3.019759	0.000000		
24	C	3.873549	2.934375	1.467792	0.000000	
25	O	2.773248	1.796900	1.451028	1.449394	0.000000
26	H	4.043903	3.223769	1.087760	2.209195	2.147633
27	H	4.718899	3.783673	1.086649	2.215998	2.133115
28	H	4.585415	3.655640	2.191475	1.089028	2.108620
29	C	4.039532	3.291701	2.600732	1.503470	2.522401
30	H	3.872684	3.271925	3.427645	2.150785	2.908430
31	H	5.132037	4.377144	3.165574	2.135125	3.427785
32	H	3.774788	3.144909	2.715055	2.151901	2.746743

		26	27	28	29	30
26	H	0.000000				
27	H	1.852516	0.000000			
28	H	3.121346	2.502756	0.000000		
29	C	2.812075	3.539520	2.208564	0.000000	
30	H	3.740163	4.339220	2.587163	1.094162	0.000000
31	H	3.336902	3.956512	2.530498	1.094449	1.769998
32	H	2.502841	3.769760	3.100143	1.091864	1.785828

		31	32
31	H	0.000000	
32	H	1.767410	0.000000

Stoichiometry C10H17BrN2O2
Framework group C1[X(C10H17BrN2O2)]
Deg. of freedom 90
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.703542	2.139706	-0.405564
2	6	0	-3.770095	1.370909	-0.068109
3	7	0	-3.298381	0.068482	0.063529
4	6	0	-1.974493	0.060883	-0.186956
5	7	0	-1.598051	1.305659	-0.477376
6	6	0	-0.201594	1.703914	-0.749544
7	6	0	0.493537	2.253411	0.507746
8	1	0	-2.637512	3.195579	-0.604425
9	1	0	-4.801351	1.634998	0.079058
10	1	0	0.318629	0.812760	-1.104169

11	1	0	-0.212924	2.460570	-1.535261
12	1	0	-0.093161	3.082635	0.923218
13	1	0	0.541091	1.459920	1.262464
14	35	0	0.497339	-2.084352	-0.215874
15	1	0	-1.277606	-0.806719	-0.162657
16	6	0	-4.017837	-1.111096	0.399790
17	6	0	-5.320511	-1.157091	0.646314
18	1	0	-3.375604	-1.982414	0.434435
19	1	0	-5.776416	-2.105127	0.895725
20	1	0	-5.967516	-0.289731	0.612664
21	8	0	1.766340	2.732302	0.159404
22	1	0	2.439047	2.063181	0.396394
23	6	0	3.724300	-0.527364	1.265962
24	6	0	4.523279	0.011334	0.158781
25	8	0	3.681124	0.887804	0.948285
26	1	0	2.811817	-1.073963	1.038308
27	1	0	4.203128	-0.745900	2.216631
28	1	0	5.579919	0.193307	0.349515
29	6	0	4.142172	-0.200466	-1.280080
30	1	0	4.355656	0.693235	-1.874146
31	1	0	4.725303	-1.028447	-1.695081
32	1	0	3.084650	-0.456235	-1.371710

Rotational constants (GHZ): 0.5908450 0.2231960 0.1733828

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.

475 basis functions, 751 primitive gaussians, 492 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1307.6484237588 Hartrees.

NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 475 RedAO= T EigKep= 3.76D-06 NBF= 475

NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999998 0.000329 -0.000140 -0.001862 Ang= 0.22 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3225.52360173 A.U. after 11 cycles
NFock= 11 Conv=0.23D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000197950	0.000079624	-0.000290847
2	6	-0.000112994	-0.000115758	0.000413127
3	7	0.000270630	0.000037459	-0.000290767
4	6	0.000149954	-0.000260940	0.000120961
5	7	-0.000135010	0.000319083	-0.000030388
6	6	-0.000005397	0.000198491	0.000284502
7	6	-0.000745742	0.000430980	0.000049871
8	1	0.000008038	0.000025008	-0.000040682
9	1	0.000014697	-0.000007551	0.000054498
10	1	-0.000133191	-0.000178651	0.000094133
11	1	-0.000021172	0.000084483	-0.000010632
12	1	0.000177684	-0.000078612	0.000183715
13	1	0.000143797	-0.000116181	-0.000044302
14	35	0.000150501	-0.000006002	0.000076826
15	1	-0.000482099	-0.000190193	-0.000164623
16	6	-0.000022025	0.000065179	-0.000041445
17	6	0.000072786	-0.000036458	0.000005550
18	1	-0.000017281	-0.000008679	0.000012356
19	1	0.000016738	-0.000015088	0.000012197
20	1	-0.000020837	0.000019539	0.000005448
21	8	0.000717069	-0.000016793	-0.000542312
22	1	-0.000553756	-0.000280538	0.000027284

23	6	-0.000061773	0.000164277	0.000026854
24	6	0.000323989	0.000282037	-0.000777633
25	8	0.000173098	-0.000240264	0.000658463
26	1	0.000133777	-0.000050877	-0.000151726
27	1	-0.000079250	-0.000058107	0.000014963
28	1	-0.000078621	0.000034748	0.000233706
29	6	-0.000152306	-0.000030501	0.000279615
30	1	0.000035840	-0.000025656	-0.000066696
31	1	-0.000006159	-0.000016423	-0.000047363
32	1	0.000041062	-0.000007638	-0.000054653

Cartesian Forces: Max 0.000777633 RMS 0.000225092

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000479265 RMS 0.000116425
Search for a local minimum.
Step number 23 out of a maximum of 177
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 19 20 21 22 23
DE= -5.51D-05 DEPred=-3.74D-05 R= 1.47D+00
TightC=F SS= 1.41D+00 RLast= 1.18D-01 DXNew= 3.2661D+00 3.5509D-01
Trust test= 1.47D+00 RLast= 1.18D-01 DXMaxT set to 1.94D+00
ITU= 1 1 1 1 1 1 -1 1 1 1 1 1 1 1 1 1 1 1 0 1
ITU= 0 1 0

Eigenvalues ---	0.00004	0.00211	0.00229	0.00298	0.00405
Eigenvalues ---	0.00535	0.00902	0.01175	0.01285	0.01401
Eigenvalues ---	0.01610	0.01737	0.01892	0.02053	0.02157
Eigenvalues ---	0.02178	0.02315	0.02385	0.02615	0.03053
Eigenvalues ---	0.03061	0.03163	0.03433	0.03747	0.04170
Eigenvalues ---	0.04641	0.05044	0.05243	0.05424	0.05660
Eigenvalues ---	0.05942	0.06320	0.07523	0.09410	0.09534
Eigenvalues ---	0.10386	0.10969	0.11509	0.11735	0.13007
Eigenvalues ---	0.13944	0.14308	0.15240	0.15972	0.15994
Eigenvalues ---	0.16000	0.16001	0.16003	0.16014	0.16078
Eigenvalues ---	0.16458	0.17447	0.19703	0.21300	0.22044
Eigenvalues ---	0.22916	0.23435	0.23861	0.24215	0.25065
Eigenvalues ---	0.27680	0.28282	0.31195	0.32434	0.33106
Eigenvalues ---	0.33411	0.34031	0.34285	0.34498	0.34841

Eigenvalues --- 0.35159 0.35686 0.35691 0.35858 0.36358
Eigenvalues --- 0.36438 0.36676 0.37213 0.37260 0.37728
Eigenvalues --- 0.39684 0.42102 0.42803 0.43682 0.45849
Eigenvalues --- 0.49603 0.54058 0.55289 0.59164 0.60599
Eigenvalue 1 is 4.25D-05 Eigenvector:

	D54	D55	D52	D53	D47
1	0.50151	0.50150	-0.49969	0.49307	0.02655
	R18	D46	D42	D35	D41
1	-0.01999	0.01853	0.01545	-0.01395	-0.01327

En-DIIS/RFO-DIIS IScMMF= 0 using points: 23 22 21 20 19
RFO step: Lambda=-7.39746157D-06.
DidBck=F Rises=F RFO-DIIS coefs: 1.54756 -0.46779 -0.08468 -0.00156 0.00647
Iteration 1 RMS(Cart)= 0.01930091 RMS(Int)= 0.00145357
Iteration 2 RMS(Cart)= 0.00029590 RMS(Int)= 0.00010702
Iteration 3 RMS(Cart)= 0.00000333 RMS(Int)= 0.00010702
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00010702

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56506	-0.00001	-0.00014	-0.00008	-0.00021	2.56485
R2	2.62046	-0.00011	0.00026	-0.00026	-0.00001	2.62045
R3	2.03422	-0.00001	0.00007	-0.00002	0.00005	2.03427
R4	2.62948	-0.00002	-0.00020	0.00004	-0.00014	2.62934
R5	2.03081	-0.00002	0.00005	-0.00006	0.00000	2.03081
R6	2.54621	-0.00023	0.00036	-0.00025	0.00011	2.54632
R7	2.68720	0.00000	-0.00023	-0.00012	-0.00035	2.68684
R8	2.51804	-0.00044	0.00143	-0.00060	0.00090	2.51894
R9	2.10344	-0.00033	0.00177	-0.00094	0.00094	2.10438
R10	2.79192	-0.00018	0.00065	-0.00066	-0.00002	2.79190
R11	2.90670	0.00012	0.00171	0.00020	0.00189	2.90859
R12	2.06192	-0.00012	0.00040	-0.00035	0.00005	2.06198
R13	2.06145	-0.00008	0.00035	-0.00025	0.00010	2.06155
R14	2.07392	-0.00017	0.00019	-0.00034	-0.00014	2.07378
R15	2.07137	-0.00010	0.00030	-0.00029	0.00002	2.07139
R16	2.65283	0.00048	0.00019	-0.00020	-0.00001	2.65282
R17	4.13397	0.00019	0.00053	0.00212	0.00274	4.13672
R18	8.51960	0.00008	-0.01533	-0.00999	-0.02534	8.49426
R19	2.50690	-0.00007	0.00018	-0.00012	0.00006	2.50696
R20	2.04655	-0.00001	0.00003	-0.00007	-0.00003	2.04651
R21	2.04303	-0.00002	0.00004	-0.00005	-0.00002	2.04301
R22	2.04585	-0.00001	0.00007	-0.00002	0.00004	2.04589
R23	1.84809	-0.00038	0.00023	-0.00048	-0.00036	1.84773
R24	3.39565	0.00017	0.00916	0.00391	0.01297	3.40861
R25	2.77372	-0.00014	0.00032	0.00014	0.00045	2.77417

R26	2.74205	0.00009	0.00045	-0.00087	-0.00041	2.74164
R27	2.05557	-0.00020	0.00015	-0.00035	-0.00020	2.05537
R28	2.05347	-0.00007	-0.00014	0.00004	-0.00010	2.05337
R29	2.73896	-0.00003	0.00213	-0.00011	0.00202	2.74097
R30	2.05796	-0.00014	0.00043	-0.00044	-0.00001	2.05795
R31	2.84115	0.00015	0.00182	-0.00034	0.00147	2.84262
R32	2.06767	0.00003	-0.00011	0.00010	-0.00001	2.06766
R33	2.06821	-0.00004	0.00023	-0.00021	0.00002	2.06823
R34	2.06332	-0.00005	0.00021	-0.00009	0.00012	2.06345
A1	1.87405	-0.00006	0.00047	-0.00016	0.00029	1.87434
A2	2.27796	0.00003	0.00008	0.00018	0.00026	2.27822
A3	2.13116	0.00002	-0.00055	-0.00003	-0.00057	2.13058
A4	1.86220	-0.00010	-0.00009	-0.00015	-0.00022	1.86197
A5	2.27690	0.00005	0.00009	0.00009	0.00017	2.27707
A6	2.14406	0.00005	-0.00002	0.00007	0.00005	2.14411
A7	1.89735	0.00001	0.00045	0.00012	0.00057	1.89793
A8	2.24887	0.00004	-0.00057	-0.00009	-0.00065	2.24822
A9	2.13696	-0.00005	0.00012	-0.00004	0.00008	2.13704
A10	1.88897	0.00006	-0.00042	-0.00016	-0.00061	1.88836
A11	2.23381	-0.00001	0.00039	0.00053	0.00092	2.23474
A12	2.16039	-0.00005	0.00003	-0.00039	-0.00035	2.16005
A13	1.90220	0.00008	-0.00042	0.00037	-0.00003	1.90217
A14	2.21547	-0.00011	-0.00160	-0.00110	-0.00262	2.21285
A15	2.16397	0.00002	0.00183	0.00078	0.00250	2.16647
A16	1.95290	-0.00016	0.00014	-0.00123	-0.00111	1.95180
A17	1.86540	0.00003	0.00073	0.00041	0.00107	1.86648
A18	1.88582	-0.00002	-0.00024	-0.00103	-0.00119	1.88464
A19	1.91981	0.00018	-0.00119	0.00173	0.00057	1.92038
A20	1.92372	0.00004	0.00025	-0.00007	0.00016	1.92388
A21	1.91491	-0.00008	0.00034	0.00017	0.00051	1.91542
A22	1.91535	-0.00008	-0.00063	-0.00053	-0.00111	1.91423
A23	1.90054	0.00006	-0.00134	0.00047	-0.00093	1.89962
A24	1.90581	0.00024	0.00161	0.00109	0.00272	1.90854
A25	1.88546	0.00008	-0.00009	0.00095	0.00085	1.88632
A26	1.89746	-0.00020	0.00020	-0.00188	-0.00160	1.89586
A27	1.95894	-0.00011	0.00021	-0.00013	0.00000	1.95893
A28	1.75348	0.00021	0.00791	0.00720	0.01497	1.76845
A29	2.86752	-0.00022	-0.00602	-0.00597	-0.01204	2.85547
A30	2.17673	0.00001	0.00032	-0.00003	0.00029	2.17702
A31	1.95511	0.00001	0.00014	0.00019	0.00033	1.95543
A32	2.15135	-0.00001	-0.00046	-0.00016	-0.00062	2.15073
A33	2.07987	-0.00003	0.00003	-0.00015	-0.00013	2.07974
A34	2.15712	0.00005	-0.00008	0.00018	0.00010	2.15722
A35	2.04620	-0.00001	0.00005	-0.00003	0.00003	2.04622

A36	1.90724	0.00006	0.00060	0.00009	-0.00026	1.90698
A37	3.07005	-0.00001	-0.00903	-0.00765	-0.01645	3.05361
A38	2.07508	0.00018	0.00108	0.00024	0.00146	2.07654
A39	2.08733	-0.00013	0.00088	0.00017	0.00090	2.08823
A40	2.00347	-0.00012	-0.00073	-0.00104	-0.00178	2.00170
A41	1.98317	0.00010	0.00005	0.00017	0.00022	1.98339
A42	2.03945	-0.00003	-0.00137	0.00005	-0.00132	2.03812
A43	2.04583	0.00012	0.00129	-0.00064	0.00066	2.04649
A44	2.13201	-0.00006	-0.00020	0.00056	0.00035	2.13236
A45	1.94691	0.00023	0.00003	0.00062	0.00069	1.94760
A46	2.04790	-0.00023	-0.00038	-0.00131	-0.00174	2.04616
A47	2.02317	-0.00006	-0.00054	0.00050	-0.00005	2.02312
A48	1.43414	-0.00017	-0.00450	-0.00381	-0.00865	1.42550
A49	0.96986	0.00020	0.00924	0.00836	0.01797	0.98784
A50	2.38293	0.00001	0.00311	0.00175	0.00458	2.38751
A51	2.25220	0.00028	0.00766	0.00866	0.01633	2.26853
A52	1.93380	-0.00010	-0.00207	0.00018	-0.00189	1.93191
A53	1.91177	0.00000	0.00057	-0.00043	0.00014	1.91191
A54	1.93781	-0.00003	-0.00202	0.00069	-0.00133	1.93647
A55	1.88398	0.00004	0.00100	-0.00045	0.00055	1.88453
A56	1.91213	0.00006	0.00143	-0.00011	0.00131	1.91344
A57	1.88285	0.00004	0.00128	0.00008	0.00136	1.88421
A58	3.68635	0.00011	0.00315	0.00485	0.00768	3.69403
A59	4.99531	-0.00003	0.00087	0.00539	0.00639	5.00169
D1	0.00070	0.00019	-0.00087	0.00327	0.00239	0.00309
D2	-3.13281	0.00008	0.00170	0.00125	0.00295	-3.12986
D3	3.13504	0.00006	-0.00260	0.00143	-0.00118	3.13386
D4	0.00154	-0.00006	-0.00004	-0.00059	-0.00062	0.00092
D5	-0.00416	-0.00015	-0.00064	-0.00035	-0.00098	-0.00514
D6	-3.08746	-0.00017	0.00308	-0.00133	0.00174	-3.08572
D7	-3.13925	-0.00003	0.00091	0.00130	0.00222	-3.13703
D8	0.06064	-0.00005	0.00463	0.00032	0.00494	0.06558
D9	0.00295	-0.00016	0.00207	-0.00507	-0.00299	-0.00004
D10	-3.13774	-0.00009	0.00061	-0.00207	-0.00145	-3.13918
D11	3.13722	-0.00006	-0.00025	-0.00324	-0.00350	3.13372
D12	-0.00347	0.00001	-0.00171	-0.00025	-0.00195	-0.00542
D13	-0.00557	0.00007	-0.00249	0.00490	0.00241	-0.00316
D14	3.13123	0.00004	-0.00370	0.00142	-0.00225	3.12898
D15	3.13518	0.00000	-0.00114	0.00213	0.00098	3.13617
D16	-0.01120	-0.00003	-0.00236	-0.00134	-0.00367	-0.01487
D17	0.00697	-0.00003	-0.00211	-0.00327	-0.00538	0.00159
D18	-3.13348	-0.00005	-0.00175	-0.00420	-0.00595	-3.13942
D19	-3.13361	0.00005	-0.00375	0.00010	-0.00365	-3.13726
D20	0.00913	0.00003	-0.00338	-0.00083	-0.00421	0.00492

D21	0.00602	0.00005	0.00194	-0.00284	-0.00090	0.00511
D22	3.09142	0.00007	-0.00176	-0.00197	-0.00374	3.08768
D23	-3.13103	0.00008	0.00309	0.00045	0.00350	-3.12753
D24	-0.04563	0.00009	-0.00061	0.00132	0.00066	-0.04497
D25	-3.05419	0.00007	-0.00666	-0.00733	-0.01397	-3.06816
D26	0.08193	0.00004	-0.00805	-0.01130	-0.01929	0.06264
D27	1.40692	-0.00003	0.00543	0.00845	0.01387	1.42080
D28	-2.77367	0.00012	0.00453	0.01012	0.01461	-2.75906
D29	-0.71395	0.00003	0.00520	0.01000	0.01516	-0.69878
D30	-1.66818	-0.00005	0.00976	0.00736	0.01710	-1.65108
D31	0.43440	0.00010	0.00885	0.00902	0.01784	0.45224
D32	2.49413	0.00001	0.00952	0.00891	0.01839	2.51252
D33	-0.96499	0.00001	0.00273	0.00715	0.00980	-0.95518
D34	1.09552	0.00010	0.00146	0.00826	0.00965	1.10517
D35	-3.04320	0.00015	0.00189	0.00909	0.01078	-3.03242
D36	-3.03558	-0.00005	0.00250	0.00628	0.00879	-3.02679
D37	-0.97507	0.00004	0.00123	0.00740	0.00864	-0.96644
D38	1.16939	0.00009	0.00166	0.00822	0.00977	1.17916
D39	1.13390	-0.00009	0.00269	0.00499	0.00768	1.14158
D40	-3.08878	0.00000	0.00142	0.00611	0.00753	-3.08125
D41	-0.94432	0.00005	0.00185	0.00693	0.00866	-0.93566
D42	-1.74667	0.00003	0.00555	0.00863	0.01431	-1.73236
D43	2.44722	0.00009	0.00525	0.00975	0.01501	2.46223
D44	0.36253	0.00020	0.00510	0.00989	0.01501	0.37754
D45	0.43847	0.00008	0.00747	0.00552	0.01313	0.45159
D46	-0.36318	-0.00007	0.00187	0.00884	0.01086	-0.35233
D47	2.59081	-0.00016	-0.00477	-0.00288	-0.00738	2.58344
D48	-3.13999	-0.00002	0.00018	-0.00127	-0.00109	-3.14108
D49	0.00188	-0.00001	-0.00017	-0.00067	-0.00083	0.00105
D50	0.00033	0.00000	-0.00022	-0.00024	-0.00047	-0.00014
D51	-3.14098	0.00001	-0.00057	0.00036	-0.00021	-3.14119
D52	-1.54236	-0.00022	-0.03440	-0.03296	-0.06739	-1.60975
D53	2.14725	-0.00003	0.02430	0.01733	0.04176	2.18900
D54	1.92174	-0.00018	0.01419	0.00144	0.01539	1.93713
D55	-2.84806	0.00000	0.02342	0.01194	0.03537	-2.81269
D56	-2.72996	0.00002	-0.00184	-0.00043	-0.00230	-2.73226
D57	-0.03036	0.00000	-0.00056	0.00073	0.00015	-0.03021
D58	-0.02362	0.00007	-0.00071	0.00075	0.00002	-0.02361
D59	2.67597	0.00004	0.00058	0.00191	0.00246	2.67844
D60	-0.14778	-0.00005	-0.00181	-0.00565	-0.00736	-0.15514
D61	0.12412	0.00008	0.00862	0.01192	0.02059	0.14471
D62	-2.55926	0.00001	0.00121	-0.00472	-0.00342	-2.56268
D63	-2.28736	0.00015	0.01164	0.01285	0.02453	-2.26282
D64	2.13092	0.00001	-0.00453	-0.00064	-0.00515	2.12577

D65	-0.26286	0.00010	-0.00327	-0.00067	-0.00391	-0.26676
D66	2.48431	-0.00002	0.00164	0.00254	0.00418	2.48849
D67	-1.72231	-0.00003	0.00196	0.00183	0.00378	-1.71852
D68	0.35533	0.00000	0.00266	0.00208	0.00473	0.36006
D69	1.26770	0.00002	0.00227	0.00345	0.00573	1.27343
D70	-2.93892	0.00001	0.00259	0.00274	0.00534	-2.93358
D71	-0.86128	0.00004	0.00329	0.00299	0.00629	-0.85500
D72	-1.09395	0.00000	0.00335	0.00342	0.00676	-1.08719
D73	0.98262	-0.00001	0.00366	0.00270	0.00637	0.98898
D74	3.06025	0.00002	0.00436	0.00296	0.00731	3.06756

Item	Value	Threshold	Converged?
Maximum Force	0.000479	0.000450	NO
RMS Force	0.000116	0.000300	YES
Maximum Displacement	0.076090	0.001800	NO
RMS Displacement	0.019305	0.001200	NO

Predicted change in Energy=-2.509019D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.387175	-1.917208	-0.256743
2	6	0	-2.510572	-1.161169	-0.164331
3	7	0	-2.104462	0.112001	0.223057
4	6	0	-0.763930	0.116088	0.359426
5	7	0	-0.313057	-1.106001	0.076574
6	6	0	1.116800	-1.477057	0.052598
7	6	0	1.708461	-1.384319	-1.365271
8	1	0	-1.260986	-2.953505	-0.519405
9	1	0	-3.540445	-1.418990	-0.330995
10	1	0	1.635586	-0.787007	0.719907
11	1	0	1.206872	-2.495508	0.433079
12	1	0	1.109145	-1.990764	-2.056159
13	1	0	1.662649	-0.341693	-1.700444
14	35	0	1.632880	2.218317	1.097807
15	1	0	-0.105909	0.967548	0.645975
16	6	0	-2.898788	1.267183	0.460048
17	6	0	-4.219558	1.313074	0.344320
18	1	0	-2.298454	2.120690	0.749781
19	1	0	-4.734107	2.242147	0.546488
20	1	0	-4.825539	0.463664	0.055530
21	8	0	3.021090	-1.881909	-1.355029

22	1	0	3.649284	-1.133861	-1.312060
23	6	0	4.786171	1.666258	-1.111626
24	6	0	5.691761	0.779630	-0.370741
25	8	0	4.811945	0.242904	-1.391372
26	1	0	3.878517	2.017442	-0.626009
27	1	0	5.175413	2.276677	-1.921917
28	1	0	6.733762	0.754481	-0.686287
29	6	0	5.425662	0.370533	1.052144
30	1	0	5.721271	-0.669964	1.216966
31	1	0	6.011558	0.999492	1.729627
32	1	0	4.370619	0.496440	1.303820

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357261	0.000000			
3	N	2.205085	1.391387	0.000000		
4	C	2.214135	2.226312	1.347456	0.000000	
5	N	1.386682	2.211369	2.171202	1.332965	0.000000
6	C	2.561116	3.647557	3.595927	2.483828	1.477412
7	C	3.331031	4.392300	4.393193	3.367272	2.498582
8	H	1.076488	2.213597	3.264970	3.231379	2.160331
9	H	2.211404	1.074656	2.170934	3.246872	3.268043
10	H	3.371689	4.255878	3.878535	2.589055	2.076738
11	H	2.745790	3.994590	4.219969	3.272601	2.089978
12	H	3.078136	4.167685	4.465839	3.712451	2.711828
13	H	3.723969	4.521831	4.254036	3.215729	2.765026
14	Br	5.296991	5.493825	4.378297	3.272503	3.985057
15	H	3.283041	3.312165	2.214731	1.113592	2.160263
16	C	3.597097	2.537213	1.421817	2.427501	3.530589
17	C	4.338017	3.049793	2.435346	3.657098	4.602648
18	H	4.260063	3.413384	2.085642	2.554519	3.847927
19	H	5.398830	4.126976	3.399583	4.507485	5.565663
20	H	4.193854	2.836810	2.748817	4.087766	4.777739
21	O	4.543157	5.704078	5.721653	4.610610	3.710532
22	H	5.205118	6.265929	6.083942	4.881875	4.198717
23	C	7.189037	7.882523	7.188735	5.947322	5.924471
24	C	7.576098	8.431344	7.847255	6.530649	6.309796
25	O	6.662023	7.556210	7.103534	5.845662	5.499096
26	H	6.583718	7.151026	6.336218	5.112587	5.274354
27	H	7.964235	8.601294	7.891978	6.719261	6.749798
28	H	8.559910	9.455151	8.908080	7.597135	7.328097
29	C	7.304909	8.173722	7.580039	6.233431	6.005396
30	H	7.365965	8.361370	7.927258	6.588710	6.156601

31	H	8.197198	8.993455	8.302239	6.968866	6.867783
32	H	6.435313	7.228688	6.575904	5.234515	5.100076

		6	7	8	9	10
6	C	0.000000				
7	C	1.539161	0.000000			
8	H	2.856737	3.463445	0.000000		
9	H	4.673376	5.349948	2.754300	0.000000	
10	H	1.091151	2.170268	3.823576	5.319313	0.000000
11	H	1.090926	2.172648	2.684643	4.927445	1.784668
12	H	2.170440	1.097397	2.984293	4.992175	3.071273
13	H	2.158740	1.096133	4.094393	5.487089	2.461125
14	Br	3.874867	4.364797	6.143092	6.483423	3.028992
15	H	2.797000	3.587246	4.250526	4.294889	2.473203
16	C	4.880759	5.620409	4.632055	2.872803	4.984753
17	C	6.028818	6.733502	5.263351	2.895067	6.231702
18	H	5.009372	5.728342	5.332413	3.903838	4.892061
19	H	6.950505	7.636280	6.339834	3.949522	7.055412
20	H	6.251224	6.937354	4.971281	2.311980	6.614508
21	O	2.402424	1.403814	4.492522	6.657077	2.724664
22	H	2.897163	1.957640	5.296240	7.261955	2.881698
23	C	4.969923	4.340812	7.632891	8.914071	4.393087
24	C	5.118801	4.640952	7.892977	9.490476	4.482903
25	O	4.324051	3.504304	6.917937	8.581883	3.950630
26	H	4.505454	4.102150	7.150956	8.181509	3.834993
27	H	5.870398	5.072722	8.411247	9.599748	5.375479
28	H	6.089005	5.503557	8.814364	10.507594	5.508627
29	C	4.793640	4.768751	7.630875	9.246975	3.976803
30	H	4.817501	4.825028	7.548606	9.420011	4.117474
31	H	5.736234	5.811849	8.577542	10.066577	4.833244
32	H	4.005945	4.212883	6.851368	8.302194	3.077109

		11	12	13	14	15
11	H	0.000000				
12	H	2.541776	0.000000			
13	H	3.065709	1.775481	0.000000		
14	Br	4.779487	5.285657	3.792723	0.000000	
15	H	3.709646	4.186824	3.216767	2.189055	0.000000
16	C	5.569112	5.745350	5.297444	4.674121	2.815053
17	C	6.630182	6.713622	6.443576	5.969777	4.139141
18	H	5.804902	6.032336	5.268517	3.947916	2.479469
19	H	7.599570	7.670392	7.255579	6.390857	4.801533
20	H	6.729727	6.760468	6.769685	6.773207	4.783036
21	O	2.620157	2.039354	2.082531	4.975479	4.679909
22	H	3.296206	2.782134	2.173727	4.594611	4.727716
23	C	5.702437	5.271287	3.759649	3.889680	5.244979

24	C	5.611318	5.613919	4.388532	4.549831	5.889142
25	O	4.880991	4.375151	3.217972	4.494966	5.372260
26	H	5.350334	5.077447	3.410279	2.838094	4.312293
27	H	6.638455	5.896067	4.386847	4.655285	6.016665
28	H	6.508604	6.406968	5.286426	5.598643	6.971472
29	C	5.137667	5.819758	4.716383	4.219193	5.578502
30	H	4.932230	5.807716	5.009137	5.007126	6.079762
31	H	6.081206	6.878042	5.698875	4.588851	6.212787
32	H	4.440635	5.302156	4.130517	3.240759	4.549067

		16	17	18	19	20
16	C	0.000000				
17	C	1.326625	0.000000			
18	H	1.082968	2.123037	0.000000		
19	H	2.080006	1.081115	2.447139	0.000000	
20	H	2.126417	1.082641	3.100626	1.847269	0.000000
21	O	6.946671	8.094608	6.982017	8.987029	8.310293
22	H	7.196015	8.405342	7.086528	9.226749	8.731840
23	C	7.854171	9.129494	7.339159	9.680738	9.756713
24	C	8.644388	9.951387	8.179091	10.567828	10.530676
25	O	7.995768	9.258830	7.659529	9.943812	9.747993
26	H	6.904656	8.186360	6.329173	8.694973	8.867882
27	H	8.478535	9.712355	7.938576	10.212385	10.354534
28	H	9.714060	11.015870	9.247148	11.629485	11.586730
29	C	8.393511	9.716979	7.925683	10.343092	10.299954
30	H	8.867406	10.174185	8.504234	10.874046	10.670954
31	H	9.004319	10.329237	8.442362	10.881789	10.978724
32	H	7.358687	8.682090	6.886340	9.301457	9.280552

		21	22	23	24	25
21	O	0.000000				
22	H	0.977778	0.000000			
23	C	3.970421	3.028754	0.000000		
24	C	3.896806	2.952836	1.468030	0.000000	
25	O	2.779085	1.803761	1.450812	1.450461	0.000000
26	H	4.058521	3.233253	1.087653	2.210247	2.146171
27	H	4.717660	3.785864	1.086597	2.216734	2.133031
28	H	4.602359	3.670345	2.192114	1.089022	2.110032
29	C	4.080434	3.317858	2.601875	1.504251	2.522638
30	H	3.921091	3.302167	3.428511	2.150118	2.909232
31	H	5.173053	4.402658	3.165260	2.135920	3.428138
32	H	3.814086	3.165602	2.715794	2.151689	2.742828

		26	27	28	29	30
26	H	0.000000				
27	H	1.851626	0.000000			
28	H	3.122679	2.504459	0.000000		

29	C	2.814634	3.541334	2.209227	0.000000	
30	H	3.743588	4.339729	2.583903	1.094159	0.000000
31	H	3.336931	3.957792	2.533427	1.094462	1.770359
32	H	2.505963	3.771248	3.100251	1.091929	1.786702

		31	32
31	H	0.000000	
32	H	1.768347	0.000000

Stoichiometry C10H17BrN2O2

Framework group C1[X(C10H17BrN2O2)]

Deg. of freedom 90

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.715932	2.129086	-0.414760
2	6	0	-3.782477	1.359506	-0.079523
3	7	0	-3.308441	0.058808	0.059876
4	6	0	-1.983904	0.051858	-0.187495
5	7	0	-1.608694	1.296878	-0.480642
6	6	0	-0.212783	1.700990	-0.746861
7	6	0	0.479635	2.235831	0.519441
8	1	0	-2.651009	3.184086	-0.618687
9	1	0	-4.815137	1.621760	0.060909
10	1	0	0.310033	0.816094	-1.113239
11	1	0	-0.226350	2.468416	-1.522100
12	1	0	-0.115344	3.051570	0.949384
13	1	0	0.535969	1.429251	1.259550
14	35	0	0.509316	-2.067738	-0.208479
15	1	0	-1.284348	-0.813980	-0.155354
16	6	0	-4.027252	-1.120128	0.398970
17	6	0	-5.329752	-1.166363	0.646538
18	1	0	-3.385144	-1.991481	0.434486
19	1	0	-5.785005	-2.114388	0.897142
20	1	0	-5.977231	-0.299347	0.612397
21	8	0	1.747002	2.735596	0.180756
22	1	0	2.425682	2.064562	0.393260
23	6	0	3.755176	-0.512814	1.266719
24	6	0	4.538255	0.016658	0.143527
25	8	0	3.692039	0.896280	0.927123
26	1	0	2.845717	-1.071633	1.057928

```
      27        1        0        4.243980     -0.710549      2.216806
      28        1        0        5.594460      0.213870      0.321030
      29        6        0        4.145383     -0.220313     -1.289046
      30        1        0        4.349335      0.665897     -1.897504
      31        1        0        4.729633     -1.051382     -1.696261
      32        1        0        3.088202     -0.482607     -1.365726
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.5958532           0.2219560           0.1730421
 Standard basis: 6-311++G(d,p) (5D, 7F)
 There are     492 symmetry adapted cartesian basis functions of A      symmetry.
 There are     475 symmetry adapted basis functions of A      symmetry.
   475 basis functions,      751 primitive gaussians,      492 cartesian basis functions
    71 alpha electrons              71 beta electrons
         nuclear repulsion energy           1307.4324432254 Hartrees.
 NAtoms=       32 NActive=       32 NUniq=       32 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      475 RedAO= T EigKep=    3.77D-06    NBF=      475
 NBsUse=      475 1.00D-06 EigRej= -1.00D+00 NBFU=      475
 Initial guess from the checkpoint file:    "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"
 B after Tr=          0.000000        0.000000        0.000000
             Rot=        0.999999        0.000681     -0.000267     -0.001326 Ang=      0.17 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn=                5 AccDes=
0.00D+00
 Harris functional with IExCor=    402 and IRadAn=             5 diagonalized for initial guess.
 HarFok:    IExCor=    402 AccDes= 0.00D+00 IRadAn=                5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=    3500011 ScaDFX=    1.000000    1.000000    1.000000    1.000000
 FoFCou: FMM=F IPFlag=                  0 FMFlag=           100000 FMFlg1=                  0
             NFxFlg=                    0 DoJE=T BraDBF=F KetDBF=T FulRan=T
             wScrn=      0.000000  ICntrl=             500  IOpCl=      0  I1Cent=        200000004  NGrid=
0
             NMat0=         1 NMatS0=             1 NMatT0=         0 NMatD0=         1 NMtDS0=         0
NMtDT0=         0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                       energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3225.52363408          A.U. after      11 cycles
                   NFock= 11    Conv=0.33D-08         -V/T= 2.0018
 Calling FoFJK, ICntrl=             2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
```

NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000243773	0.000040504	-0.000019957
2	6	-0.000084629	-0.000049290	0.000208291
3	7	0.000171420	0.000065550	0.000032024
4	6	0.000501785	-0.000318859	-0.000318197
5	7	-0.000268267	0.000482804	-0.000048866
6	6	0.000220623	0.000226185	0.000133573
7	6	-0.000945822	0.000407928	0.000206810
8	1	-0.000002374	0.000048689	-0.000077393
9	1	0.000024719	0.000012815	0.000001467
10	1	-0.000155863	-0.000157895	0.000038274
11	1	0.000014825	0.000120542	-0.000068917
12	1	0.000164563	-0.000068058	0.000186899
13	1	0.000115619	-0.000167028	-0.000046401
14	35	0.000192537	0.000052574	0.000021603
15	1	-0.000597104	-0.000571933	-0.000129835
16	6	-0.000092691	0.000136456	0.000060924
17	6	0.000082329	-0.000060822	0.000015302
18	1	-0.000001206	-0.000019381	-0.000015535
19	1	0.000007900	-0.000007189	-0.000015746
20	1	-0.000008348	0.000036000	0.000009141
21	8	0.000721672	0.000216498	-0.000155986
22	1	-0.000446886	-0.000309606	-0.000224685
23	6	-0.000266469	-0.000094452	-0.000060311
24	6	-0.000350587	-0.000062628	-0.000670999
25	8	0.000649532	-0.000047418	0.000948904
26	1	0.000186516	-0.000036029	0.000076813
27	1	0.000065107	-0.000029997	0.000002111
28	1	-0.000121888	0.000086430	0.000134968
29	6	-0.000075074	0.000179088	-0.000324452
30	1	-0.000022467	-0.000021848	0.000053851
31	1	-0.000036816	-0.000050127	-0.000011103
32	1	0.000113572	-0.000039501	0.000057427

Cartesian Forces: Max 0.000948904 RMS 0.000255900

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000729037 RMS 0.000137697
Search for a local minimum.
Step number 24 out of a maximum of 177
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 19 20 21 22 23
24
DE= -3.24D-05 DEPred=-2.51D-05 R= 1.29D+00
TightC=F SS= 1.41D+00 RLast= 1.25D-01 DXNew= 3.2661D+00 3.7524D-01
Trust test= 1.29D+00 RLast= 1.25D-01 DXMaxT set to 1.94D+00
ITU= 1 1 1 1 1 1 1 -1 1 1 1 1 1 1 1 1 1 1 1 0
ITU= 1 0 1 0
Eigenvalues --- 0.00006 0.00172 0.00232 0.00283 0.00364
Eigenvalues --- 0.00543 0.00884 0.01223 0.01246 0.01404
Eigenvalues --- 0.01533 0.01779 0.01909 0.02070 0.02160
Eigenvalues --- 0.02181 0.02315 0.02385 0.02717 0.03058
Eigenvalues --- 0.03062 0.03134 0.03373 0.03923 0.04190
Eigenvalues --- 0.04657 0.04962 0.05194 0.05432 0.05662
Eigenvalues --- 0.05936 0.06129 0.07293 0.09293 0.09561
Eigenvalues --- 0.10407 0.11006 0.11546 0.11686 0.13039
Eigenvalues --- 0.13948 0.14168 0.15395 0.15978 0.15993
Eigenvalues --- 0.16000 0.16002 0.16004 0.16009 0.16077
Eigenvalues --- 0.16499 0.17404 0.19707 0.21528 0.22049
Eigenvalues --- 0.22927 0.23553 0.23981 0.24246 0.25046
Eigenvalues --- 0.27644 0.28355 0.31374 0.32579 0.33106
Eigenvalues --- 0.33473 0.34047 0.34288 0.34483 0.34849
Eigenvalues --- 0.35169 0.35684 0.35689 0.35857 0.36169
Eigenvalues --- 0.36439 0.36670 0.37224 0.37261 0.37765
Eigenvalues --- 0.41123 0.42119 0.43286 0.44034 0.45861
Eigenvalues --- 0.49721 0.54196 0.55230 0.59977 0.61246
Eigenvalue 1 is 5.84D-05 Eigenvector:
D55 D52 D54 D53 D47
1 -0.50157 0.50060 -0.49996 -0.49152 -0.03191
R18 D46 D42 D35 D41
1 0.02504 -0.02349 -0.01891 0.01659 0.01604
En-DIIS/RFO-DIIS IScMMF= 0 using points: 24 23 22 21 20
RFO step: Lambda=-6.14485838D-06.
DidBck=F Rises=F RFO-DIIS coefs: 1.41040 -0.21095 -0.36527 0.06787
0.09795
Iteration 1 RMS(Cart)= 0.01989238 RMS(Int)= 0.00080676
Iteration 2 RMS(Cart)= 0.00024814 RMS(Int)= 0.00007069

Iteration 3 RMS(Cart)= 0.00000114 RMS(Int)= 0.00007069

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00007069

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56485	0.00005	0.00003	0.00007	0.00010	2.56496
R2	2.62045	-0.00016	-0.00011	-0.00016	-0.00028	2.62017
R3	2.03427	-0.00003	0.00004	-0.00008	-0.00004	2.03423
R4	2.62934	-0.00003	-0.00010	0.00001	-0.00008	2.62926
R5	2.03081	-0.00003	0.00000	-0.00004	-0.00004	2.03077
R6	2.54632	-0.00019	-0.00013	0.00000	-0.00014	2.54619
R7	2.68684	0.00008	0.00002	-0.00007	-0.00006	2.68679
R8	2.51894	-0.00073	0.00038	-0.00081	-0.00038	2.51855
R9	2.10438	-0.00064	-0.00048	-0.00076	-0.00117	2.10321
R10	2.79190	-0.00017	0.00010	-0.00004	0.00007	2.79198
R11	2.90859	-0.00025	0.00074	-0.00065	0.00009	2.90868
R12	2.06198	-0.00015	-0.00003	-0.00019	-0.00022	2.06176
R13	2.06155	-0.00014	0.00011	-0.00033	-0.00022	2.06133
R14	2.07378	-0.00017	-0.00026	-0.00019	-0.00044	2.07334
R15	2.07139	-0.00015	-0.00019	-0.00016	-0.00035	2.07104
R16	2.65282	0.00050	0.00143	0.00008	0.00153	2.65435
R17	4.13672	0.00019	0.00563	0.00458	0.01026	4.14698
R18	8.49426	-0.00005	-0.00698	-0.01193	-0.01894	8.47532
R19	2.50696	-0.00008	0.00003	-0.00009	-0.00006	2.50690
R20	2.04651	-0.00002	0.00001	-0.00007	-0.00006	2.04645
R21	2.04301	-0.00001	0.00002	-0.00005	-0.00002	2.04299
R22	2.04589	-0.00002	0.00004	-0.00006	-0.00002	2.04587
R23	1.84773	-0.00054	-0.00075	-0.00011	-0.00092	1.84682
R24	3.40861	-0.00002	0.00806	-0.00336	0.00464	3.41325
R25	2.77417	-0.00030	0.00059	-0.00082	-0.00016	2.77401
R26	2.74164	-0.00007	0.00042	-0.00050	-0.00011	2.74153
R27	2.05537	-0.00013	0.00003	-0.00055	-0.00052	2.05485
R28	2.05337	0.00000	0.00003	-0.00024	-0.00021	2.05316
R29	2.74097	-0.00057	0.00039	-0.00086	-0.00052	2.74045
R30	2.05795	-0.00016	0.00014	-0.00037	-0.00023	2.05773
R31	2.84262	-0.00022	0.00102	-0.00032	0.00071	2.84333
R32	2.06766	0.00002	0.00017	-0.00015	0.00002	2.06768
R33	2.06823	-0.00006	0.00014	-0.00024	-0.00010	2.06813
R34	2.06345	-0.00010	0.00015	-0.00033	-0.00017	2.06328
A1	1.87434	-0.00006	0.00022	-0.00004	0.00017	1.87451
A2	2.27822	0.00002	0.00004	0.00010	0.00014	2.27836
A3	2.13058	0.00004	-0.00027	-0.00006	-0.00033	2.13025
A4	1.86197	-0.00012	-0.00014	-0.00012	-0.00024	1.86173
A5	2.27707	0.00006	0.00011	0.00010	0.00020	2.27728
A6	2.14411	0.00005	0.00003	0.00000	0.00003	2.14413

A7	1.89793	-0.00010	0.00014	-0.00015	-0.00001	1.89792
A8	2.24822	0.00010	-0.00010	-0.00003	-0.00014	2.24808
A9	2.13704	0.00000	-0.00004	0.00018	0.00014	2.13718
A10	1.88836	0.00020	-0.00001	0.00019	0.00017	1.88853
A11	2.23474	-0.00015	0.00009	0.00010	0.00021	2.23495
A12	2.16005	-0.00004	-0.00011	-0.00026	-0.00036	2.15969
A13	1.90217	0.00008	-0.00023	0.00011	-0.00011	1.90206
A14	2.21285	0.00002	-0.00101	0.00006	-0.00091	2.21194
A15	2.16647	-0.00010	0.00120	-0.00009	0.00106	2.16753
A16	1.95180	-0.00017	-0.00148	0.00078	-0.00072	1.95108
A17	1.86648	0.00000	0.00087	-0.00034	0.00048	1.86696
A18	1.88464	0.00005	-0.00064	0.00000	-0.00058	1.88406
A19	1.92038	0.00022	0.00104	0.00024	0.00131	1.92169
A20	1.92388	-0.00005	0.00020	-0.00085	-0.00067	1.92321
A21	1.91542	-0.00006	0.00001	0.00018	0.00019	1.91561
A22	1.91423	-0.00007	-0.00101	0.00003	-0.00097	1.91327
A23	1.89962	0.00014	0.00005	0.00005	0.00008	1.89969
A24	1.90854	0.00006	0.00164	0.00000	0.00168	1.91022
A25	1.88632	0.00005	0.00101	0.00039	0.00140	1.88772
A26	1.89586	-0.00012	-0.00134	-0.00034	-0.00164	1.89421
A27	1.95893	-0.00005	-0.00041	-0.00012	-0.00059	1.95834
A28	1.76845	0.00006	0.00542	0.00490	0.01014	1.77860
A29	2.85547	-0.00001	-0.00464	-0.00376	-0.00848	2.84699
A30	2.17702	-0.00001	0.00024	-0.00014	0.00010	2.17712
A31	1.95543	-0.00001	0.00010	0.00005	0.00015	1.95559
A32	2.15073	0.00002	-0.00035	0.00009	-0.00026	2.15048
A33	2.07974	-0.00002	-0.00015	0.00000	-0.00015	2.07959
A34	2.15722	0.00004	0.00021	0.00002	0.00024	2.15745
A35	2.04622	-0.00002	-0.00006	-0.00002	-0.00009	2.04614
A36	1.90698	0.00016	-0.00079	0.00141	0.00006	1.90703
A37	3.05361	0.00020	-0.00662	-0.00448	-0.01099	3.04262
A38	2.07654	0.00007	0.00067	-0.00061	0.00017	2.07671
A39	2.08823	-0.00010	0.00008	0.00025	0.00023	2.08847
A40	2.00170	0.00004	0.00020	-0.00065	-0.00043	2.00127
A41	1.98339	0.00005	-0.00011	0.00005	-0.00005	1.98334
A42	2.03812	0.00004	-0.00060	0.00056	-0.00004	2.03809
A43	2.04649	0.00010	0.00098	-0.00025	0.00075	2.04724
A44	2.13236	-0.00015	-0.00024	0.00005	-0.00020	2.13217
A45	1.94760	0.00007	0.00101	0.00030	0.00134	1.94894
A46	2.04616	-0.00013	-0.00069	-0.00019	-0.00090	2.04525
A47	2.02312	0.00002	-0.00067	0.00006	-0.00062	2.02250
A48	1.42550	-0.00014	-0.00339	-0.00156	-0.00511	1.42039
A49	0.98784	0.00005	0.00730	0.00410	0.01175	0.99959
A50	2.38751	-0.00013	0.00164	-0.00061	0.00083	2.38834

A51	2.26853	0.00016	0.00657	0.00768	0.01429	2.28283
A52	1.93191	0.00005	-0.00142	0.00006	-0.00137	1.93055
A53	1.91191	0.00002	0.00055	-0.00024	0.00030	1.91222
A54	1.93647	0.00011	-0.00078	0.00022	-0.00056	1.93591
A55	1.88453	-0.00004	0.00042	-0.00015	0.00027	1.88480
A56	1.91344	-0.00008	0.00053	0.00034	0.00086	1.91430
A57	1.88421	-0.00006	0.00080	-0.00024	0.00056	1.88477
A58	3.69403	0.00002	0.00318	0.00612	0.00919	3.70322
A59	5.00169	0.00007	0.00406	0.00828	0.01249	5.01418
D1	0.00309	0.00008	0.00214	-0.00169	0.00044	0.00352
D2	-3.12986	0.00004	0.00156	0.00022	0.00179	-3.12807
D3	3.13386	0.00003	0.00003	-0.00128	-0.00124	3.13262
D4	0.00092	-0.00001	-0.00054	0.00064	0.00010	0.00102
D5	-0.00514	-0.00010	-0.00195	-0.00013	-0.00207	-0.00721
D6	-3.08572	-0.00013	-0.00144	-0.00150	-0.00293	-3.08864
D7	-3.13703	-0.00006	-0.00006	-0.00050	-0.00057	-3.13759
D8	0.06558	-0.00009	0.00045	-0.00188	-0.00142	0.06416
D9	-0.00004	-0.00003	-0.00161	0.00293	0.00132	0.00128
D10	-3.13918	0.00000	-0.00080	0.00234	0.00155	-3.13763
D11	3.13372	0.00001	-0.00109	0.00119	0.00010	3.13382
D12	-0.00542	0.00003	-0.00028	0.00060	0.00033	-0.00509
D13	-0.00316	-0.00003	0.00041	-0.00304	-0.00263	-0.00579
D14	3.12898	0.00007	-0.00052	0.00038	-0.00010	3.12888
D15	3.13617	-0.00006	-0.00034	-0.00249	-0.00283	3.13333
D16	-0.01487	0.00004	-0.00127	0.00093	-0.00031	-0.01518
D17	0.00159	-0.00001	-0.00209	-0.00144	-0.00353	-0.00194
D18	-3.13942	0.00000	-0.00229	-0.00114	-0.00344	3.14033
D19	-3.13726	0.00002	-0.00117	-0.00210	-0.00327	-3.14053
D20	0.00492	0.00002	-0.00138	-0.00181	-0.00318	0.00174
D21	0.00511	0.00009	0.00094	0.00197	0.00290	0.00802
D22	3.08768	0.00012	0.00034	0.00331	0.00365	3.09133
D23	-3.12753	-0.00001	0.00181	-0.00127	0.00051	-3.12702
D24	-0.04497	0.00002	0.00121	0.00006	0.00125	-0.04371
D25	-3.06816	-0.00006	-0.00915	-0.00988	-0.01904	-3.08720
D26	0.06264	0.00005	-0.01022	-0.00597	-0.01615	0.04649
D27	1.42080	-0.00010	0.00675	0.00587	0.01259	1.43339
D28	-2.75906	0.00007	0.00771	0.00641	0.01409	-2.74498
D29	-0.69878	0.00003	0.00785	0.00644	0.01427	-0.68452
D30	-1.65108	-0.00014	0.00740	0.00429	0.01166	-1.63942
D31	0.45224	0.00003	0.00836	0.00483	0.01316	0.46540
D32	2.51252	-0.00001	0.00851	0.00486	0.01334	2.52586
D33	-0.95518	-0.00002	0.00413	0.00486	0.00895	-0.94623
D34	1.10517	0.00008	0.00481	0.00537	0.01013	1.11530
D35	-3.03242	0.00014	0.00537	0.00526	0.01052	-3.02191

D36	-3.02679	-0.00006	0.00331	0.00463	0.00794	-3.01885
D37	-0.96644	0.00003	0.00398	0.00514	0.00912	-0.95731
D38	1.17916	0.00009	0.00455	0.00503	0.00951	1.18867
D39	1.14158	-0.00010	0.00249	0.00480	0.00729	1.14887
D40	-3.08125	0.00000	0.00316	0.00531	0.00847	-3.07278
D41	-0.93566	0.00005	0.00373	0.00520	0.00886	-0.92680
D42	-1.73236	-0.00004	0.00605	0.00863	0.01472	-1.71763
D43	2.46223	0.00009	0.00710	0.00880	0.01589	2.47812
D44	0.37754	0.00014	0.00698	0.00861	0.01559	0.39313
D45	0.45159	0.00000	0.00725	-0.00039	0.00694	0.45853
D46	-0.35233	0.00008	0.00534	0.00959	0.01503	-0.33729
D47	2.58344	-0.00006	-0.00334	-0.00267	-0.00580	2.57763
D48	-3.14108	0.00001	-0.00034	0.00033	-0.00001	-3.14110
D49	0.00105	0.00000	-0.00042	-0.00002	-0.00043	0.00062
D50	-0.00014	0.00001	-0.00011	0.00000	-0.00011	-0.00025
D51	-3.14119	0.00000	-0.00019	-0.00035	-0.00053	3.14146
D52	-1.60975	-0.00012	-0.03205	-0.02660	-0.05866	-1.66841
D53	2.18900	0.00003	0.01983	0.01547	0.03540	2.22441
D54	1.93713	-0.00011	0.00754	-0.00016	0.00725	1.94437
D55	-2.81269	-0.00004	0.01576	0.00720	0.02291	-2.78978
D56	-2.73226	0.00005	0.00066	0.00000	0.00063	-2.73163
D57	-0.03021	-0.00002	0.00070	-0.00036	0.00033	-0.02989
D58	-0.02361	0.00006	0.00093	0.00065	0.00156	-0.02205
D59	2.67844	-0.00002	0.00097	0.00029	0.00125	2.67969
D60	-0.15514	0.00008	-0.00431	-0.00622	-0.01041	-0.16556
D61	0.14471	0.00023	0.00891	0.01166	0.02057	0.16528
D62	-2.56268	-0.00009	-0.00349	-0.00642	-0.00980	-2.57248
D63	-2.26282	0.00006	0.00973	0.01146	0.02118	-2.24164
D64	2.12577	0.00006	-0.00249	0.00161	-0.00084	2.12494
D65	-0.26676	0.00009	-0.00183	0.00140	-0.00040	-0.26717
D66	2.48849	0.00004	0.00072	-0.00058	0.00013	2.48862
D67	-1.71852	0.00003	0.00071	-0.00088	-0.00019	-1.71871
D68	0.36006	0.00004	0.00157	-0.00120	0.00035	0.36041
D69	1.27343	-0.00003	0.00117	-0.00068	0.00051	1.27394
D70	-2.93358	-0.00004	0.00116	-0.00098	0.00019	-2.93339
D71	-0.85500	-0.00004	0.00202	-0.00130	0.00073	-0.85427
D72	-1.08719	-0.00001	0.00115	-0.00100	0.00015	-1.08704
D73	0.98898	-0.00002	0.00114	-0.00130	-0.00017	0.98881
D74	3.06756	-0.00002	0.00200	-0.00162	0.00037	3.06794

Item	Value	Threshold	Converged?
Maximum Force	0.000729	0.000450	NO
RMS Force	0.000138	0.000300	YES
Maximum Displacement	0.079039	0.001800	NO
RMS Displacement	0.019886	0.001200	NO

Predicted change in Energy=-1.357383D-05
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.388913	-1.919260	-0.253963
2	6	0	-2.513967	-1.166371	-0.155380
3	7	0	-2.108710	0.108753	0.226272
4	6	0	-0.767187	0.117305	0.351517
5	7	0	-0.314969	-1.104483	0.070474
6	6	0	1.115249	-1.473841	0.040340
7	6	0	1.702703	-1.368686	-1.378464
8	1	0	-1.261362	-2.955990	-0.514163
9	1	0	-3.544329	-1.427742	-0.313125
10	1	0	1.634970	-0.789967	0.713068
11	1	0	1.206388	-2.495763	0.410796
12	1	0	1.096216	-1.962909	-2.073330
13	1	0	1.664302	-0.321921	-1.700812
14	35	0	1.644225	2.212864	1.074396
15	1	0	-0.109676	0.970767	0.630776
16	6	0	-2.904862	1.261678	0.467896
17	6	0	-4.226348	1.304077	0.359594
18	1	0	-2.305421	2.116880	0.754339
19	1	0	-4.742077	2.231802	0.564862
20	1	0	-4.831852	0.453363	0.073700
21	8	0	3.011991	-1.877332	-1.381407
22	1	0	3.645965	-1.136234	-1.318534
23	6	0	4.813402	1.654629	-1.123004
24	6	0	5.702103	0.771265	-0.358320
25	8	0	4.829247	0.227004	-1.380541
26	1	0	3.903446	2.021004	-0.653813
27	1	0	5.217239	2.248818	-1.938054
28	1	0	6.747664	0.732155	-0.659954
29	6	0	5.414985	0.385544	1.067400
30	1	0	5.699881	-0.655024	1.249765
31	1	0	5.998131	1.019039	1.742943
32	1	0	4.358031	0.524194	1.303484

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				

2	C	1.357316	0.000000			
3	N	2.204897	1.391342	0.000000		
4	C	2.213763	2.226210	1.347384	0.000000	
5	N	1.386534	2.211432	2.171110	1.332761	0.000000
6	C	2.560438	3.647473	3.596260	2.484380	1.477450
7	C	3.335524	4.395131	4.391454	3.361750	2.498044
8	H	1.076468	2.213703	3.264796	3.230907	2.159986
9	H	2.211540	1.074637	2.170892	3.246759	3.268090
10	H	3.369618	4.255533	3.880697	2.593110	2.077044
11	H	2.740411	3.991100	4.219885	3.275154	2.089499
12	H	3.080238	4.164904	4.455502	3.698574	2.706332
13	H	3.737243	4.534246	4.258492	3.212026	2.769002
14	Br	5.295178	5.497466	4.385329	3.275488	3.981342
15	H	3.281991	3.311498	2.214233	1.112970	2.159339
16	C	3.596880	2.537064	1.421786	2.427506	3.530468
17	C	4.337902	3.049682	2.435358	3.657088	4.602569
18	H	4.259940	3.413330	2.085695	2.554747	3.847954
19	H	5.398656	4.126839	3.399500	4.507367	5.565473
20	H	4.194106	2.837006	2.749097	4.087985	4.777983
21	O	4.543220	5.704807	5.722827	4.611268	3.711323
22	H	5.205424	6.268860	6.087093	4.882248	4.197541
23	C	7.210869	7.911048	7.219828	5.973320	5.944517
24	C	7.585007	8.443899	7.860628	6.540890	6.317235
25	O	6.673915	7.573989	7.122575	5.859363	5.508290
26	H	6.610191	7.182686	6.370029	5.142914	5.299838
27	H	7.990637	8.637881	7.933077	6.752691	6.773783
28	H	8.567305	9.467672	8.922409	7.607503	7.334000
29	C	7.304187	8.171408	7.575625	6.229261	6.003867
30	H	7.355984	8.348845	7.912332	6.574672	6.145825
31	H	8.196929	8.990854	8.297577	6.965537	6.867440
32	H	6.436108	7.225694	6.568997	5.228734	5.099984

		6	7	8	9	10
6	C	0.000000				
7	C	1.539209	0.000000			
8	H	2.855262	3.471632	0.000000		
9	H	4.673193	5.354417	2.754614	0.000000	
10	H	1.091035	2.171178	3.819227	5.318362	0.000000
11	H	1.090811	2.172115	2.675285	4.922809	1.784598
12	H	2.169597	1.097163	2.995894	4.991932	3.070841
13	H	2.158701	1.095947	4.111686	5.502577	2.459013
14	Br	3.865343	4.341364	6.138648	6.488476	3.024506
15	H	2.797349	3.576982	4.249316	4.294257	2.480070
16	C	4.881307	5.617607	4.631874	2.872610	4.987929
17	C	6.029214	6.731876	5.263342	2.894916	6.234182

18	H	5.010395	5.723904	5.332277	3.903681	4.896749
19	H	6.950912	7.633820	6.339784	3.949395	7.058313
20	H	6.251659	6.937510	4.971687	2.312121	6.616226
21	O	2.404537	1.404623	4.491899	6.657980	2.732284
22	H	2.892238	1.958033	5.295317	7.266096	2.879480
23	C	4.981670	4.345359	7.650572	8.944752	4.410175
24	C	5.122369	4.649225	7.899783	9.504430	4.486300
25	O	4.324992	3.510201	6.926585	8.601996	3.952320
26	H	4.524360	4.105897	7.173926	8.214576	3.862111
27	H	5.882053	5.074588	8.431474	9.639635	5.394007
28	H	6.089411	5.511935	8.818626	10.521909	5.508328
29	C	4.795820	4.779186	7.631566	9.244629	3.974404
30	H	4.811655	4.836770	7.540875	9.407186	4.102408
31	H	5.740718	5.821951	8.578789	10.063434	4.834285
32	H	4.012893	4.222157	6.855152	8.298842	3.080693

		11	12	13	14	15
11	H	0.000000				
12	H	2.543020	0.000000			
13	H	3.064989	1.776044	0.000000		
14	Br	4.775273	5.257906	3.758632	0.000000	
15	H	3.714464	4.168071	3.202240	2.194486	0.000000
16	C	5.569919	5.732749	5.299843	4.686874	2.815000
17	C	6.629934	6.702388	6.448946	5.983349	4.139037
18	H	5.807521	6.017601	5.266329	3.963755	2.479948
19	H	7.599858	7.657762	7.259233	6.406624	4.801426
20	H	6.728396	6.752044	6.778641	6.785042	4.782989
21	O	2.618139	2.038695	2.082688	4.963009	4.680315
22	H	3.284880	2.784660	2.176288	4.577066	4.726954
23	C	5.708664	5.273251	3.762638	3.896650	5.270684
24	C	5.610389	5.624160	4.393311	4.538420	5.898719
25	O	4.873136	4.383058	3.228122	4.484944	5.384379
26	H	5.367373	5.076134	3.405770	2.850894	4.342615
27	H	6.641917	5.894046	4.391850	4.673604	6.050481
28	H	6.501669	6.418713	5.294812	5.589773	6.981835
29	C	5.142504	5.833625	4.714989	4.190200	5.572701
30	H	4.927846	5.826428	5.010266	4.970301	6.064429
31	H	6.090094	6.890916	5.695585	4.563844	6.208425
32	H	4.455321	5.313003	4.122849	3.204502	4.540084

		16	17	18	19	20
16	C	0.000000				
17	C	1.326594	0.000000			
18	H	1.082936	2.122836	0.000000		
19	H	2.079880	1.081103	2.446712	0.000000	
20	H	2.126512	1.082628	3.100550	1.847199	0.000000

21	O	6.948558	8.096049	6.984985	8.988799	8.311158
22	H	7.201017	8.410978	7.092147	9.233097	8.737191
23	C	7.890309	9.167229	7.376703	9.720556	9.793164
24	C	8.660427	9.968623	8.195678	10.586138	10.547602
25	O	8.018960	9.283963	7.683283	9.970659	9.772558
26	H	6.941748	8.224022	6.367269	8.733536	8.904616
27	H	8.528280	9.764890	7.991045	10.269024	10.404568
28	H	9.732610	11.036101	9.266932	11.651749	11.606083
29	C	8.387304	9.710819	7.918346	10.335720	10.295130
30	H	8.850236	10.156797	8.486093	10.855291	10.655001
31	H	8.997105	10.321573	8.433954	10.872476	10.972460
32	H	7.347905	8.671258	6.873122	9.288350	9.272073

		21	22	23	24	25
21	O	0.000000				
22	H	0.977293	0.000000			
23	C	3.973236	3.031511	0.000000		
24	C	3.911327	2.964501	1.467945	0.000000	
25	O	2.780405	1.806217	1.450755	1.450184	0.000000
26	H	4.064617	3.236711	1.087378	2.210052	2.145618
27	H	4.711485	3.783026	1.086485	2.216712	2.132859
28	H	4.613586	3.680373	2.192428	1.088903	2.110627
29	C	4.109944	3.337352	2.601989	1.504625	2.522030
30	H	3.954979	3.323597	3.427882	2.149476	2.907660
31	H	5.202649	4.421597	3.165629	2.136429	3.427792
32	H	3.845490	3.184186	2.715343	2.151550	2.741233

		26	27	28	29	30
26	H	0.000000				
27	H	1.851277	0.000000			
28	H	3.122619	2.505195	0.000000		
29	C	2.814614	3.541701	2.209055	0.000000	
30	H	3.743250	4.339059	2.582468	1.094169	0.000000
31	H	3.337077	3.958773	2.533380	1.094410	1.770498
32	H	2.505614	3.770959	3.099787	1.091838	1.787178

		31	32
31	H	0.000000	
32	H	1.768593	0.000000

Stoichiometry C10H17BrN2O2
Framework group C1[X(C10H17BrN2O2)]
Deg. of freedom 90
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.723503	2.122365	-0.420245
2	6	0	-3.791269	1.352133	-0.090209
3	7	0	-3.316149	0.052561	0.055414
4	6	0	-1.989777	0.047414	-0.181556
5	7	0	-1.614831	1.291665	-0.477370
6	6	0	-0.218678	1.698034	-0.739052
7	6	0	0.471429	2.223133	0.532636
8	1	0	-2.658651	3.176738	-0.627308
9	1	0	-4.825402	1.612926	0.041707
10	1	0	0.304665	0.816812	-1.113105
11	1	0	-0.232326	2.472460	-1.507131
12	1	0	-0.129779	3.028819	0.972164
13	1	0	0.536136	1.408141	1.262499
14	35	0	0.520510	-2.056658	-0.194290
15	1	0	-1.289215	-0.816514	-0.142259
16	6	0	-4.035782	-1.126863	0.390917
17	6	0	-5.339463	-1.174198	0.631808
18	1	0	-3.393339	-1.997779	0.429942
19	1	0	-5.795034	-2.122658	0.880126
20	1	0	-5.987628	-0.307831	0.594724
21	8	0	1.734689	2.739358	0.199992
22	1	0	2.418076	2.067249	0.390659
23	6	0	3.780973	-0.496714	1.261674
24	6	0	4.544153	0.019284	0.118799
25	8	0	3.704395	0.906280	0.900515
26	1	0	2.871833	-1.063463	1.075530
27	1	0	4.284580	-0.676193	2.207517
28	1	0	5.601866	0.224545	0.276343
29	6	0	4.130664	-0.242027	-1.304100
30	1	0	4.321249	0.636323	-1.928107
31	1	0	4.713014	-1.076153	-1.707628
32	1	0	3.073807	-0.510441	-1.359931

Rotational constants (GHZ): 0.5997321 0.2212557 0.1728136
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 492 symmetry adapted cartesian basis functions of A symmetry.
There are 475 symmetry adapted basis functions of A symmetry.
475 basis functions, 751 primitive gaussians, 492 cartesian basis functions
71 alpha electrons 71 beta electrons
nuclear repulsion energy 1307.5373783703 Hartrees.
NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F

Big=F
 Integral buffers will be 131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis= 475 RedAO= T EigKep= 3.79D-06 NBF= 475
 NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475
 Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"
 B after Tr= 0.000000 0.000000 0.000000
 Rot= 0.999999 0.000957 -0.000399 -0.000913 Ang= 0.16 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
 Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
 HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
 FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
 NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
 wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
 NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on energy=1.00D-06.
 No special actions if energy rises.
 SCF Done: E(RB3LYP) = -3225.52365497 A.U. after 11 cycles
 NFock= 11 Conv=0.21D-08 -V/T= 2.0018
 Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****

 Center Atomic Forces (Hartrees/Bohr)
 Number Number X Y Z

1	6	0.000123605	-0.000031828	0.000114162
2	6	-0.000005077	-0.000084561	0.000268894
3	7	0.000082664	0.000155705	-0.000156623
4	6	0.000512617	-0.000214321	0.000016026
5	7	-0.000196228	0.000390110	-0.000235553
6	6	0.000272310	0.000184870	-0.000000994
7	6	-0.000409223	0.000199509	0.000237508
8	1	-0.000011040	0.000035780	-0.000090648
9	1	0.000018096	0.000008884	-0.000014777

10	1	-0.000100786	-0.000064443	0.000022245
11	1	-0.000022899	0.000058791	-0.000043606
12	1	0.000141866	-0.000064347	0.000093213
13	1	0.000030847	-0.000112106	-0.000101884
14	35	0.000068015	-0.000002473	-0.000042609
15	1	-0.000444817	-0.000507065	-0.000021676
16	6	-0.000073735	0.000147992	-0.000019829
17	6	0.000050768	-0.000038830	0.000004868
18	1	0.000009173	-0.000015894	-0.000013613
19	1	-0.000004231	-0.000003648	0.000000354
20	1	0.000002743	0.000021494	0.000012377
21	8	0.000016080	0.000147738	0.000092410
22	1	-0.000165266	-0.000054289	-0.000393912
23	6	-0.000242915	-0.000202605	-0.000202151
24	6	-0.000496398	-0.000167280	-0.000219012
25	8	0.000706215	0.000049830	0.000891736
26	1	0.000062781	-0.000021418	0.000208425
27	1	0.000118856	0.000021471	-0.000041720
28	1	-0.000069859	0.000090221	-0.000030512
29	6	0.000023914	0.000187636	-0.000621449
30	1	-0.000037805	-0.000022400	0.000135383
31	1	-0.000024581	-0.000042018	0.000016105
32	1	0.000064308	-0.000050509	0.000136861

Cartesian Forces: Max 0.000891736 RMS 0.000209126

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000619562 RMS 0.000115700
Search for a local minimum.
Step number 25 out of a maximum of 177
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 19 20 21 22 23
24 25
DE= -2.09D-05 DEPred=-1.36D-05 R= 1.54D+00
TightC=F SS= 1.41D+00 RLast= 1.06D-01 DXNew= 3.2661D+00 3.1900D-01
Trust test= 1.54D+00 RLast= 1.06D-01 DXMaxT set to 1.94D+00
ITU= 1 1 1 1 1 1 1 1 -1 1 1 1 1 1 1 1 1 1 1 1
ITU= 0 1 0 1 0

Eigenvalues --- 0.00007 0.00152 0.00231 0.00275 0.00330
Eigenvalues --- 0.00566 0.00870 0.01129 0.01205 0.01401
Eigenvalues --- 0.01481 0.01795 0.01917 0.02061 0.02102
Eigenvalues --- 0.02180 0.02316 0.02385 0.02746 0.03055
Eigenvalues --- 0.03063 0.03243 0.03493 0.03936 0.04498
Eigenvalues --- 0.04828 0.04982 0.05139 0.05440 0.05661
Eigenvalues --- 0.05937 0.05981 0.07063 0.09321 0.09637
Eigenvalues --- 0.10370 0.11209 0.11545 0.11729 0.13105
Eigenvalues --- 0.13982 0.14160 0.15617 0.15967 0.15993
Eigenvalues --- 0.16000 0.16002 0.16004 0.16016 0.16065
Eigenvalues --- 0.16651 0.17432 0.19641 0.21621 0.22061
Eigenvalues --- 0.22949 0.23438 0.23993 0.24489 0.25048
Eigenvalues --- 0.27640 0.28486 0.31164 0.32487 0.33103
Eigenvalues --- 0.33341 0.34044 0.34279 0.34496 0.34842
Eigenvalues --- 0.35177 0.35685 0.35690 0.35859 0.36049
Eigenvalues --- 0.36439 0.36666 0.37230 0.37253 0.37783
Eigenvalues --- 0.39479 0.42136 0.42705 0.45679 0.46159
Eigenvalues --- 0.49307 0.53629 0.54939 0.56644 0.60410
Eigenvalue 1 is 6.87D-05 Eigenvector:

	D55	D52	D54	D53	D47
1	0.50168	-0.50002	0.49988	0.49061	0.03616

	D46	R18	D42	D35	D41
1	0.02703	-0.02381	0.02030	-0.01853	-0.01823

En-DIIS/RFO-DIIS IScMMF= 0 using points: 25 24 23 22 21
RFO step: Lambda=-4.90724418D-06.
DidBck=F Rises=F RFO-DIIS coefs: 1.60534 -0.27416 -0.73090 0.32707 0.07266
Iteration 1 RMS(Cart)= 0.01850718 RMS(Int)= 0.00030928
Iteration 2 RMS(Cart)= 0.00018637 RMS(Int)= 0.00003294
Iteration 3 RMS(Cart)= 0.00000024 RMS(Int)= 0.00003294

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56496	0.00002	0.00011	0.00007	0.00019	2.56514
R2	2.62017	-0.00009	-0.00037	0.00008	-0.00029	2.61988
R3	2.03423	-0.00001	-0.00006	0.00000	-0.00006	2.03417
R4	2.62926	0.00001	0.00005	0.00002	0.00007	2.62932
R5	2.03077	-0.00002	-0.00006	0.00001	-0.00005	2.03072
R6	2.54619	-0.00010	-0.00033	0.00014	-0.00019	2.54599
R7	2.68679	0.00009	0.00003	0.00012	0.00015	2.68694
R8	2.51855	-0.00053	-0.00099	-0.00009	-0.00108	2.51748
R9	2.10321	-0.00062	-0.00180	-0.00039	-0.00220	2.10101
R10	2.79198	-0.00011	-0.00042	0.00037	-0.00003	2.79195
R11	2.90868	-0.00025	-0.00057	0.00003	-0.00053	2.90815
R12	2.06176	-0.00008	-0.00041	0.00013	-0.00028	2.06147

R13	2.06133	-0.00007	-0.00035	0.00014	-0.00021	2.06112
R14	2.07334	-0.00010	-0.00048	-0.00004	-0.00052	2.07282
R15	2.07104	-0.00007	-0.00045	0.00010	-0.00035	2.07069
R16	2.65435	0.00004	0.00094	0.00007	0.00102	2.65537
R17	4.14698	0.00003	0.00716	-0.00007	0.00707	4.15405
R18	8.47532	-0.00008	-0.00933	0.00506	-0.00429	8.47102
R19	2.50690	-0.00005	-0.00015	0.00006	-0.00009	2.50681
R20	2.04645	-0.00001	-0.00007	0.00000	-0.00007	2.04638
R21	2.04299	0.00000	-0.00004	0.00003	-0.00001	2.04297
R22	2.04587	-0.00002	-0.00005	-0.00002	-0.00006	2.04581
R23	1.84682	-0.00020	-0.00089	0.00019	-0.00068	1.84614
R24	3.41325	-0.00005	0.00127	0.00445	0.00574	3.41899
R25	2.77401	-0.00020	-0.00016	-0.00008	-0.00013	2.77388
R26	2.74153	-0.00015	-0.00048	-0.00011	-0.00064	2.74089
R27	2.05485	0.00003	-0.00049	0.00026	-0.00024	2.05461
R28	2.05316	0.00009	-0.00007	0.00013	0.00006	2.05322
R29	2.74045	-0.00057	-0.00127	-0.00032	-0.00166	2.73879
R30	2.05773	-0.00006	-0.00045	0.00023	-0.00022	2.05751
R31	2.84333	-0.00033	-0.00036	-0.00018	-0.00054	2.84279
R32	2.06768	0.00004	0.00010	0.00003	0.00013	2.06781
R33	2.06813	-0.00003	-0.00021	0.00018	-0.00004	2.06810
R34	2.06328	-0.00004	-0.00021	0.00001	-0.00020	2.06308
A1	1.87451	-0.00006	-0.00015	0.00008	-0.00007	1.87444
A2	2.27836	0.00001	0.00011	-0.00005	0.00006	2.27842
A3	2.13025	0.00005	0.00002	-0.00001	0.00001	2.13026
A4	1.86173	-0.00004	-0.00016	0.00009	-0.00006	1.86167
A5	2.27728	0.00002	0.00011	-0.00003	0.00009	2.27736
A6	2.14413	0.00002	0.00004	-0.00005	-0.00001	2.14413
A7	1.89792	-0.00011	-0.00016	-0.00026	-0.00042	1.89749
A8	2.24808	0.00010	0.00014	0.00009	0.00023	2.24831
A9	2.13718	0.00002	0.00001	0.00017	0.00019	2.13737
A10	1.88853	0.00015	0.00023	0.00032	0.00056	1.88909
A11	2.23495	-0.00015	0.00014	-0.00009	0.00006	2.23501
A12	2.15969	0.00000	-0.00037	-0.00022	-0.00061	2.15907
A13	1.90206	0.00007	0.00022	-0.00022	-0.00001	1.90205
A14	2.21194	0.00005	-0.00018	0.00014	-0.00004	2.21190
A15	2.16753	-0.00011	0.00008	0.00020	0.00030	2.16783
A16	1.95108	-0.00009	-0.00095	0.00041	-0.00052	1.95056
A17	1.86696	-0.00002	0.00011	0.00006	0.00018	1.86714
A18	1.88406	0.00002	-0.00057	-0.00013	-0.00072	1.88334
A19	1.92169	0.00017	0.00193	0.00029	0.00221	1.92390
A20	1.92321	-0.00006	-0.00053	-0.00070	-0.00123	1.92198
A21	1.91561	-0.00002	-0.00002	0.00008	0.00007	1.91568
A22	1.91327	0.00000	-0.00052	-0.00050	-0.00102	1.91224

A23	1.89969	0.00016	0.00079	0.00066	0.00144	1.90114
A24	1.91022	-0.00007	0.00079	0.00043	0.00124	1.91147
A25	1.88772	-0.00001	0.00126	-0.00038	0.00088	1.88860
A26	1.89421	-0.00009	-0.00174	-0.00083	-0.00259	1.89162
A27	1.95834	0.00001	-0.00059	0.00058	-0.00001	1.95833
A28	1.77860	0.00003	0.00520	0.00198	0.00705	1.78565
A29	2.84699	0.00002	-0.00450	-0.00123	-0.00579	2.84120
A30	2.17712	-0.00002	-0.00007	0.00004	-0.00003	2.17709
A31	1.95559	-0.00001	0.00009	-0.00009	0.00000	1.95559
A32	2.15048	0.00003	-0.00002	0.00005	0.00003	2.15051
A33	2.07959	0.00000	-0.00016	0.00013	-0.00003	2.07956
A34	2.15745	0.00001	0.00025	-0.00011	0.00015	2.15760
A35	2.04614	-0.00001	-0.00009	-0.00002	-0.00011	2.04602
A36	1.90703	0.00017	-0.00060	0.00218	0.00166	1.90869
A37	3.04262	0.00033	-0.00515	0.00137	-0.00377	3.03885
A38	2.07671	0.00002	-0.00016	-0.00086	-0.00102	2.07570
A39	2.08847	-0.00010	-0.00021	-0.00033	-0.00053	2.08794
A40	2.00127	0.00008	-0.00027	0.00074	0.00048	2.00175
A41	1.98334	0.00002	-0.00004	0.00047	0.00043	1.98378
A42	2.03809	0.00007	0.00053	0.00038	0.00091	2.03900
A43	2.04724	0.00002	-0.00019	-0.00006	-0.00024	2.04700
A44	2.13217	-0.00010	0.00011	-0.00018	-0.00007	2.13210
A45	1.94894	-0.00003	0.00113	-0.00044	0.00069	1.94963
A46	2.04525	-0.00003	-0.00086	0.00099	0.00014	2.04540
A47	2.02250	0.00005	-0.00009	-0.00008	-0.00017	2.02233
A48	1.42039	-0.00010	-0.00246	-0.00063	-0.00299	1.41740
A49	0.99959	-0.00005	0.00599	0.00022	0.00644	1.00602
A50	2.38834	-0.00018	-0.00036	-0.00237	-0.00280	2.38554
A51	2.28283	0.00010	0.00819	0.00643	0.01466	2.29748
A52	1.93055	0.00015	0.00001	-0.00001	0.00000	1.93055
A53	1.91222	0.00000	-0.00015	0.00050	0.00035	1.91257
A54	1.93591	0.00019	0.00068	0.00005	0.00074	1.93665
A55	1.88480	-0.00009	-0.00036	-0.00031	-0.00067	1.88413
A56	1.91430	-0.00016	-0.00010	0.00003	-0.00006	1.91424
A57	1.88477	-0.00010	-0.00013	-0.00028	-0.00041	1.88436
A58	3.70322	0.00000	0.00572	0.00580	0.01167	3.71489
A59	5.01418	0.00005	0.00921	0.00349	0.01279	5.02697
D1	0.00352	0.00005	0.00186	0.00045	0.00231	0.00583
D2	-3.12807	-0.00002	0.00081	-0.00084	-0.00003	-3.12810
D3	3.13262	0.00007	0.00088	0.00130	0.00218	3.13480
D4	0.00102	0.00000	-0.00017	0.00001	-0.00015	0.00087
D5	-0.00721	0.00000	-0.00122	0.00026	-0.00096	-0.00817
D6	-3.08864	-0.00005	-0.00376	-0.00186	-0.00560	-3.09424
D7	-3.13759	-0.00002	-0.00034	-0.00050	-0.00084	-3.13844

D8	0.06416	-0.00007	-0.00288	-0.00262	-0.00549	0.05867
D9	0.00128	-0.00009	-0.00188	-0.00100	-0.00288	-0.00160
D10	-3.13763	-0.00003	-0.00005	-0.00008	-0.00014	-3.13777
D11	3.13382	-0.00002	-0.00093	0.00016	-0.00076	3.13306
D12	-0.00509	0.00004	0.00089	0.00109	0.00198	-0.00311
D13	-0.00579	0.00008	0.00114	0.00117	0.00231	-0.00347
D14	3.12888	0.00013	0.00205	0.00189	0.00394	3.13282
D15	3.13333	0.00003	-0.00054	0.00032	-0.00022	3.13311
D16	-0.01518	0.00008	0.00037	0.00104	0.00140	-0.01378
D17	-0.00194	-0.00001	-0.00229	0.00039	-0.00190	-0.00384
D18	3.14033	-0.00002	-0.00272	0.00018	-0.00254	3.13779
D19	-3.14053	0.00006	-0.00025	0.00143	0.00118	-3.13935
D20	0.00174	0.00004	-0.00067	0.00122	0.00054	0.00228
D21	0.00802	-0.00005	0.00004	-0.00089	-0.00085	0.00716
D22	3.09133	0.00000	0.00245	0.00116	0.00363	3.09496
D23	-3.12702	-0.00009	-0.00084	-0.00157	-0.00240	-3.12942
D24	-0.04371	-0.00004	0.00158	0.00048	0.00209	-0.04162
D25	-3.08720	-0.00005	-0.01156	-0.00622	-0.01778	-3.10498
D26	0.04649	0.00000	-0.01051	-0.00540	-0.01592	0.03057
D27	1.43339	-0.00011	0.00827	0.00064	0.00892	1.44230
D28	-2.74498	0.00004	0.01016	0.00128	0.01145	-2.73353
D29	-0.68452	0.00002	0.00990	0.00134	0.01125	-0.67327
D30	-1.63942	-0.00017	0.00538	-0.00177	0.00362	-1.63580
D31	0.46540	-0.00003	0.00727	-0.00113	0.00615	0.47155
D32	2.52586	-0.00005	0.00702	-0.00107	0.00595	2.53181
D33	-0.94623	-0.00003	0.00632	0.00094	0.00727	-0.93897
D34	1.11530	0.00004	0.00801	0.00057	0.00858	1.12388
D35	-3.02191	0.00012	0.00828	0.00199	0.01029	-3.01162
D36	-3.01885	-0.00006	0.00551	0.00040	0.00592	-3.01293
D37	-0.95731	0.00001	0.00720	0.00004	0.00723	-0.95008
D38	1.18867	0.00009	0.00747	0.00146	0.00894	1.19761
D39	1.14887	-0.00011	0.00462	0.00057	0.00519	1.15406
D40	-3.07278	-0.00003	0.00631	0.00020	0.00651	-3.06628
D41	-0.92680	0.00004	0.00658	0.00162	0.00821	-0.91859
D42	-1.71763	-0.00006	0.00947	0.00707	0.01654	-1.70109
D43	2.47812	0.00004	0.01067	0.00792	0.01860	2.49672
D44	0.39313	0.00011	0.01062	0.00859	0.01922	0.41234
D45	0.45853	0.00000	0.00342	0.00069	0.00408	0.46261
D46	-0.33729	0.00017	0.01120	0.00775	0.01893	-0.31836
D47	2.57763	0.00003	-0.00253	0.00052	-0.00202	2.57561
D48	-3.14110	-0.00001	-0.00051	-0.00016	-0.00068	3.14141
D49	0.00062	0.00000	-0.00043	-0.00005	-0.00047	0.00014
D50	-0.00025	0.00000	-0.00004	0.00007	0.00003	-0.00022
D51	3.14146	0.00001	0.00005	0.00019	0.00023	-3.14149

D52	-1.66841	-0.00001	-0.03208	-0.01936	-0.05142	-1.71983
D53	2.22441	0.00005	0.01719	0.01332	0.03053	2.25494
D54	1.94437	-0.00007	-0.00105	0.00499	0.00401	1.94839
D55	-2.78978	0.00000	0.00798	0.00983	0.01775	-2.77203
D56	-2.73163	0.00001	0.00110	0.00078	0.00186	-2.72976
D57	-0.02989	-0.00004	0.00066	-0.00006	0.00059	-0.02930
D58	-0.02205	0.00001	0.00166	-0.00120	0.00046	-0.02159
D59	2.67969	-0.00004	0.00122	-0.00204	-0.00081	2.67888
D60	-0.16556	0.00013	-0.00769	0.00105	-0.00657	-0.17212
D61	0.16528	0.00027	0.01257	0.01092	0.02343	0.18872
D62	-2.57248	-0.00009	-0.00819	-0.00097	-0.00910	-2.58158
D63	-2.24164	0.00006	0.01207	0.00891	0.02090	-2.22074
D64	2.12494	0.00013	0.00116	0.00313	0.00431	2.12924
D65	-0.26717	0.00012	0.00093	0.00266	0.00360	-0.26356
D66	2.48862	0.00006	0.00016	-0.00112	-0.00098	2.48764
D67	-1.71871	0.00003	-0.00037	-0.00120	-0.00158	-1.72029
D68	0.36041	0.00003	-0.00020	-0.00119	-0.00140	0.35901
D69	1.27394	-0.00002	0.00043	-0.00159	-0.00115	1.27279
D70	-2.93339	-0.00004	-0.00011	-0.00166	-0.00175	-2.93515
D71	-0.85427	-0.00005	0.00006	-0.00165	-0.00157	-0.85584
D72	-1.08704	0.00000	-0.00030	-0.00195	-0.00225	-1.08930
D73	0.98881	-0.00002	-0.00084	-0.00202	-0.00286	0.98595
D74	3.06794	-0.00003	-0.00067	-0.00202	-0.00268	3.06526

Item	Value	Threshold	Converged?
Maximum Force	0.000620	0.000450	NO
RMS Force	0.000116	0.000300	YES
Maximum Displacement	0.069504	0.001800	NO
RMS Displacement	0.018513	0.001200	NO

Predicted change in Energy=-1.037704D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.388036	-1.920176	-0.249729
2	6	0	-2.515483	-1.171833	-0.142876
3	7	0	-2.111927	0.106982	0.228210
4	6	0	-0.769573	0.120625	0.342521
5	7	0	-0.314861	-1.099782	0.062209
6	6	0	1.116282	-1.464950	0.026145
7	6	0	1.697193	-1.356051	-1.394764
8	1	0	-1.258338	-2.957115	-0.507903

9	1	0	-3.546117	-1.438052	-0.290205
10	1	0	1.636304	-0.782300	0.699641
11	1	0	1.210734	-2.487842	0.392736
12	1	0	1.084644	-1.945257	-2.088150
13	1	0	1.663043	-0.308184	-1.713363
14	35	0	1.649534	2.214288	1.051008
15	1	0	-0.113561	0.976035	0.614617
16	6	0	-2.910411	1.257809	0.472585
17	6	0	-4.232929	1.294624	0.376054
18	1	0	-2.311829	2.116241	0.750914
19	1	0	-4.750455	2.220964	0.583008
20	1	0	-4.837705	0.440670	0.098527
21	8	0	3.003734	-1.873004	-1.408714
22	1	0	3.643384	-1.138762	-1.330372
23	6	0	4.836207	1.641970	-1.129785
24	6	0	5.710222	0.762309	-0.344322
25	8	0	4.846853	0.211606	-1.369897
26	1	0	3.923741	2.019335	-0.674678
27	1	0	5.254019	2.224333	-1.946366
28	1	0	6.759090	0.714298	-0.632471
29	6	0	5.403895	0.395407	1.082066
30	1	0	5.679131	-0.645024	1.279822
31	1	0	5.984061	1.031988	1.757241
32	1	0	4.345622	0.544464	1.305047

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357414	0.000000			
3	N	2.204952	1.391377	0.000000		
4	C	2.213171	2.225817	1.347281	0.000000	
5	N	1.386382	2.211332	2.171009	1.332191	0.000000
6	C	2.560263	3.647493	3.596266	2.484067	1.477436
7	C	3.338859	4.398613	4.391344	3.359116	2.497359
8	H	1.076438	2.213796	3.264838	3.230263	2.159829
9	H	2.211650	1.074609	2.170896	3.246385	3.267971
10	H	3.367892	4.254281	3.881018	2.594427	2.077056
11	H	2.736533	3.987914	4.219035	3.275399	2.088875
12	H	3.081325	4.164516	4.449188	3.689736	2.701385
13	H	3.748310	4.546691	4.265263	3.213745	2.773335
14	Br	5.292688	5.498959	4.389342	3.276806	3.977391
15	H	3.280155	3.310039	2.213149	1.111807	2.157474
16	C	3.597076	2.537306	1.421865	2.427611	3.530372
17	C	4.338198	3.049970	2.435365	3.657080	4.602492

18	H	4.259969	3.413468	2.085738	2.554960	3.847727
19	H	5.398921	4.127114	3.399504	4.507402	5.565346
20	H	4.194650	2.837455	2.749188	4.087990	4.778120
21	O	4.542369	5.705764	5.724495	4.612941	3.711409
22	H	5.205150	6.272391	6.091359	4.884549	4.196249
23	C	7.225274	7.933399	7.244094	5.992240	5.955800
24	C	7.588804	8.452438	7.870404	6.547614	6.319357
25	O	6.683794	7.591013	7.140693	5.872384	5.514885
26	H	6.626862	7.206246	6.395435	5.164009	5.313910
27	H	8.010770	8.669007	7.966750	6.778514	6.789443
28	H	8.571033	9.477072	8.933339	7.614711	7.335820
29	C	7.298351	8.165371	7.569665	6.223676	5.998323
30	H	7.342369	8.333865	7.897593	6.561290	6.133297
31	H	8.190911	8.983848	8.290874	6.960142	6.862507
32	H	6.431688	7.219205	6.561318	5.222194	5.095909

		6	7	8	9	10
6	C	0.000000				
7	C	1.538927	0.000000			
8	H	2.854923	3.476362	0.000000		
9	H	4.673196	5.359018	2.754791	0.000000	
10	H	1.090885	2.172425	3.816666	5.316700	0.000000
11	H	1.090697	2.170887	2.669773	4.918953	1.784425
12	H	2.168395	1.096888	3.001766	4.993376	3.070598
13	H	2.159384	1.095763	4.123644	5.517004	2.459287
14	Br	3.856358	4.327978	6.134276	6.491012	3.017147
15	H	2.795929	3.571424	4.247380	4.292896	2.482137
16	C	4.881289	5.616874	4.632094	2.872915	4.988609
17	C	6.029240	6.732623	5.263730	2.895364	6.234278
18	H	5.010206	5.721276	5.332298	3.903895	4.898155
19	H	6.950874	7.634053	6.340147	3.949852	7.058603
20	H	6.251926	6.939957	4.972380	2.312771	6.615874
21	O	2.405785	1.405163	4.489099	6.658888	2.739464
22	H	2.886655	1.959342	5.292423	7.270519	2.876871
23	C	4.982666	4.348764	7.660404	8.969659	4.411719
24	C	5.118810	4.657819	7.900741	9.514427	4.480233
25	O	4.321681	3.518313	6.932329	8.621429	3.946956
26	H	4.529152	4.107222	7.186572	8.240153	3.869145
27	H	5.884087	5.076852	8.445554	9.674623	5.397134
28	H	6.084749	5.521797	8.818954	10.533140	5.500660
29	C	4.791610	4.789774	7.625796	9.238367	3.965852
30	H	4.802455	4.849206	7.527962	9.391436	4.086552
31	H	5.738176	5.832247	8.572991	10.055716	4.828369
32	H	4.012726	4.232624	6.852168	8.291848	3.076885

		11	12	13	14	15

11	H	0.000000				
12	H	2.542654	0.000000			
13	H	3.064498	1.776237	0.000000		
14	Br	4.768218	5.241682	3.742298	0.000000	
15	H	3.715029	4.156272	3.197661	2.198230	0.000000
16	C	5.569571	5.725160	5.305392	4.694947	2.814593
17	C	6.628786	6.696694	6.457333	5.992055	4.138550
18	H	5.808126	6.007668	5.267837	3.973924	2.480126
19	H	7.599002	7.651200	7.266558	6.417081	4.801211
20	H	6.726541	6.748957	6.789952	6.792438	4.782311
21	O	2.614975	2.037095	2.083008	4.958835	4.682779
22	H	3.272140	2.787797	2.181351	4.570487	4.729692
23	C	5.702409	5.278341	3.769964	3.903625	5.290237
24	C	5.599297	5.636295	4.404530	4.532590	5.906073
25	O	4.859553	4.395698	3.244194	4.482673	5.397069
26	H	5.367907	5.077043	3.406900	2.861471	4.364695
27	H	6.635070	5.898244	4.400346	4.687927	6.076825
28	H	6.487604	6.433628	5.308813	5.584947	6.989783
29	C	5.135260	5.846786	4.722651	4.171872	5.567582
30	H	4.914211	5.843214	5.020117	4.946278	6.051910
31	H	6.085698	6.903282	5.701960	4.548046	6.204008
32	H	4.455862	5.324140	4.127231	3.181468	4.532909

		16	17	18	19	20
16	C	0.000000				
17	C	1.326547	0.000000			
18	H	1.082900	2.122781	0.000000		
19	H	2.079813	1.081096	2.446641	0.000000	
20	H	2.126523	1.082596	3.100515	1.847101	0.000000
21	O	6.951143	8.098676	6.988081	8.991939	8.313424
22	H	7.207388	8.418406	7.098687	9.241499	8.744440
23	C	7.919927	9.199860	7.406509	9.755663	9.825296
24	C	8.673417	9.983414	8.208896	10.602517	10.562117
25	O	8.041419	9.309334	7.705335	9.997983	9.797928
26	H	6.971497	8.255938	6.397190	8.767217	8.936048
27	H	8.569913	9.811227	8.032998	10.319265	10.450164
28	H	9.747605	11.053433	9.282282	11.671206	11.623032
29	C	8.381103	9.704402	7.912227	10.329208	10.288817
30	H	8.834740	10.140412	8.471114	10.838620	10.638516
31	H	8.989603	10.313270	8.426748	10.863807	10.964105
32	H	7.338383	8.661253	6.862885	9.277424	9.262826

		21	22	23	24	25
21	O	0.000000				
22	H	0.976934	0.000000			
23	C	3.973764	3.032414	0.000000		

24	C	3.924651	2.976271	1.467875	0.000000	
25	O	2.782839	1.809252	1.450416	1.449305	0.000000
26	H	4.066390	3.237609	1.087254	2.209245	2.145541
27	H	4.705425	3.779419	1.086517	2.216344	2.132879
28	H	4.625947	3.691683	2.192117	1.088788	2.110248
29	C	4.136478	3.357519	2.601629	1.504339	2.521150
30	H	3.986717	3.346813	3.427399	2.149278	2.906460
31	H	5.229207	4.441202	3.166160	2.136418	3.427136
32	H	3.874185	3.204968	2.715437	2.151745	2.741778

		26	27	28	29	30
26	H	0.000000				
27	H	1.851717	0.000000			
28	H	3.121555	2.504349	0.000000		
29	C	2.813209	3.541021	2.208592	0.000000	
30	H	3.741693	4.338458	2.582814	1.094239	0.000000
31	H	3.336765	3.958706	2.532256	1.094390	1.770107
32	H	2.504503	3.770787	3.099620	1.091733	1.787110

		31	32
31	H	0.000000	
32	H	1.768232	0.000000

Stoichiometry C10H17BrN2O2
Framework group C1[X(C10H17BrN2O2)]
Deg. of freedom 90
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.725511	2.118366	-0.427392
2	6	0	-3.796235	1.348638	-0.105458
3	7	0	-3.321564	0.050137	0.051109
4	6	0	-1.993424	0.045074	-0.175135
5	7	0	-1.616294	1.287867	-0.471730
6	6	0	-0.218748	1.693039	-0.727698
7	6	0	0.466404	2.215524	0.547400
8	1	0	-2.658941	3.172151	-0.636737
9	1	0	-4.831636	1.609379	0.015959
10	1	0	0.304467	0.812616	-1.103374
11	1	0	-0.229655	2.470033	-1.493060
12	1	0	-0.140203	3.015791	0.988721
13	1	0	0.535879	1.398206	1.273940

14	35	0	0.525503	-2.050744	-0.178449
15	1	0	-1.293609	-0.817620	-0.128958
16	6	0	-4.043486	-1.128656	0.384236
17	6	0	-5.349224	-1.175985	0.613445
18	1	0	-3.400988	-1.999076	0.431525
19	1	0	-5.806518	-2.123980	0.860334
20	1	0	-5.997591	-0.310215	0.567882
21	8	0	1.726717	2.743847	0.220338
22	1	0	2.414359	2.071749	0.393063
23	6	0	3.802328	-0.483936	1.251872
24	6	0	4.548671	0.019311	0.092402
25	8	0	3.718731	0.913962	0.874248
26	1	0	2.892395	-1.054910	1.084148
27	1	0	4.319892	-0.651355	2.192413
28	1	0	5.608173	0.227195	0.232758
29	6	0	4.116221	-0.260291	-1.321050
30	1	0	4.295512	0.611021	-1.958253
31	1	0	4.695563	-1.097181	-1.723128
32	1	0	3.059739	-0.532762	-1.359598

Rotational constants (GHZ): 0.6023315 0.2207589 0.1725842

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.

475 basis functions, 751 primitive gaussians, 492 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1307.5472710018 Hartrees.

NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 475 RedAO= T EigKep= 3.80D-06 NBF= 475

NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999999 0.001009 -0.000351 -0.000335 Ang= 0.13 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3225.52367319 A.U. after 11 cycles
NFock= 11 Conv=0.19D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000056704	-0.000066425	0.000216722
2	6	0.000069482	-0.000004404	-0.000058159
3	7	-0.000042994	0.000020659	0.000105227
4	6	0.000307386	0.000083023	-0.000103707
5	7	-0.000075232	0.000063889	-0.000134223
6	6	0.000183514	0.000013876	-0.000065235
7	6	0.000102440	-0.000055266	0.000137987
8	1	-0.000014089	0.000002542	-0.000037647
9	1	0.000000187	0.000002458	-0.000042637
10	1	-0.000005164	0.000069991	-0.000008305
11	1	-0.000020418	-0.000007882	-0.000004318
12	1	0.000047615	-0.000033847	-0.000013033
13	1	-0.000035623	-0.000013617	-0.000078062
14	35	0.000032202	-0.000014935	-0.000076660
15	1	-0.000167432	-0.000150492	0.000083389
16	6	-0.000022602	0.000046437	0.000011685
17	6	0.000010963	-0.000005946	0.000005317
18	1	0.000014664	0.000001761	-0.000020340
19	1	-0.000005326	0.000008228	-0.000010680
20	1	0.000005132	-0.000003292	0.000003699
21	8	-0.000331479	0.000046282	0.000222075
22	1	-0.000035970	0.000181292	-0.000428547
23	6	-0.000102913	-0.000068828	-0.000171518
24	6	-0.000342714	-0.000077279	0.000004681
25	8	0.000441727	-0.000066864	0.000637686

26	1	-0.000054684	-0.000032351	0.000151783
27	1	0.000032265	0.000016613	-0.000047272
28	1	0.000022644	0.000045069	-0.000092830
29	6	0.000105691	0.000047095	-0.000386682
30	1	-0.000034527	-0.000014043	0.000099165
31	1	0.000003203	0.000000642	0.000001693
32	1	-0.000031245	-0.000034386	0.000098744

Cartesian Forces: Max 0.000637686 RMS 0.000135282

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000322630 RMS 0.000071195
Search for a local minimum.
Step number 26 out of a maximum of 177
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 21 22 23 24 25
26
DE= -1.82D-05 DEPred=-1.04D-05 R= 1.76D+00
TightC=F SS= 1.41D+00 RLast= 9.46D-02 DXNew= 3.2661D+00 2.8368D-01
Trust test= 1.76D+00 RLast= 9.46D-02 DXMaxT set to 1.94D+00
ITU= 1 1 1 1 1 1 1 1 1 -1 1 1 1 1 1 1 1 1 1 1
ITU= 1 0 1 0 1 0

Eigenvalues ---	0.00007	0.00141	0.00231	0.00270	0.00314
Eigenvalues ---	0.00573	0.00842	0.01074	0.01216	0.01401
Eigenvalues ---	0.01456	0.01816	0.01920	0.02028	0.02097
Eigenvalues ---	0.02179	0.02315	0.02386	0.02803	0.03055
Eigenvalues ---	0.03064	0.03307	0.03382	0.03787	0.04461
Eigenvalues ---	0.04662	0.04990	0.05241	0.05446	0.05665
Eigenvalues ---	0.05943	0.06425	0.06823	0.09399	0.09590
Eigenvalues ---	0.10514	0.11381	0.11524	0.11606	0.13031
Eigenvalues ---	0.13995	0.14209	0.15083	0.15940	0.15992
Eigenvalues ---	0.16000	0.16001	0.16004	0.16019	0.16042
Eigenvalues ---	0.16637	0.17383	0.19154	0.21276	0.22052
Eigenvalues ---	0.22937	0.23477	0.23900	0.24472	0.25083
Eigenvalues ---	0.27642	0.28538	0.30539	0.32050	0.33107
Eigenvalues ---	0.33331	0.34047	0.34352	0.34530	0.34847
Eigenvalues ---	0.35339	0.35685	0.35689	0.35855	0.36016
Eigenvalues ---	0.36440	0.36671	0.37222	0.37272	0.37581

Eigenvalues --- 0.38136 0.42155 0.42567 0.44890 0.46016
Eigenvalues --- 0.49601 0.53986 0.55003 0.56692 0.60399
Eigenvalue 1 is 6.82D-05 Eigenvector:

	D52	D55	D53	D54	D47
1	0.50867	-0.49858	-0.49224	-0.49148	-0.03554
	D46	D42	R18	D44	D43
1	-0.03425	-0.02584	0.02497	-0.02432	-0.02386

En-DIIS/RFO-DIIS IScMMF= 0 using points: 26 25 24 23 22
RFO step: Lambda=-2.73709930D-06.
DidBck=F Rises=F RFO-DIIS coefs: 1.63806 -0.54670 -0.32610 0.23415 0.00059
Iteration 1 RMS(Cart)= 0.01456912 RMS(Int)= 0.00012972
Iteration 2 RMS(Cart)= 0.00023224 RMS(Int)= 0.00004358
Iteration 3 RMS(Cart)= 0.00000007 RMS(Int)= 0.00004358

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56514	-0.00004	0.00018	-0.00012	0.00006	2.56520
R2	2.61988	0.00002	-0.00021	0.00010	-0.00010	2.61978
R3	2.03417	0.00001	-0.00005	0.00001	-0.00004	2.03413
R4	2.62932	0.00002	0.00007	0.00005	0.00010	2.62943
R5	2.03072	0.00001	-0.00004	0.00001	-0.00002	2.03069
R6	2.54599	0.00002	-0.00016	0.00002	-0.00014	2.54585
R7	2.68694	0.00002	0.00017	-0.00008	0.00009	2.68703
R8	2.51748	-0.00007	-0.00094	0.00002	-0.00093	2.51655
R9	2.10101	-0.00023	-0.00173	0.00006	-0.00172	2.09929
R10	2.79195	0.00001	-0.00001	0.00003	0.00004	2.79199
R11	2.90815	-0.00014	-0.00078	0.00023	-0.00054	2.90761
R12	2.06147	0.00003	-0.00021	0.00012	-0.00010	2.06138
R13	2.06112	0.00000	-0.00018	0.00002	-0.00016	2.06096
R14	2.07282	0.00000	-0.00034	-0.00002	-0.00036	2.07246
R15	2.07069	0.00002	-0.00026	0.00015	-0.00011	2.07058
R16	2.65537	-0.00026	0.00079	-0.00064	0.00017	2.65554
R17	4.15405	-0.00005	0.00481	0.00001	0.00478	4.15883
R18	8.47102	-0.00009	0.00151	-0.00303	-0.00152	8.46950
R19	2.50681	-0.00001	-0.00008	-0.00002	-0.00009	2.50672
R20	2.04638	0.00000	-0.00004	0.00000	-0.00004	2.04634
R21	2.04297	0.00001	-0.00001	-0.00001	-0.00002	2.04295
R22	2.04581	0.00000	-0.00005	0.00001	-0.00004	2.04577
R23	1.84614	0.00005	-0.00043	0.00013	-0.00026	1.84588
R24	3.41899	-0.00006	0.00103	0.00035	0.00142	3.42042
R25	2.77388	-0.00002	-0.00020	0.00005	-0.00009	2.77379
R26	2.74089	-0.00010	-0.00032	-0.00014	-0.00049	2.74040
R27	2.05461	0.00010	-0.00015	-0.00008	-0.00023	2.05438
R28	2.05322	0.00005	0.00004	-0.00010	-0.00006	2.05316

R29	2.73879	-0.00032	-0.00158	-0.00014	-0.00176	2.73703
R30	2.05751	0.00004	-0.00016	0.00003	-0.00013	2.05738
R31	2.84279	-0.00018	-0.00063	0.00015	-0.00048	2.84231
R32	2.06781	0.00002	0.00009	0.00000	0.00008	2.06790
R33	2.06810	0.00000	-0.00004	-0.00001	-0.00005	2.06805
R34	2.06308	0.00005	-0.00017	0.00010	-0.00007	2.06301
A1	1.87444	-0.00002	-0.00010	-0.00009	-0.00018	1.87426
A2	2.27842	-0.00001	-0.00001	0.00003	0.00001	2.27843
A3	2.13026	0.00003	0.00011	0.00008	0.00018	2.13045
A4	1.86167	0.00002	-0.00001	0.00003	0.00002	1.86169
A5	2.27736	-0.00002	0.00003	-0.00008	-0.00005	2.27732
A6	2.14413	0.00000	-0.00001	0.00005	0.00004	2.14416
A7	1.89749	-0.00003	-0.00041	0.00010	-0.00031	1.89718
A8	2.24831	0.00002	0.00029	-0.00005	0.00024	2.24855
A9	2.13737	0.00000	0.00011	-0.00004	0.00007	2.13744
A10	1.88909	0.00001	0.00052	-0.00018	0.00035	1.88944
A11	2.23501	-0.00007	-0.00016	0.00018	0.00001	2.23502
A12	2.15907	0.00006	-0.00034	0.00002	-0.00034	2.15873
A13	1.90205	0.00002	-0.00001	0.00015	0.00013	1.90218
A14	2.21190	0.00004	0.00051	0.00002	0.00049	2.21238
A15	2.16783	-0.00006	-0.00030	-0.00013	-0.00040	2.16743
A16	1.95056	-0.00002	-0.00014	0.00019	0.00007	1.95063
A17	1.86714	-0.00002	-0.00009	-0.00026	-0.00033	1.86680
A18	1.88334	0.00001	-0.00023	-0.00012	-0.00039	1.88295
A19	1.92390	0.00005	0.00140	0.00010	0.00148	1.92538
A20	1.92198	-0.00004	-0.00089	-0.00016	-0.00104	1.92094
A21	1.91568	0.00002	-0.00006	0.00026	0.00020	1.91588
A22	1.91224	0.00004	-0.00048	0.00029	-0.00020	1.91204
A23	1.90114	0.00009	0.00115	0.00024	0.00140	1.90254
A24	1.91147	-0.00012	0.00030	0.00023	0.00053	1.91200
A25	1.88860	-0.00004	0.00049	-0.00026	0.00022	1.88882
A26	1.89162	-0.00002	-0.00143	-0.00076	-0.00222	1.88940
A27	1.95833	0.00005	-0.00006	0.00026	0.00023	1.95856
A28	1.78565	0.00000	0.00190	0.00142	0.00329	1.78894
A29	2.84120	-0.00004	-0.00164	-0.00155	-0.00320	2.83800
A30	2.17709	-0.00002	-0.00008	-0.00006	-0.00014	2.17695
A31	1.95559	0.00000	-0.00006	0.00001	-0.00005	1.95554
A32	2.15051	0.00003	0.00014	0.00005	0.00019	2.15070
A33	2.07956	0.00001	0.00000	0.00004	0.00004	2.07960
A34	2.15760	-0.00001	0.00009	-0.00008	0.00001	2.15761
A35	2.04602	0.00000	-0.00009	0.00004	-0.00005	2.04597
A36	1.90869	0.00011	0.00112	0.00023	0.00171	1.91040
A37	3.03885	0.00029	0.00046	0.00154	0.00189	3.04073
A38	2.07570	0.00002	-0.00098	0.00007	-0.00097	2.07472

A39	2.08794	-0.00005	-0.00053	0.00042	-0.00004	2.08790
A40	2.00175	0.00003	0.00069	-0.00099	-0.00030	2.00146
A41	1.98378	0.00001	0.00022	0.00004	0.00027	1.98404
A42	2.03900	0.00004	0.00089	0.00008	0.00096	2.03996
A43	2.04700	0.00000	-0.00024	-0.00016	-0.00040	2.04660
A44	2.13210	-0.00003	-0.00014	0.00048	0.00034	2.13244
A45	1.94963	-0.00003	0.00040	0.00016	0.00055	1.95018
A46	2.04540	0.00001	0.00042	-0.00034	0.00010	2.04550
A47	2.02233	0.00002	-0.00016	-0.00014	-0.00030	2.02203
A48	1.41740	0.00003	-0.00034	-0.00001	-0.00019	1.41721
A49	1.00602	-0.00018	0.00095	-0.00079	0.00019	1.00622
A50	2.38554	-0.00017	-0.00279	-0.00305	-0.00580	2.37974
A51	2.29748	0.00006	0.00682	0.00711	0.01395	2.31144
A52	1.93055	0.00012	0.00032	0.00006	0.00038	1.93093
A53	1.91257	-0.00004	0.00022	-0.00039	-0.00017	1.91239
A54	1.93665	0.00012	0.00073	0.00006	0.00079	1.93745
A55	1.88413	-0.00005	-0.00053	0.00004	-0.00049	1.88364
A56	1.91424	-0.00012	-0.00027	0.00011	-0.00016	1.91408
A57	1.88436	-0.00005	-0.00053	0.00013	-0.00040	1.88397
A58	3.71489	0.00009	0.00648	0.00710	0.01376	3.72864
A59	5.02697	0.00000	0.00780	0.00353	0.01130	5.03828
D1	0.00583	-0.00007	0.00095	-0.00088	0.00008	0.00592
D2	-3.12810	-0.00005	-0.00055	-0.00069	-0.00124	-3.12934
D3	3.13480	0.00001	0.00156	0.00007	0.00163	3.13643
D4	0.00087	0.00003	0.00006	0.00026	0.00032	0.00118
D5	-0.00817	0.00007	-0.00057	0.00050	-0.00007	-0.00823
D6	-3.09424	0.00004	-0.00425	-0.00026	-0.00451	-3.09875
D7	-3.13844	0.00000	-0.00111	-0.00035	-0.00146	-3.13990
D8	0.05867	-0.00003	-0.00480	-0.00110	-0.00590	0.05277
D9	-0.00160	0.00005	-0.00102	0.00095	-0.00007	-0.00167
D10	-3.13777	0.00004	0.00039	0.00068	0.00106	-3.13671
D11	3.13306	0.00003	0.00034	0.00078	0.00112	3.13418
D12	-0.00311	0.00002	0.00175	0.00050	0.00225	-0.00086
D13	-0.00347	-0.00001	0.00067	-0.00065	0.00002	-0.00345
D14	3.13282	0.00007	0.00304	0.00098	0.00400	3.13682
D15	3.13311	0.00000	-0.00063	-0.00039	-0.00102	3.13209
D16	-0.01378	0.00007	0.00173	0.00124	0.00296	-0.01082
D17	-0.00384	0.00002	-0.00027	0.00064	0.00037	-0.00347
D18	3.13779	0.00002	-0.00054	0.00066	0.00013	3.13792
D19	-3.13935	0.00001	0.00132	0.00033	0.00164	-3.13770
D20	0.00228	0.00001	0.00105	0.00035	0.00140	0.00368
D21	0.00716	-0.00004	-0.00007	0.00010	0.00003	0.00719
D22	3.09496	-0.00001	0.00353	0.00084	0.00436	3.09932
D23	-3.12942	-0.00010	-0.00231	-0.00145	-0.00374	-3.13315

D24	-0.04162	-0.00008	0.00129	-0.00071	0.00060	-0.04102
D25	-3.10498	-0.00008	-0.00980	-0.00625	-0.01606	-3.12103
D26	0.03057	0.00000	-0.00709	-0.00439	-0.01152	0.01905
D27	1.44230	-0.00007	0.00358	-0.00124	0.00234	1.44465
D28	-2.73353	-0.00004	0.00516	-0.00118	0.00399	-2.72954
D29	-0.67327	-0.00001	0.00492	-0.00108	0.00385	-0.66942
D30	-1.63580	-0.00010	-0.00065	-0.00212	-0.00276	-1.63856
D31	0.47155	-0.00007	0.00093	-0.00206	-0.00111	0.47044
D32	2.53181	-0.00005	0.00069	-0.00196	-0.00125	2.53056
D33	-0.93897	-0.00003	0.00315	0.00004	0.00322	-0.93575
D34	1.12388	0.00000	0.00414	0.00003	0.00420	1.12808
D35	-3.01162	0.00004	0.00500	0.00066	0.00573	-3.00589
D36	-3.01293	-0.00003	0.00244	0.00019	0.00262	-3.01031
D37	-0.95008	0.00000	0.00342	0.00018	0.00359	-0.94649
D38	1.19761	0.00004	0.00428	0.00081	0.00513	1.20274
D39	1.15406	-0.00006	0.00217	-0.00009	0.00208	1.15614
D40	-3.06628	-0.00003	0.00316	-0.00010	0.00306	-3.06322
D41	-0.91859	0.00001	0.00402	0.00053	0.00459	-0.91400
D42	-1.70109	-0.00003	0.00853	0.00794	0.01643	-1.68466
D43	2.49672	0.00000	0.00979	0.00791	0.01769	2.51441
D44	0.41234	0.00004	0.01016	0.00857	0.01873	0.43107
D45	0.46261	-0.00003	0.00015	0.00111	0.00118	0.46379
D46	-0.31836	0.00017	0.01090	0.00731	0.01819	-0.30017
D47	2.57561	0.00005	-0.00008	-0.00040	-0.00061	2.57500
D48	3.14141	0.00001	-0.00018	0.00008	-0.00010	3.14131
D49	0.00014	0.00001	-0.00015	0.00010	-0.00004	0.00010
D50	-0.00022	0.00000	0.00012	0.00005	0.00017	-0.00005
D51	-3.14149	0.00000	0.00015	0.00007	0.00022	-3.14126
D52	-1.71983	0.00005	-0.02231	-0.04776	-0.07007	-1.78990
D53	2.25494	0.00004	0.01289	0.04308	0.05590	2.31084
D54	1.94839	-0.00002	-0.00040	0.03461	0.03437	1.98276
D55	-2.77203	0.00004	0.00509	0.03955	0.04459	-2.72744
D56	-2.72976	-0.00005	0.00179	-0.00101	0.00078	-2.72898
D57	-0.02930	-0.00006	0.00037	-0.00061	-0.00023	-0.02953
D58	-0.02159	-0.00001	0.00044	0.00043	0.00088	-0.02071
D59	2.67888	-0.00002	-0.00098	0.00083	-0.00014	2.67874
D60	-0.17212	0.00008	-0.00341	-0.00033	-0.00374	-0.17587
D61	0.18872	0.00019	0.01199	0.00995	0.02189	0.21061
D62	-2.58158	-0.00003	-0.00590	0.00065	-0.00526	-2.58684
D63	-2.22074	0.00008	0.00950	0.01094	0.02038	-2.20036
D64	2.12924	0.00016	0.00388	0.00438	0.00826	2.13750
D65	-0.26356	0.00015	0.00318	0.00481	0.00797	-0.25559
D66	2.48764	0.00003	-0.00159	0.00174	0.00015	2.48779
D67	-1.72029	0.00001	-0.00192	0.00158	-0.00034	-1.72063

D68	0.35901	0.00000	-0.00198	0.00153	-0.00045	0.35856
D69	1.27279	0.00000	-0.00203	0.00181	-0.00022	1.27257
D70	-2.93515	-0.00002	-0.00236	0.00165	-0.00070	-2.93585
D71	-0.85584	-0.00002	-0.00241	0.00160	-0.00082	-0.85666
D72	-1.08930	0.00001	-0.00301	0.00213	-0.00088	-1.09018
D73	0.98595	0.00000	-0.00334	0.00197	-0.00136	0.98459
D74	3.06526	-0.00001	-0.00340	0.00192	-0.00148	3.06378

Item	Value	Threshold	Converged?
Maximum Force	0.000323	0.000450	YES
RMS Force	0.000071	0.000300	YES
Maximum Displacement	0.047430	0.001800	NO
RMS Displacement	0.014775	0.001200	NO

Predicted change in Energy=-8.509334D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.385260	-1.919321	-0.246586
2	6	0	-2.514591	-1.174668	-0.133644
3	7	0	-2.112793	0.107155	0.229088
4	6	0	-0.769692	0.125758	0.332508
5	7	0	-0.312856	-1.093629	0.053552
6	6	0	1.119313	-1.454347	0.012848
7	6	0	1.693382	-1.351016	-1.410945
8	1	0	-1.253718	-2.956459	-0.502938
9	1	0	-3.545290	-1.445024	-0.272654
10	1	0	1.639586	-0.767477	0.681762
11	1	0	1.218166	-2.475492	0.382886
12	1	0	1.077703	-1.943109	-2.098779
13	1	0	1.658993	-0.304746	-1.734521
14	35	0	1.652527	2.220800	1.030452
15	1	0	-0.115186	0.982888	0.599056
16	6	0	-2.913373	1.255937	0.476496
17	6	0	-4.236821	1.287182	0.392198
18	1	0	-2.315478	2.117601	0.746088
19	1	0	-4.756095	2.212235	0.600463
20	1	0	-4.840770	0.429812	0.123626
21	8	0	2.998908	-1.870588	-1.430425
22	1	0	3.641240	-1.139945	-1.342640
23	6	0	4.848349	1.630555	-1.131317
24	6	0	5.713711	0.755705	-0.331130

25	8	0	4.859569	0.198527	-1.359616
26	1	0	3.932577	2.012094	-0.686741
27	1	0	5.274594	2.205996	-1.948405
28	1	0	6.765150	0.704894	-0.608990
29	6	0	5.394250	0.400112	1.094974
30	1	0	5.666188	-0.639135	1.303468
31	1	0	5.969673	1.040802	1.770277
32	1	0	4.334511	0.552518	1.308346

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357443	0.000000			
3	N	2.205034	1.391433	0.000000		
4	C	2.212832	2.225551	1.347206	0.000000	
5	N	1.386327	2.211164	2.170823	1.331699	0.000000
6	C	2.560545	3.647593	3.596047	2.483395	1.477457
7	C	3.340171	4.401095	4.393511	3.359647	2.497196
8	H	1.076417	2.213811	3.264905	3.229909	2.159870
9	H	2.211643	1.074596	2.170956	3.246155	3.267800
10	H	3.367234	4.252984	3.879464	2.593157	2.076788
11	H	2.735578	3.986529	4.217701	3.274235	2.088547
12	H	3.081781	4.166154	4.449923	3.688392	2.699592
13	H	3.753436	4.553941	4.272212	3.218145	2.776280
14	Br	5.291463	5.499926	4.391732	3.277723	3.975236
15	H	3.278874	3.308933	2.212288	1.110899	2.156054
16	C	3.597255	2.537545	1.421914	2.427634	3.530161
17	C	4.338329	3.050129	2.435274	3.656973	4.602222
18	H	4.259982	3.413591	2.085728	2.554983	3.847350
19	H	5.399053	4.127271	3.399459	4.507393	5.565090
20	H	4.194763	2.837544	2.749016	4.087757	4.777844
21	O	4.541452	5.706542	5.726687	4.614725	3.711285
22	H	5.203313	6.273526	6.093807	4.885125	4.193610
23	C	7.227880	7.942135	7.254581	5.997464	5.955092
24	C	7.586719	8.454010	7.873286	6.547653	6.315657
25	O	6.687452	7.600454	7.151655	5.878534	5.515495
26	H	6.627907	7.212998	6.404220	5.168023	5.311991
27	H	8.016738	8.682951	7.982487	6.786998	6.790799
28	H	8.570124	9.480100	8.937424	7.615488	7.332926
29	C	7.289809	8.157156	7.562492	6.216977	5.990566
30	H	7.332426	8.323294	7.888206	6.553501	6.125179
31	H	8.180777	8.973068	8.280895	6.951512	6.853693
32	H	6.422117	7.209210	6.552167	5.214142	5.087468

	6	7	8	9	10

6	C	0.000000				
7	C	1.538641	0.000000			
8	H	2.855459	3.476682	0.000000		
9	H	4.673341	5.361737	2.754772	0.000000	
10	H	1.090834	2.173208	3.816590	5.315347	0.000000
11	H	1.090613	2.169816	2.669498	4.917530	1.784442
12	H	2.167853	1.096700	3.001518	4.995486	3.070705
13	H	2.160124	1.095704	4.127016	5.524658	2.460268
14	Br	3.850524	4.326657	6.132010	6.492584	3.008580
15	H	2.794233	3.571853	4.246068	4.291881	2.479888
16	C	4.880898	5.619682	4.632281	2.873279	4.986559
17	C	6.028934	6.736373	5.263901	2.895719	6.231984
18	H	5.009415	5.723203	5.332305	3.904173	4.895952
19	H	6.950505	7.637950	6.340311	3.950180	7.056204
20	H	6.251793	6.944163	4.972561	2.313075	6.613625
21	O	2.406070	1.405252	4.485998	6.659435	2.743346
22	H	2.880332	1.960451	5.288235	7.272149	2.871159
23	C	4.973072	4.349917	7.659685	8.980516	4.397042
24	C	5.109907	4.665546	7.896502	9.517128	4.465930
25	O	4.313371	3.525402	6.932540	8.632751	3.933025
26	H	4.518860	4.104750	7.184563	8.248734	3.854429
27	H	5.874605	5.076049	8.447435	9.691668	5.382621
28	H	6.076552	5.531069	8.815837	10.537572	5.486832
29	C	4.783838	4.800261	7.616782	9.229859	3.953671
30	H	4.796285	4.863949	7.517858	9.380029	4.076336
31	H	5.730648	5.841886	8.562883	10.044273	4.817094
32	H	4.005412	4.241881	6.842659	8.281365	3.065554

		11	12	13	14	15
11	H	0.000000				
12	H	2.542011	0.000000			
13	H	3.064291	1.776180	0.000000		
14	Br	4.760584	5.240290	3.744796	0.000000	
15	H	3.712808	4.154847	3.201764	2.200758	0.000000
16	C	5.567938	5.726659	5.313272	4.699497	2.814148
17	C	6.626815	6.699545	6.466668	5.996951	4.138026
18	H	5.806466	6.008020	5.274240	3.979520	2.480015
19	H	7.596967	7.654148	7.276036	6.423036	4.800972
20	H	6.724486	6.752641	6.799942	6.796534	4.781534
21	O	2.612480	2.035433	2.083197	4.960657	4.686012
22	H	3.260738	2.790796	2.186420	4.569589	4.731526
23	C	5.686006	5.284395	3.779052	3.903193	5.296258
24	C	5.582148	5.648075	4.419819	4.526989	5.907022
25	O	4.842160	4.408569	3.261522	4.481867	5.403685
26	H	5.352621	5.078167	3.410978	2.861982	4.370003

27	H	6.618599	5.903522	4.407055	4.689689	6.085662
28	H	6.470526	6.448135	5.325320	5.578948	6.991115
29	C	5.120141	5.858611	4.738672	4.161677	5.562324
30	H	4.899447	5.859166	5.039722	4.935914	6.045779
31	H	6.071738	6.914093	5.716298	4.536242	6.196824
32	H	4.442627	5.333241	4.141539	3.170715	4.526381

		16	17	18	19	20
16	C	0.000000				
17	C	1.326498	0.000000			
18	H	1.082877	2.122826	0.000000		
19	H	2.079783	1.081085	2.446788	0.000000	
20	H	2.126466	1.082574	3.100514	1.847045	0.000000
21	O	6.954609	8.102422	6.991822	8.996334	8.316699
22	H	7.211966	8.424040	7.103300	9.248134	8.749775
23	C	7.935347	9.218423	7.421744	9.776643	9.843561
24	C	8.679233	9.990934	8.214806	10.611606	10.569299
25	O	8.056553	9.327289	7.719983	10.017880	9.815808
26	H	6.985121	8.272162	6.411109	8.785782	8.951644
27	H	8.592180	9.838173	8.054645	10.349468	10.477057
28	H	9.754780	11.062766	9.289230	11.682206	11.632273
29	C	8.374458	9.697335	7.906415	10.322685	10.281052
30	H	8.825194	10.129694	8.462698	10.828135	10.626893
31	H	8.979347	10.302054	8.417374	10.852779	10.952189
32	H	7.329298	8.651404	6.854778	9.267949	9.252265

		21	22	23	24	25
21	O	0.000000				
22	H	0.976799	0.000000			
23	C	3.970882	3.029428	0.000000		
24	C	3.933957	2.985259	1.467826	0.000000	
25	O	2.783579	1.810006	1.450155	1.448375	0.000000
26	H	4.062022	3.232712	1.087134	2.208487	2.145018
27	H	4.697402	3.772282	1.086485	2.216246	2.132802
28	H	4.635994	3.701416	2.191757	1.088720	2.109759
29	C	4.155885	3.374430	2.601609	1.504086	2.520225
30	H	4.013107	3.369437	3.427613	2.149360	2.905913
31	H	5.248441	4.457298	3.166137	2.136050	3.426075
32	H	3.893090	3.220680	2.716275	2.152060	2.742083

		26	27	28	29	30
26	H	0.000000				
27	H	1.852135	0.000000			
28	H	3.120623	2.503816	0.000000		
29	C	2.812381	3.540860	2.208111	0.000000	
30	H	3.741037	4.338524	2.582949	1.094283	0.000000
31	H	3.336182	3.958460	2.531112	1.094362	1.769803

32 H 2.504454 3.771495 3.099581 1.091696 1.787015
31 32
31 H 0.000000
32 H 1.767924 0.000000

Stoichiometry C10H17BrN2O2
Framework group C1[X(C10H17BrN2O2)]
Deg. of freedom 90
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.723931	2.116423	-0.433291
2	6	0	-3.797400	1.347716	-0.118003
3	7	0	-3.324100	0.049686	0.046889
4	6	0	-1.994171	0.044286	-0.168106
5	7	0	-1.614588	1.285625	-0.465453
6	6	0	-0.215306	1.688292	-0.715955
7	6	0	0.463582	2.216054	0.559973
8	1	0	-2.655348	3.169742	-0.644214
9	1	0	-4.833615	1.609075	-0.005276
10	1	0	0.308294	0.805901	-1.086291
11	1	0	-0.221977	2.462699	-1.483865
12	1	0	-0.146241	3.016566	0.995916
13	1	0	0.533046	1.401989	1.290069
14	35	0	0.527873	-2.049213	-0.163435
15	1	0	-1.295649	-0.817988	-0.116655
16	6	0	-4.048793	-1.128443	0.376543
17	6	0	-5.356662	-1.175462	0.593023
18	1	0	-3.406435	-1.998420	0.432563
19	1	0	-5.816149	-2.122819	0.838240
20	1	0	-6.004781	-0.310055	0.538443
21	8	0	1.723135	2.748649	0.236548
22	1	0	2.412314	2.075628	0.398446
23	6	0	3.812322	-0.475541	1.240439
24	6	0	4.549083	0.016909	0.070315
25	8	0	3.728720	0.919089	0.851894
26	1	0	2.899865	-1.045597	1.084502
27	1	0	4.338123	-0.636649	2.177470
28	1	0	5.610346	0.222652	0.199555
29	6	0	4.103730	-0.272714	-1.336829

```
      30        1        0        4.279139       0.593028      -1.982723
      31        1        0        4.678158      -1.113667      -1.737404
      32        1        0        3.046601      -0.543818      -1.364779
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.6034650           0.2206220           0.1724540
 Standard basis: 6-311++G(d,p) (5D, 7F)
 There are     492 symmetry adapted cartesian basis functions of A      symmetry.
 There are     475 symmetry adapted basis functions of A      symmetry.
   475 basis functions,      751 primitive gaussians,      492 cartesian basis functions
    71 alpha electrons              71 beta electrons
         nuclear repulsion energy           1307.6149226731 Hartrees.
 NAtoms=       32 NActive=       32 NUniq=       32 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      475 RedAO= T EigKep=    3.81D-06    NBF=      475
 NBsUse=      475 1.00D-06 EigRej= -1.00D+00 NBFU=      475
 Initial guess from the checkpoint file:    "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"
 B after Tr=          0.000000        0.000000        0.000000
             Rot=        1.000000        0.000877      -0.000187      -0.000023 Ang=      0.10 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn=                5 AccDes=
0.00D+00
 Harris functional with IExCor=    402 and IRadAn=             5 diagonalized for initial guess.
 HarFok:    IExCor=    402 AccDes= 0.00D+00 IRadAn=                5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=    3500011 ScaDFX=    1.000000    1.000000    1.000000    1.000000
 FoFCou: FMM=F IPFlag=                  0 FMFlag=           100000 FMFlg1=                  0
             NFxFlg=                    0 DoJE=T BraDBF=F KetDBF=T FulRan=T
             wScrn=      0.000000 ICntrl=             500 IOpCl=      0 I1Cent=        200000004 NGrid=
0
             NMat0=        1 NMatS0=            1 NMatT0=        0 NMatD0=        1 NMtDS0=        0
NMtDT0=        0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                       energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3225.52368674          A.U. after      10 cycles
                  NFock= 10    Conv=0.72D-08         -V/T= 2.0018
 Calling FoFJK, ICntrl=              2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 ---------------------------------------------------------------------
```

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000114546	-0.000032727	0.000152128
2	6	0.000069722	0.000039185	-0.000127356
3	7	-0.000120780	-0.000022320	0.000097191
4	6	0.000034922	0.000205271	0.000006086
5	7	0.000100252	-0.000207252	-0.000063682
6	6	0.000043554	-0.000107430	-0.000109104
7	6	0.000370946	-0.000206157	0.000032994
8	1	-0.000007127	-0.000018870	0.000008281
9	1	-0.000014140	-0.000002497	-0.000029293
10	1	0.000065710	0.000132729	-0.000028443
11	1	-0.000009125	-0.000054441	0.000036295
12	1	-0.000048990	-0.000001192	-0.000053161
13	1	-0.000083119	0.000056819	-0.000035236
14	35	-0.000019284	-0.000037054	-0.000078432
15	1	0.000048926	0.000160260	0.000121970
16	6	0.000021565	-0.000026465	-0.000018660
17	6	-0.000031486	0.000024802	0.000004133
18	1	0.000007811	0.000015924	-0.000013345
19	1	-0.000008770	0.000016269	-0.000006295
20	1	0.000003219	-0.000016117	-0.000001142
21	8	-0.000385854	-0.000041131	0.000208548
22	1	0.000056026	0.000265683	-0.000349440
23	6	-0.000090390	0.000004111	-0.000103920
24	6	-0.000160234	-0.000026534	0.000185758
25	8	0.000218429	-0.000244040	0.000275385
26	1	-0.000116855	0.000055539	0.000112830
27	1	0.000007351	0.000045453	-0.000048559
28	1	0.000090575	-0.000004031	-0.000125977
29	6	0.000149042	0.000014567	-0.000153588
30	1	-0.000026427	-0.000010653	0.000034908
31	1	0.000012864	0.000027362	0.000025377
32	1	-0.000063785	-0.000005062	0.000043750

Cartesian Forces: Max 0.000385854 RMS 0.000114491

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000300565 RMS 0.000065244

Search for a local minimum.
Step number 27 out of a maximum of 177
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 21 22 23 24 25
26 27
DE= -1.36D-05 DEPred=-8.51D-06 R= 1.59D+00
TightC=F SS= 1.41D+00 RLast= 1.22D-01 DXNew= 3.2661D+00 3.6598D-01
Trust test= 1.59D+00 RLast= 1.22D-01 DXMaxT set to 1.94D+00
ITU= 1 1 1 1 1 1 1 1 1 1 -1 1 1 1 1 1 1 1 1 1
ITU= 1 1 0 1 0 1 0
Eigenvalues --- 0.00006 0.00127 0.00232 0.00262 0.00293
Eigenvalues --- 0.00566 0.00752 0.01037 0.01242 0.01409
Eigenvalues --- 0.01474 0.01773 0.01900 0.01961 0.02100
Eigenvalues --- 0.02182 0.02315 0.02387 0.02758 0.03029
Eigenvalues --- 0.03063 0.03178 0.03423 0.03586 0.04153
Eigenvalues --- 0.04614 0.04993 0.05240 0.05439 0.05666
Eigenvalues --- 0.05930 0.06198 0.07087 0.09405 0.09599
Eigenvalues --- 0.10663 0.11083 0.11536 0.11778 0.13013
Eigenvalues --- 0.14016 0.14335 0.14704 0.15960 0.15992
Eigenvalues --- 0.16000 0.16000 0.16005 0.16020 0.16041
Eigenvalues --- 0.16490 0.17426 0.19104 0.21486 0.22053
Eigenvalues --- 0.22959 0.23706 0.23873 0.24259 0.25078
Eigenvalues --- 0.27670 0.28514 0.30753 0.32293 0.33108
Eigenvalues --- 0.33433 0.34055 0.34402 0.34527 0.34868
Eigenvalues --- 0.35333 0.35685 0.35690 0.35857 0.36243
Eigenvalues --- 0.36441 0.36677 0.37223 0.37275 0.37735
Eigenvalues --- 0.39872 0.42148 0.42857 0.44175 0.46087
Eigenvalues --- 0.49976 0.54146 0.55156 0.60159 0.62129
Eigenvalue 1 is 5.68D-05 Eigenvector:
D52 D55 D53 D54 D46
1 0.51126 -0.49660 -0.49453 -0.48810 -0.03786
D47 D42 D44 D43 R18
1 -0.03329 -0.02790 -0.02768 -0.02665 0.01962
En-DIIS/RFO-DIIS IScMMF= 0 using points: 27 26 25 24 23
RFO step: Lambda=-2.13445150D-06.
DidBck=F Rises=F RFO-DIIS coefs: 2.45207 -1.82210 -0.01280 0.55717 -0.17433
Iteration 1 RMS(Cart)= 0.01333863 RMS(Int)= 0.00033912
Iteration 2 RMS(Cart)= 0.00074269 RMS(Int)= 0.00007131
Iteration 3 RMS(Cart)= 0.00000037 RMS(Int)= 0.00007131
Variable Old X -DE/DX Delta X Delta X Delta X New X
(Linear) (Quad) (Total)

R1	2.56520	-0.00002	-0.00006	0.00005	-0.00002	2.56518
R2	2.61978	0.00007	0.00006	0.00000	0.00006	2.61984
R3	2.03413	0.00002	-0.00001	0.00001	-0.00001	2.03413
R4	2.62943	0.00001	0.00014	-0.00010	0.00003	2.62946
R5	2.03069	0.00002	0.00000	0.00002	0.00002	2.03071
R6	2.54585	0.00011	-0.00006	0.00018	0.00012	2.54597
R7	2.68703	0.00000	0.00004	0.00001	0.00005	2.68708
R8	2.51655	0.00030	-0.00065	0.00040	-0.00030	2.51625
R9	2.09929	0.00008	-0.00106	0.00040	-0.00074	2.09855
R10	2.79199	0.00009	0.00004	0.00017	0.00022	2.79221
R11	2.90761	-0.00003	-0.00029	0.00005	-0.00023	2.90738
R12	2.06138	0.00009	0.00006	0.00010	0.00016	2.06154
R13	2.06096	0.00006	-0.00005	0.00004	-0.00001	2.06095
R14	2.07246	0.00006	-0.00018	0.00002	-0.00017	2.07230
R15	2.07058	0.00007	0.00010	0.00013	0.00023	2.07081
R16	2.65554	-0.00029	-0.00072	0.00002	-0.00070	2.65485
R17	4.15883	-0.00010	0.00087	-0.00001	0.00079	4.15962
R18	8.46950	-0.00005	0.00221	-0.00185	0.00037	8.46988
R19	2.50672	0.00004	-0.00007	0.00006	-0.00001	2.50671
R20	2.04634	0.00001	-0.00002	0.00000	-0.00002	2.04632
R21	2.04295	0.00001	-0.00002	0.00002	0.00000	2.04296
R22	2.04577	0.00001	-0.00002	0.00001	-0.00001	2.04576
R23	1.84588	0.00019	0.00017	0.00006	0.00030	1.84619
R24	3.42042	-0.00004	0.00043	-0.00137	-0.00087	3.41955
R25	2.77379	0.00012	0.00005	-0.00003	0.00005	2.77384
R26	2.74040	0.00004	-0.00051	0.00057	0.00005	2.74044
R27	2.05438	0.00017	-0.00008	0.00022	0.00014	2.05452
R28	2.05316	0.00006	-0.00005	0.00010	0.00006	2.05322
R29	2.73703	-0.00003	-0.00138	0.00009	-0.00131	2.73572
R30	2.05738	0.00012	-0.00002	0.00015	0.00013	2.05751
R31	2.84231	-0.00006	-0.00051	-0.00012	-0.00063	2.84168
R32	2.06790	0.00001	0.00006	-0.00003	0.00003	2.06792
R33	2.06805	0.00004	-0.00002	0.00007	0.00005	2.06810
R34	2.06301	0.00007	0.00006	-0.00004	0.00002	2.06303
A1	1.87426	0.00003	-0.00025	0.00022	-0.00002	1.87423
A2	2.27843	-0.00002	-0.00001	-0.00005	-0.00007	2.27836
A3	2.13045	-0.00001	0.00029	-0.00017	0.00011	2.13056
A4	1.86169	0.00007	0.00010	0.00001	0.00010	1.86179
A5	2.27732	-0.00004	-0.00015	0.00001	-0.00013	2.27718
A6	2.14416	-0.00003	0.00005	-0.00002	0.00004	2.14420
A7	1.89718	0.00001	-0.00019	-0.00004	-0.00024	1.89694
A8	2.24855	-0.00002	0.00020	-0.00009	0.00012	2.24867
A9	2.13744	0.00001	-0.00001	0.00012	0.00012	2.13756
A10	1.88944	-0.00006	0.00012	0.00009	0.00023	1.88967

A11	2.23502	0.00000	0.00007	-0.00010	-0.00001	2.23501
A12	2.15873	0.00005	-0.00020	0.00002	-0.00022	2.15850
A13	1.90218	-0.00005	0.00023	-0.00028	-0.00006	1.90212
A14	2.21238	0.00002	0.00061	-0.00026	0.00033	2.21271
A15	2.16743	0.00003	-0.00066	0.00050	-0.00012	2.16731
A16	1.95063	0.00002	0.00038	-0.00003	0.00036	1.95099
A17	1.86680	0.00000	-0.00055	-0.00015	-0.00066	1.86614
A18	1.88295	0.00001	-0.00028	0.00036	0.00003	1.88298
A19	1.92538	-0.00005	0.00093	-0.00044	0.00048	1.92586
A20	1.92094	-0.00001	-0.00077	0.00004	-0.00072	1.92021
A21	1.91588	0.00004	0.00028	0.00023	0.00052	1.91640
A22	1.91204	0.00003	0.00026	-0.00029	-0.00007	1.91196
A23	1.90254	-0.00001	0.00131	-0.00074	0.00062	1.90315
A24	1.91200	-0.00009	0.00015	0.00064	0.00077	1.91277
A25	1.88882	-0.00004	-0.00039	-0.00028	-0.00068	1.88815
A26	1.88940	0.00004	-0.00192	0.00042	-0.00153	1.88787
A27	1.95856	0.00006	0.00056	0.00023	0.00085	1.95941
A28	1.78894	0.00003	0.00090	0.00116	0.00212	1.79107
A29	2.83800	-0.00011	-0.00135	-0.00177	-0.00315	2.83486
A30	2.17695	0.00000	-0.00018	0.00014	-0.00004	2.17690
A31	1.95554	0.00000	-0.00008	0.00002	-0.00005	1.95548
A32	2.15070	0.00000	0.00026	-0.00016	0.00010	2.15080
A33	2.07960	0.00001	0.00010	0.00002	0.00012	2.07972
A34	2.15761	-0.00002	-0.00011	-0.00002	-0.00013	2.15748
A35	2.04597	0.00001	0.00001	0.00000	0.00001	2.04598
A36	1.91040	0.00006	0.00180	0.00040	0.00280	1.91320
A37	3.04073	0.00020	0.00548	0.00022	0.00534	3.04608
A38	2.07472	0.00005	-0.00085	-0.00026	-0.00119	2.07353
A39	2.08790	-0.00005	0.00020	-0.00043	-0.00014	2.08776
A40	2.00146	0.00008	-0.00075	0.00113	0.00036	2.00182
A41	1.98404	-0.00004	0.00028	0.00035	0.00065	1.98469
A42	2.03996	0.00000	0.00084	-0.00013	0.00072	2.04068
A43	2.04660	-0.00001	-0.00067	0.00007	-0.00065	2.04595
A44	2.13244	-0.00001	0.00066	-0.00035	0.00036	2.13280
A45	1.95018	-0.00007	0.00015	-0.00051	-0.00039	1.94979
A46	2.04550	0.00007	0.00014	0.00080	0.00096	2.04646
A47	2.02203	0.00001	-0.00014	0.00000	-0.00014	2.02189
A48	1.41721	0.00008	0.00127	-0.00041	0.00111	1.41832
A49	1.00622	-0.00020	-0.00347	0.00017	-0.00347	1.00274
A50	2.37974	-0.00013	-0.00691	-0.00205	-0.00889	2.37084
A51	2.31144	0.00006	0.01221	0.00639	0.01861	2.33004
A52	1.93093	0.00005	0.00074	-0.00034	0.00040	1.93133
A53	1.91239	0.00000	-0.00047	0.00048	0.00001	1.91240
A54	1.93745	0.00004	0.00086	-0.00033	0.00053	1.93798

A55	1.88364	-0.00002	-0.00048	0.00026	-0.00022	1.88342
A56	1.91408	-0.00005	-0.00031	0.00004	-0.00027	1.91381
A57	1.88397	-0.00002	-0.00041	-0.00009	-0.00050	1.88347
A58	3.72864	0.00014	0.01349	0.00597	0.01972	3.74836
A59	5.03828	-0.00003	0.00802	0.00184	0.00981	5.04809
D1	0.00592	-0.00008	-0.00049	-0.00007	-0.00056	0.00536
D2	-3.12934	-0.00005	-0.00195	0.00010	-0.00186	-3.13119
D3	3.13643	-0.00001	0.00183	-0.00015	0.00168	3.13812
D4	0.00118	0.00003	0.00037	0.00002	0.00038	0.00157
D5	-0.00823	0.00008	0.00088	-0.00003	0.00084	-0.00739
D6	-3.09875	0.00008	-0.00305	0.00073	-0.00233	-3.10109
D7	-3.13990	0.00002	-0.00120	0.00004	-0.00116	-3.14106
D8	0.05277	0.00001	-0.00513	0.00079	-0.00434	0.04843
D9	-0.00167	0.00005	-0.00006	0.00015	0.00009	-0.00158
D10	-3.13671	0.00003	0.00075	-0.00001	0.00073	-3.13597
D11	3.13418	0.00002	0.00127	0.00000	0.00127	3.13545
D12	-0.00086	0.00001	0.00207	-0.00016	0.00191	0.00105
D13	-0.00345	0.00000	0.00060	-0.00017	0.00043	-0.00301
D14	3.13682	0.00002	0.00400	0.00031	0.00429	3.14112
D15	3.13209	0.00001	-0.00014	-0.00002	-0.00016	3.13193
D16	-0.01082	0.00004	0.00325	0.00046	0.00370	-0.00712
D17	-0.00347	0.00002	0.00166	0.00024	0.00190	-0.00157
D18	3.13792	0.00002	0.00141	0.00012	0.00153	3.13945
D19	-3.13770	0.00000	0.00256	0.00006	0.00263	-3.13508
D20	0.00368	0.00000	0.00232	-0.00006	0.00226	0.00594
D21	0.00719	-0.00005	-0.00091	0.00013	-0.00079	0.00640
D22	3.09932	-0.00005	0.00294	-0.00063	0.00230	3.10163
D23	-3.13315	-0.00007	-0.00412	-0.00033	-0.00444	-3.13759
D24	-0.04102	-0.00007	-0.00027	-0.00109	-0.00135	-0.04237
D25	-3.12103	-0.00005	-0.01188	-0.00291	-0.01480	-3.13583
D26	0.01905	-0.00002	-0.00801	-0.00235	-0.01039	0.00866
D27	1.44465	-0.00002	-0.00230	-0.00235	-0.00466	1.43999
D28	-2.72954	-0.00008	-0.00129	-0.00300	-0.00428	-2.73382
D29	-0.66942	-0.00003	-0.00139	-0.00263	-0.00401	-0.67343
D30	-1.63856	-0.00002	-0.00683	-0.00146	-0.00829	-1.64685
D31	0.47044	-0.00008	-0.00582	-0.00211	-0.00791	0.46253
D32	2.53056	-0.00003	-0.00592	-0.00173	-0.00764	2.52292
D33	-0.93575	-0.00001	0.00027	-0.00036	-0.00005	-0.93580
D34	1.12808	-0.00004	0.00072	-0.00131	-0.00055	1.12753
D35	-3.00589	-0.00003	0.00237	-0.00109	0.00140	-3.00449
D36	-3.01031	0.00002	0.00011	0.00013	0.00023	-3.01008
D37	-0.94649	-0.00002	0.00056	-0.00082	-0.00027	-0.94676
D38	1.20274	0.00000	0.00220	-0.00060	0.00167	1.20441
D39	1.15614	0.00001	-0.00035	0.00010	-0.00026	1.15588

D40	-3.06322	-0.00003	0.00010	-0.00085	-0.00076	-3.06398
D41	-0.91400	-0.00001	0.00175	-0.00063	0.00119	-0.91281
D42	-1.68466	0.00001	0.01460	0.00665	0.02114	-1.66352
D43	2.51441	-0.00001	0.01534	0.00638	0.02169	2.53610
D44	0.43107	-0.00002	0.01674	0.00631	0.02302	0.45409
D45	0.46379	-0.00002	-0.00017	0.00083	0.00060	0.46439
D46	-0.30017	0.00011	0.01554	0.00463	0.02011	-0.28006
D47	2.57500	0.00004	0.00080	-0.00106	-0.00041	2.57459
D48	3.14131	0.00000	-0.00008	-0.00006	-0.00014	3.14117
D49	0.00010	0.00001	0.00013	-0.00006	0.00007	0.00017
D50	-0.00005	0.00000	0.00020	0.00007	0.00027	0.00022
D51	-3.14126	0.00000	0.00041	0.00008	0.00048	-3.14078
D52	-1.78990	0.00005	-0.07200	-0.04547	-0.11754	-1.90743
D53	2.31084	0.00001	0.06359	0.04200	0.10549	2.41633
D54	1.98276	0.00001	0.04834	0.03559	0.08406	2.06682
D55	-2.72744	0.00004	0.05558	0.04015	0.09568	-2.63176
D56	-2.72898	-0.00004	-0.00020	0.00091	0.00073	-2.72825
D57	-0.02953	-0.00004	-0.00065	0.00022	-0.00042	-0.02995
D58	-0.02071	-0.00004	0.00051	-0.00118	-0.00065	-0.02136
D59	2.67874	-0.00005	0.00005	-0.00188	-0.00180	2.67694
D60	-0.17587	0.00006	-0.00030	0.00236	0.00202	-0.17384
D61	0.21061	0.00012	0.01883	0.00995	0.02873	0.23933
D62	-2.58684	0.00003	-0.00111	0.00083	-0.00031	-2.58715
D63	-2.20036	0.00008	0.01802	0.00842	0.02639	-2.17398
D64	2.13750	0.00011	0.00982	0.00250	0.01225	2.14975
D65	-0.25559	0.00010	0.00972	0.00220	0.01185	-0.24374
D66	2.48779	0.00001	0.00125	-0.00186	-0.00060	2.48719
D67	-1.72063	0.00002	0.00083	-0.00145	-0.00061	-1.72125
D68	0.35856	0.00001	0.00056	-0.00146	-0.00089	0.35767
D69	1.27257	-0.00002	0.00091	-0.00241	-0.00151	1.27106
D70	-2.93585	-0.00001	0.00048	-0.00200	-0.00152	-2.93737
D71	-0.85666	-0.00002	0.00021	-0.00201	-0.00180	-0.85846
D72	-1.09018	0.00000	0.00068	-0.00253	-0.00185	-1.09203
D73	0.98459	0.00001	0.00025	-0.00212	-0.00187	0.98272
D74	3.06378	0.00000	-0.00002	-0.00213	-0.00215	3.06163

Item	Value	Threshold	Converged?
Maximum Force	0.000301	0.000450	YES
RMS Force	0.000065	0.000300	YES
Maximum Displacement	0.056894	0.001800	NO
RMS Displacement	0.014070	0.001200	NO

Predicted change in Energy=-7.048458D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.381755	-1.917098	-0.243295
2	6	0	-2.513006	-1.176107	-0.125682
3	7	0	-2.113589	0.108651	0.229269
4	6	0	-0.769824	0.132380	0.323402
5	7	0	-0.310325	-1.086105	0.045639
6	6	0	1.122976	-1.442070	-0.000780
7	6	0	1.687625	-1.352170	-1.429113
8	1	0	-1.248146	-2.954431	-0.497768
9	1	0	-3.543530	-1.450630	-0.257729
10	1	0	1.644508	-0.746024	0.657722
11	1	0	1.228021	-2.459039	0.378911
12	1	0	1.069808	-1.953909	-2.106439
13	1	0	1.647132	-0.309756	-1.764628
14	35	0	1.652778	2.228503	1.013565
15	1	0	-0.117027	0.991631	0.585637
16	6	0	-2.916716	1.255329	0.478327
17	6	0	-4.240978	1.280657	0.405733
18	1	0	-2.320005	2.120613	0.738757
19	1	0	-4.762380	2.204448	0.614296
20	1	0	-4.843574	0.419399	0.146756
21	8	0	2.993935	-1.868598	-1.452671
22	1	0	3.636805	-1.139129	-1.357567
23	6	0	4.853584	1.619285	-1.126976
24	6	0	5.716951	0.750247	-0.318294
25	8	0	4.869037	0.185994	-1.347100
26	1	0	3.935675	2.001428	-0.687167
27	1	0	5.282706	2.191627	-1.944774
28	1	0	6.769668	0.700369	-0.591710
29	6	0	5.393001	0.402526	1.108388
30	1	0	5.664867	-0.635290	1.324066
31	1	0	5.965680	1.047449	1.782036
32	1	0	4.332564	0.555433	1.317947

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357435	0.000000			
3	N	2.205121	1.391449	0.000000		
4	C	2.212683	2.225421	1.347267	0.000000	
5	N	1.386360	2.211166	2.170927	1.331540	0.000000

6	C	2.560887	3.647835	3.596250	2.483280	1.477571
7	C	3.338622	4.401730	4.396982	3.363666	2.497496
8	H	1.076414	2.213765	3.264973	3.229786	2.159963
9	H	2.211577	1.074606	2.171003	3.246086	3.267801
10	H	3.367717	4.252484	3.877801	2.590823	2.076457
11	H	2.737110	3.986955	4.216845	3.272601	2.088666
12	H	3.079418	4.167124	4.454627	3.693369	2.699868
13	H	3.751287	4.554498	4.277115	3.224442	2.776945
14	Br	5.289054	5.499364	4.392540	3.277050	3.972063
15	H	3.278318	3.308440	2.211993	1.110506	2.155446
16	C	3.597379	2.537655	1.421940	2.427789	3.530270
17	C	4.338437	3.050243	2.435266	3.657079	4.602311
18	H	4.260029	3.413630	2.085707	2.555123	3.847372
19	H	5.399188	4.127398	3.399515	4.507615	5.565241
20	H	4.194706	2.837502	2.748853	4.087668	4.777774
21	O	4.540000	5.706736	5.729332	4.617817	3.711518
22	H	5.199305	6.272087	6.094426	4.884749	4.189467
23	C	7.222627	7.942509	7.256922	5.994764	5.946437
24	C	7.583665	8.454592	7.875838	6.547655	6.311315
25	O	6.686836	7.605376	7.158770	5.881344	5.512146
26	H	6.620191	7.210928	6.404378	5.162976	5.300791
27	H	8.011972	8.684691	7.985639	6.783675	6.781392
28	H	8.568443	9.481897	8.940715	7.616034	7.329666
29	C	7.287319	8.155977	7.563604	6.218489	5.989440
30	H	7.331749	8.322972	7.890273	6.557126	6.127033
31	H	8.177732	8.970602	8.280520	6.952121	6.852399
32	H	6.419059	7.207227	6.552688	5.215597	5.086239

		6	7	8	9	10
6	C	0.000000				
7	C	1.538520	0.000000			
8	H	2.855951	3.471800	0.000000		
9	H	4.673582	5.361605	2.754601	0.000000	
10	H	1.090918	2.173511	3.818333	5.315097	0.000000
11	H	1.090609	2.169181	2.673085	4.918322	1.784831
12	H	2.167627	1.096612	2.993622	4.995388	3.070806
13	H	2.160563	1.095827	4.120907	5.524066	2.461324
14	Br	3.844827	4.334640	6.128808	6.492597	2.995747
15	H	2.793634	3.579020	4.245539	4.291483	2.475408
16	C	4.881047	5.624707	4.632383	2.873480	4.984211
17	C	6.029138	6.741422	5.263966	2.895953	6.229758
18	H	5.009366	5.728959	5.332349	3.904327	4.893009
19	H	6.950743	7.643796	6.340392	3.950395	7.053750
20	H	6.251925	6.948265	4.972449	2.313165	6.611696
21	O	2.406325	1.404884	4.481754	6.658906	2.744974

22	H	2.872626	1.962093	5.281791	7.270755	2.860973
23	C	4.955567	4.352485	7.651528	8.982844	4.367837
24	C	5.100164	4.678626	7.891098	9.518615	4.447046
25	O	4.300714	3.534693	6.928460	8.639244	3.909674
26	H	4.498898	4.104977	7.174149	8.248614	3.821867
27	H	5.855444	5.074348	8.439654	9.696112	5.351566
28	H	6.068308	5.544485	8.812021	10.540416	5.469953
29	C	4.781830	4.821585	7.612735	9.228329	3.946323
30	H	4.799467	4.890028	7.515800	9.378776	4.076710
31	H	5.729565	5.862713	8.558729	10.041221	4.811772
32	H	4.003812	4.263916	6.838149	8.278882	3.058648

		11	12	13	14	15
11	H	0.000000				
12	H	2.541093	0.000000			
13	H	3.064284	1.775775	0.000000		
14	Br	4.749343	5.250414	3.763130	0.000000	
15	H	3.709314	4.163178	3.213971	2.201178	0.000000
16	C	5.566440	5.733462	5.320624	4.702533	2.814127
17	C	6.625406	6.706554	6.473772	6.000353	4.137980
18	H	5.804411	6.015621	5.283163	3.983738	2.480153
19	H	7.595290	7.662163	7.284391	6.427616	4.801151
20	H	6.723360	6.758518	6.805463	6.799030	4.781246
21	O	2.611852	2.033951	2.083551	4.966615	4.691875
22	H	3.249578	2.795380	2.193708	4.571605	4.733649
23	C	5.660842	5.295661	3.795936	3.898490	5.294711
24	C	5.562024	5.666203	4.447349	4.525107	5.908524
25	O	4.819991	4.426050	3.286452	4.482065	5.407898
26	H	5.325757	5.086474	3.426357	2.855814	4.366247
27	H	6.593079	5.912708	4.416647	4.682895	6.082769
28	H	6.452427	6.467457	5.351304	5.576259	6.992678
29	C	5.105659	5.880298	4.774212	4.163227	5.566033
30	H	4.889273	5.884020	5.078208	4.939087	6.051648
31	H	6.058848	6.935269	5.750712	4.537242	6.199501
32	H	4.427981	5.354324	4.178799	3.173809	4.530497

		16	17	18	19	20
16	C	0.000000				
17	C	1.326493	0.000000			
18	H	1.082868	2.122868	0.000000		
19	H	2.079854	1.081087	2.446980	0.000000	
20	H	2.126383	1.082569	3.100483	1.847048	0.000000
21	O	6.958697	8.106506	6.996722	9.001249	8.319835
22	H	7.214746	8.427577	7.106622	9.252786	8.752647
23	C	7.942734	9.229026	7.429177	9.789852	9.853781
24	C	8.685040	9.998295	8.221188	10.620772	10.575936

25	O	8.068061	9.341472	7.731487	10.034213	9.829594
26	H	6.990730	8.280798	6.417243	8.797227	8.959546
27	H	8.601081	9.851665	8.062729	10.365942	10.490798
28	H	9.761095	11.070951	9.295665	11.692084	11.640089
29	C	8.377091	9.699402	7.910684	10.325833	10.281659
30	H	8.827983	10.131138	8.467336	10.830299	10.626654
31	H	8.979968	10.301673	8.419780	10.853273	10.950277
32	H	7.331226	8.652382	6.858711	9.269972	9.251578

		21	22	23	24	25
21	O	0.000000				
22	H	0.976960	0.000000			
23	C	3.966069	3.023669	0.000000		
24	C	3.944614	2.996137	1.467854	0.000000	
25	O	2.783613	1.809546	1.450179	1.447681	0.000000
26	H	4.055857	3.225191	1.087208	2.207819	2.145339
27	H	4.686797	3.761348	1.086515	2.216209	2.133284
28	H	4.647257	3.712832	2.191414	1.088787	2.108932
29	C	4.180018	3.397332	2.601601	1.503754	2.520089
30	H	4.045392	3.399713	3.427666	2.149366	2.905681
31	H	5.272374	4.479050	3.166402	2.135786	3.425817
32	H	3.917164	3.242529	2.716779	2.152154	2.743495

		26	27	28	29	30
26	H	0.000000				
27	H	1.852631	0.000000			
28	H	3.119837	2.503136	0.000000		
29	C	2.811460	3.540459	2.207771	0.000000	
30	H	3.739979	4.338528	2.583557	1.094299	0.000000
31	H	3.335860	3.957867	2.530124	1.094389	1.769699
32	H	2.503778	3.771638	3.099560	1.091707	1.786866

		31	32
31	H	0.000000	
32	H	1.767634	0.000000

Stoichiometry C10H17BrN2O2
Framework group C1[X(C10H17BrN2O2)]
Deg. of freedom 90
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.720001	2.114328	-0.441343

2	6	0	-3.796522	1.347637	-0.131639
3	7	0	-3.325636	0.049878	0.042196
4	6	0	-1.993958	0.042900	-0.162041
5	7	0	-1.610928	1.282716	-0.460608
6	6	0	-0.209457	1.682608	-0.703881
7	6	0	0.459392	2.224014	0.571487
8	1	0	-2.648830	3.167019	-0.654519
9	1	0	-4.833238	1.610509	-0.027254
10	1	0	0.316380	0.795907	-1.060753
11	1	0	-0.209694	2.449217	-1.479599
12	1	0	-0.153648	3.029256	0.993772
13	1	0	0.522679	1.418374	1.311607
14	35	0	0.527833	-2.049815	-0.148799
15	1	0	-1.297201	-0.819961	-0.105256
16	6	0	-4.053921	-1.126611	0.369895
17	6	0	-5.363952	-1.172370	0.573137
18	1	0	-3.412357	-1.996440	0.436197
19	1	0	-5.826298	-2.118449	0.817924
20	1	0	-6.011164	-0.307039	0.507755
21	8	0	1.720643	2.754656	0.253108
22	1	0	2.409312	2.079275	0.408180
23	6	0	3.814935	-0.469258	1.227798
24	6	0	4.550111	0.013508	0.052618
25	8	0	3.735797	0.923196	0.830526
26	1	0	2.900425	-1.037438	1.076587
27	1	0	4.343109	-0.627204	2.164068
28	1	0	5.612500	0.215985	0.178276
29	6	0	4.100988	-0.283791	-1.351369
30	1	0	4.276593	0.577348	-2.003360
31	1	0	4.672708	-1.128452	-1.748070
32	1	0	3.043313	-0.553145	-1.375748

Rotational constants (GHZ): 0.6037391 0.2205392 0.1722998

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.

475 basis functions, 751 primitive gaussians, 492 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1307.5034848630 Hartrees.

NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.
NBasis= 475 RedAO= T EigKep= 3.82D-06 NBF= 475
NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999999 0.000991 0.000040 0.000146 Ang= 0.11 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3225.52370069 A.U. after 10 cycles
NFock= 10 Conv=0.81D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000091248	0.000002452	0.000002362
2	6	0.000037570	0.000046264	-0.000155115
3	7	-0.000073080	-0.000074437	0.000101801
4	6	-0.000129206	0.000241348	0.000035338
5	7	0.000137762	-0.000305953	0.000044393
6	6	-0.000051612	-0.000130997	-0.000061580
7	6	0.000305891	-0.000129777	-0.000044596
8	1	-0.000006123	-0.000029834	0.000048652
9	1	-0.000014921	-0.000005777	-0.000003229
10	1	0.000081862	0.000113182	-0.000022316
11	1	-0.000007833	-0.000047731	0.000074757
12	1	-0.000038997	0.000001741	-0.000060972
13	1	-0.000057232	0.000073588	0.000001710

14	35	-0.000014393	-0.000022008	-0.000045625
15	1	0.000138794	0.000281854	0.000071490
16	6	0.000044443	-0.000063179	-0.000008996
17	6	-0.000033168	0.000023168	0.000002222
18	1	-0.000001305	0.000020787	-0.000008677
19	1	-0.000002359	0.000016946	-0.000008958
20	1	-0.000002682	-0.000014368	-0.000004959
21	8	-0.000194523	-0.000117899	0.000093830
22	1	-0.000011429	0.000177513	-0.000169654
23	6	0.000001423	0.000082069	0.000033553
24	6	0.000127670	0.000066007	0.000133959
25	8	-0.000076263	-0.000207117	0.000033398
26	1	-0.000121880	0.000052073	-0.000027144
27	1	-0.000042233	0.000009969	-0.000051860
28	1	0.000086105	-0.000031536	-0.000075629
29	6	0.000073635	-0.000041177	0.000080953
30	1	-0.000015110	-0.000008298	0.000000137
31	1	0.000021796	0.000028535	-0.000000380
32	1	-0.000071354	-0.000007408	-0.000008866

Cartesian Forces: Max 0.000305953 RMS 0.000092395

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000391762 RMS 0.000060208
Search for a local minimum.
Step number 28 out of a maximum of 177
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 24 25 26 27 28
DE= -1.39D-05 DEPred=-7.05D-06 R= 1.98D+00
TightC=F SS= 1.41D+00 RLast= 2.16D-01 DXNew= 3.2661D+00 6.4724D-01
Trust test= 1.98D+00 RLast= 2.16D-01 DXMaxT set to 1.94D+00
ITU= 1 1 1 1 1 1 1 1 1 1 1 -1 1 1 1 1 1 1 1 1
ITU= 1 1 1 0 1 0 1 0
Eigenvalues --- 0.00004 0.00118 0.00233 0.00249 0.00283
Eigenvalues --- 0.00519 0.00675 0.01076 0.01258 0.01410
Eigenvalues --- 0.01510 0.01736 0.01903 0.01965 0.02102
Eigenvalues --- 0.02182 0.02316 0.02388 0.02532 0.02974
Eigenvalues --- 0.03063 0.03083 0.03448 0.03579 0.04093

Eigenvalues --- 0.04614 0.04986 0.05223 0.05434 0.05661
Eigenvalues --- 0.05919 0.05994 0.06890 0.09370 0.09688
Eigenvalues --- 0.10632 0.11079 0.11524 0.11758 0.13124
Eigenvalues --- 0.14039 0.14293 0.15126 0.15971 0.15991
Eigenvalues --- 0.16000 0.16002 0.16010 0.16013 0.16049
Eigenvalues --- 0.16484 0.17261 0.19321 0.21645 0.22059
Eigenvalues --- 0.22960 0.23657 0.24047 0.24210 0.25057
Eigenvalues --- 0.27666 0.28527 0.30887 0.32526 0.33109
Eigenvalues --- 0.33492 0.34054 0.34342 0.34491 0.34861
Eigenvalues --- 0.35198 0.35685 0.35690 0.35857 0.36222
Eigenvalues --- 0.36439 0.36674 0.37229 0.37268 0.37780
Eigenvalues --- 0.40470 0.42148 0.43264 0.43924 0.45994
Eigenvalues --- 0.49910 0.54040 0.55101 0.60026 0.61299
Eigenvalue 1 is 4.20D-05 Eigenvector:

	D52	D55	D53	D54	D46
1	0.50737	-0.49782	-0.49598	-0.49102	-0.03436
	D47	D44	D42	D43	D39
1	-0.03010	-0.02326	-0.02324	-0.02204	0.01585

En-DIIS/RFO-DIIS IScMMF= 0 using points: 28 27 26 25 24
RFO step: Lambda=-1.26837109D-06.
DidBck=F Rises=F RFO-DIIS coefs: 1.92089 -1.20917 -0.17500 0.72262 -0.25934
Iteration 1 RMS(Cart)= 0.00718794 RMS(Int)= 0.00013352
Iteration 2 RMS(Cart)= 0.00023873 RMS(Int)= 0.00002731
Iteration 3 RMS(Cart)= 0.00000005 RMS(Int)= 0.00002731

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56518	-0.00002	-0.00009	-0.00004	-0.00013	2.56505
R2	2.61984	0.00006	0.00015	0.00002	0.00016	2.62001
R3	2.03413	0.00002	0.00002	0.00002	0.00004	2.03417
R4	2.62946	0.00001	-0.00005	0.00001	-0.00005	2.62941
R5	2.03071	0.00002	0.00004	0.00000	0.00004	2.03075
R6	2.54597	0.00008	0.00020	0.00001	0.00021	2.54618
R7	2.68708	-0.00003	-0.00007	-0.00005	-0.00011	2.68696
R8	2.51625	0.00039	0.00039	0.00027	0.00064	2.51688
R9	2.09855	0.00023	0.00053	0.00029	0.00079	2.09934
R10	2.79221	0.00006	0.00022	-0.00015	0.00007	2.79227
R11	2.90738	0.00007	0.00022	0.00023	0.00044	2.90783
R12	2.06154	0.00009	0.00025	0.00009	0.00033	2.06187
R13	2.06095	0.00007	0.00008	0.00008	0.00016	2.06111
R14	2.07230	0.00006	0.00008	-0.00001	0.00007	2.07236
R15	2.07081	0.00008	0.00032	0.00011	0.00043	2.07124
R16	2.65485	-0.00020	-0.00077	-0.00033	-0.00109	2.65375
R17	4.15962	-0.00008	-0.00126	-0.00126	-0.00254	4.15708

R18	8.46988	-0.00002	-0.00214	-0.00005	-0.00218	8.46769
R19	2.50671	0.00004	0.00004	0.00002	0.00007	2.50677
R20	2.04632	0.00001	0.00001	0.00000	0.00001	2.04634
R21	2.04296	0.00001	0.00001	0.00001	0.00002	2.04298
R22	2.04576	0.00002	0.00002	0.00001	0.00003	2.04579
R23	1.84619	0.00013	0.00043	-0.00003	0.00042	1.84661
R24	3.41955	0.00000	-0.00266	0.00122	-0.00142	3.41813
R25	2.77384	0.00016	0.00009	0.00026	0.00037	2.77421
R26	2.74044	0.00008	0.00045	-0.00013	0.00032	2.74076
R27	2.05452	0.00011	0.00017	0.00011	0.00028	2.05480
R28	2.05322	0.00003	-0.00001	0.00008	0.00007	2.05329
R29	2.73572	0.00014	-0.00007	0.00021	0.00014	2.73586
R30	2.05751	0.00010	0.00020	0.00005	0.00025	2.05776
R31	2.84168	0.00008	-0.00001	0.00008	0.00008	2.84176
R32	2.06792	0.00001	-0.00005	0.00004	-0.00001	2.06791
R33	2.06810	0.00003	0.00005	0.00000	0.00005	2.06815
R34	2.06303	0.00007	0.00009	0.00006	0.00015	2.06318
A1	1.87423	0.00003	0.00011	-0.00003	0.00008	1.87431
A2	2.27836	-0.00002	-0.00006	-0.00002	-0.00008	2.27828
A3	2.13056	-0.00001	-0.00004	0.00004	0.00000	2.13056
A4	1.86179	0.00006	0.00005	0.00001	0.00007	1.86185
A5	2.27718	-0.00003	-0.00010	0.00000	-0.00010	2.27708
A6	2.14420	-0.00002	0.00004	-0.00001	0.00003	2.14423
A7	1.89694	0.00006	0.00006	0.00013	0.00019	1.89713
A8	2.24867	-0.00005	-0.00010	-0.00012	-0.00022	2.24845
A9	2.13756	-0.00001	0.00004	-0.00001	0.00003	2.13759
A10	1.88967	-0.00011	-0.00010	-0.00020	-0.00029	1.88938
A11	2.23501	0.00005	0.00001	0.00014	0.00017	2.23518
A12	2.15850	0.00006	0.00008	0.00006	0.00012	2.15862
A13	1.90212	-0.00004	-0.00012	0.00008	-0.00003	1.90208
A14	2.21271	-0.00003	-0.00005	-0.00032	-0.00036	2.21235
A15	2.16731	0.00007	0.00014	0.00020	0.00035	2.16766
A16	1.95099	0.00000	0.00037	-0.00025	0.00011	1.95110
A17	1.86614	0.00003	-0.00047	0.00012	-0.00034	1.86580
A18	1.88298	-0.00001	0.00032	-0.00019	0.00013	1.88312
A19	1.92586	-0.00008	-0.00067	-0.00009	-0.00075	1.92512
A20	1.92021	0.00005	0.00003	0.00043	0.00045	1.92066
A21	1.91640	0.00002	0.00044	-0.00003	0.00040	1.91680
A22	1.91196	0.00005	0.00021	0.00031	0.00049	1.91246
A23	1.90315	-0.00005	-0.00049	-0.00004	-0.00049	1.90266
A24	1.91277	-0.00005	0.00041	0.00006	0.00047	1.91324
A25	1.88815	-0.00002	-0.00073	-0.00002	-0.00075	1.88740
A26	1.88787	0.00002	0.00001	-0.00056	-0.00055	1.88732
A27	1.95941	0.00005	0.00057	0.00025	0.00083	1.96023

A28	1.79107	0.00000	0.00037	0.00044	0.00087	1.79193
A29	2.83486	-0.00011	-0.00149	-0.00100	-0.00252	2.83234
A30	2.17690	0.00001	0.00005	0.00003	0.00007	2.17698
A31	1.95548	0.00001	0.00000	0.00006	0.00007	1.95555
A32	2.15080	-0.00002	-0.00005	-0.00009	-0.00014	2.15065
A33	2.07972	0.00000	0.00008	-0.00003	0.00005	2.07977
A34	2.15748	-0.00001	-0.00013	0.00002	-0.00011	2.15737
A35	2.04598	0.00001	0.00005	0.00001	0.00006	2.04605
A36	1.91320	-0.00006	0.00133	-0.00064	0.00085	1.91405
A37	3.04608	0.00003	0.00327	-0.00005	0.00302	3.04910
A38	2.07353	0.00007	-0.00030	0.00065	0.00033	2.07386
A39	2.08776	-0.00002	0.00019	0.00011	0.00032	2.08808
A40	2.00182	0.00002	0.00008	-0.00033	-0.00025	2.00156
A41	1.98469	-0.00003	0.00030	-0.00036	-0.00005	1.98464
A42	2.04068	-0.00004	-0.00005	-0.00027	-0.00032	2.04036
A43	2.04595	-0.00001	-0.00018	-0.00008	-0.00028	2.04567
A44	2.13280	0.00002	0.00021	0.00016	0.00040	2.13320
A45	1.94979	-0.00002	-0.00049	-0.00020	-0.00070	1.94909
A46	2.04646	0.00003	0.00055	-0.00043	0.00013	2.04659
A47	2.02189	0.00000	-0.00012	0.00027	0.00015	2.02203
A48	1.41832	0.00011	0.00114	0.00050	0.00174	1.42006
A49	1.00274	-0.00015	-0.00319	0.00026	-0.00301	0.99973
A50	2.37084	-0.00004	-0.00501	-0.00059	-0.00559	2.36526
A51	2.33004	0.00004	0.01003	0.00301	0.01302	2.34306
A52	1.93133	0.00001	-0.00010	0.00025	0.00016	1.93148
A53	1.91240	-0.00002	-0.00002	-0.00013	-0.00015	1.91225
A54	1.93798	-0.00002	-0.00023	0.00010	-0.00013	1.93785
A55	1.88342	0.00001	0.00032	-0.00012	0.00021	1.88363
A56	1.91381	-0.00001	0.00005	-0.00025	-0.00020	1.91360
A57	1.88347	0.00002	-0.00001	0.00014	0.00013	1.88360
A58	3.74836	0.00015	0.01117	0.00351	0.01476	3.76312
A59	5.04809	-0.00006	0.00309	0.00184	0.00493	5.05301
D1	0.00536	-0.00006	-0.00149	0.00057	-0.00093	0.00443
D2	-3.13119	-0.00001	-0.00088	0.00048	-0.00039	-3.13159
D3	3.13812	-0.00003	-0.00025	-0.00026	-0.00051	3.13761
D4	0.00157	0.00001	0.00036	-0.00034	0.00002	0.00159
D5	-0.00739	0.00004	0.00070	-0.00009	0.00062	-0.00678
D6	-3.10109	0.00006	0.00099	0.00070	0.00169	-3.09940
D7	-3.14106	0.00002	-0.00041	0.00065	0.00024	-3.14082
D8	0.04843	0.00004	-0.00012	0.00144	0.00132	0.04975
D9	-0.00158	0.00005	0.00178	-0.00085	0.00093	-0.00065
D10	-3.13597	0.00003	0.00083	-0.00059	0.00025	-3.13572
D11	3.13545	0.00002	0.00122	-0.00077	0.00045	3.13589
D12	0.00105	-0.00001	0.00028	-0.00051	-0.00023	0.00082

D13	-0.00301	-0.00003	-0.00136	0.00080	-0.00056	-0.00357
D14	3.14112	-0.00003	0.00095	-0.00058	0.00039	3.14150
D15	3.13193	0.00000	-0.00049	0.00056	0.00007	3.13200
D16	-0.00712	0.00000	0.00182	-0.00082	0.00102	-0.00611
D17	-0.00157	0.00002	0.00161	-0.00011	0.00150	-0.00007
D18	3.13945	0.00002	0.00166	-0.00023	0.00143	3.14087
D19	-3.13508	-0.00002	0.00055	0.00019	0.00074	-3.13434
D20	0.00594	-0.00001	0.00060	0.00006	0.00066	0.00660
D21	0.00640	-0.00001	0.00042	-0.00044	-0.00003	0.00637
D22	3.10163	-0.00003	0.00013	-0.00123	-0.00110	3.10053
D23	-3.13759	-0.00001	-0.00177	0.00086	-0.00092	-3.13851
D24	-0.04237	-0.00003	-0.00206	0.00008	-0.00199	-0.04436
D25	-3.13583	-0.00001	-0.00570	0.00052	-0.00518	-3.14102
D26	0.00866	-0.00001	-0.00306	-0.00106	-0.00411	0.00455
D27	1.43999	0.00001	-0.00583	-0.00210	-0.00796	1.43203
D28	-2.73382	-0.00007	-0.00674	-0.00229	-0.00903	-2.74285
D29	-0.67343	-0.00004	-0.00631	-0.00236	-0.00867	-0.68210
D30	-1.64685	0.00003	-0.00549	-0.00119	-0.00671	-1.65357
D31	0.46253	-0.00005	-0.00640	-0.00138	-0.00779	0.45473
D32	2.52292	-0.00002	-0.00597	-0.00145	-0.00743	2.51549
D33	-0.93580	0.00000	-0.00202	0.00109	-0.00092	-0.93672
D34	1.12753	-0.00002	-0.00306	0.00122	-0.00183	1.12569
D35	-3.00449	-0.00003	-0.00240	0.00155	-0.00083	-3.00531
D36	-3.01008	0.00002	-0.00123	0.00117	-0.00007	-3.01015
D37	-0.94676	-0.00001	-0.00227	0.00130	-0.00098	-0.94774
D38	1.20441	-0.00001	-0.00161	0.00162	0.00003	1.20444
D39	1.15588	0.00002	-0.00136	0.00099	-0.00038	1.15550
D40	-3.06398	-0.00001	-0.00240	0.00112	-0.00129	-3.06527
D41	-0.91281	-0.00001	-0.00174	0.00144	-0.00028	-0.91309
D42	-1.66352	0.00003	0.01088	0.00279	0.01359	-1.64993
D43	2.53610	-0.00002	0.01038	0.00270	0.01305	2.54915
D44	0.45409	-0.00003	0.01094	0.00294	0.01384	0.46793
D45	0.46439	-0.00001	0.00012	-0.00007	0.00007	0.46447
D46	-0.28006	0.00002	0.00840	0.00169	0.01008	-0.26998
D47	2.57459	0.00000	-0.00077	-0.00214	-0.00288	2.57172
D48	3.14117	0.00001	0.00021	-0.00011	0.00010	3.14128
D49	0.00017	0.00000	0.00019	-0.00008	0.00011	0.00028
D50	0.00022	0.00000	0.00016	0.00003	0.00018	0.00041
D51	-3.14078	0.00000	0.00013	0.00005	0.00019	-3.14059
D52	-1.90743	0.00002	-0.07943	-0.00337	-0.08286	-1.99029
D53	2.41633	-0.00002	0.07607	0.00151	0.07756	2.49389
D54	2.06682	0.00001	0.06752	-0.00306	0.06445	2.13127
D55	-2.63176	0.00004	0.07298	-0.00033	0.07263	-2.55912
D56	-2.72825	-0.00004	-0.00025	-0.00097	-0.00121	-2.72947

D57	-0.02995	-0.00002	-0.00050	-0.00001	-0.00051	-0.03045
D58	-0.02136	-0.00002	-0.00067	0.00020	-0.00046	-0.02182
D59	2.67694	0.00001	-0.00092	0.00116	0.00025	2.67719
D60	-0.17384	-0.00003	0.00329	-0.00201	0.00127	-0.17258
D61	0.23933	-0.00001	0.01462	0.00345	0.01806	0.25739
D62	-2.58715	0.00004	0.00290	-0.00076	0.00213	-2.58502
D63	-2.17398	0.00006	0.01423	0.00470	0.01892	-2.15505
D64	2.14975	0.00004	0.00669	0.00071	0.00737	2.15713
D65	-0.24374	0.00004	0.00684	0.00101	0.00782	-0.23592
D66	2.48719	-0.00002	-0.00011	0.00082	0.00072	2.48791
D67	-1.72125	-0.00001	0.00022	0.00075	0.00097	-1.72028
D68	0.35767	0.00000	0.00005	0.00090	0.00095	0.35862
D69	1.27106	0.00000	-0.00066	0.00116	0.00050	1.27156
D70	-2.93737	0.00001	-0.00034	0.00109	0.00075	-2.93663
D71	-0.85846	0.00001	-0.00051	0.00124	0.00073	-0.85773
D72	-1.09203	0.00000	-0.00037	0.00168	0.00131	-1.09072
D73	0.98272	0.00001	-0.00005	0.00161	0.00157	0.98429
D74	3.06163	0.00002	-0.00021	0.00177	0.00155	3.06319

Item	Value	Threshold	Converged?
Maximum Force	0.000392	0.000450	YES
RMS Force	0.000060	0.000300	YES
Maximum Displacement	0.032909	0.001800	NO
RMS Displacement	0.007421	0.001200	NO

Predicted change in Energy=-2.791625D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.379087	-1.914744	-0.242924
2	6	0	-2.511160	-1.175285	-0.124399
3	7	0	-2.113214	0.110135	0.229711
4	6	0	-0.769213	0.136343	0.321397
5	7	0	-0.308276	-1.081924	0.043448
6	6	0	1.125413	-1.435933	-0.006879
7	6	0	1.683609	-1.355884	-1.438584
8	1	0	-1.244439	-2.952113	-0.496799
9	1	0	-3.541462	-1.451456	-0.254898
10	1	0	1.648714	-0.733149	0.643302
11	1	0	1.234106	-2.449654	0.380634
12	1	0	1.064598	-1.964329	-2.108852
13	1	0	1.637959	-0.316034	-1.782043

14	35	0	1.653360	2.230693	1.009939
15	1	0	-0.117138	0.996942	0.582780
16	6	0	-2.917947	1.255476	0.479397
17	6	0	-4.242460	1.278233	0.409976
18	1	0	-2.322368	2.122244	0.737504
19	1	0	-4.765138	2.201286	0.618668
20	1	0	-4.843975	0.415452	0.153499
21	8	0	2.990529	-1.869068	-1.464536
22	1	0	3.632535	-1.139030	-1.365743
23	6	0	4.851196	1.613173	-1.122868
24	6	0	5.717845	0.748821	-0.312324
25	8	0	4.870846	0.179155	-1.339005
26	1	0	3.932032	1.993622	-0.683848
27	1	0	5.277681	2.184513	-1.942793
28	1	0	6.770452	0.700990	-0.587046
29	6	0	5.396451	0.403716	1.115615
30	1	0	5.672374	-0.632452	1.334006
31	1	0	5.967161	1.052881	1.786900
32	1	0	4.335484	0.552999	1.325517

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357364	0.000000			
3	N	2.205099	1.391423	0.000000		
4	C	2.212999	2.225642	1.347379	0.000000	
5	N	1.386447	2.211242	2.171060	1.331877	0.000000
6	C	2.560762	3.647796	3.596527	2.483834	1.477606
7	C	3.334971	4.399521	4.398668	3.367582	2.497814
8	H	1.076437	2.213681	3.264958	3.230146	2.160063
9	H	2.211480	1.074627	2.171015	3.246319	3.267883
10	H	3.368849	4.253164	3.877407	2.589597	2.076362
11	H	2.739294	3.988244	4.216615	3.271724	2.088856
12	H	3.075020	4.164936	4.457664	3.698891	2.701077
13	H	3.745307	4.549866	4.277858	3.228557	2.776118
14	Br	5.286780	5.498239	4.392334	3.275553	3.969326
15	H	3.279057	3.309080	2.212555	1.110924	2.156176
16	C	3.597240	2.537448	1.421881	2.427854	3.530421
17	C	4.338236	3.050034	2.435290	3.657213	4.602445
18	H	4.260081	3.413534	2.085708	2.555236	3.847723
19	H	5.399016	4.127201	3.399544	4.507745	5.565426
20	H	4.194331	2.837198	2.748833	4.087759	4.777742
21	O	4.537397	5.704901	5.730263	4.620270	3.711566
22	H	5.194113	6.267953	6.092578	4.883483	4.185578

23	C	7.213663	7.935788	7.252006	5.987982	5.936665
24	C	7.580623	8.453048	7.875735	6.546652	6.308116
25	O	6.681877	7.602881	7.158403	5.879544	5.506796
26	H	6.608913	7.202061	6.397430	5.153805	5.288492
27	H	8.000377	8.675301	7.977979	6.773957	6.768876
28	H	8.565949	9.480653	8.940678	7.615159	7.326984
29	C	7.288951	8.158505	7.567436	6.222354	5.991709
30	H	7.338535	8.330177	7.898499	6.565857	6.134797
31	H	8.178897	8.972164	8.282878	6.954602	6.854059
32	H	6.419197	7.208728	6.556113	5.219176	5.087355

		6	7	8	9	10
6	C	0.000000				
7	C	1.538755	0.000000			
8	H	2.855699	3.465309	0.000000		
9	H	4.673487	5.358322	2.754415	0.000000	
10	H	1.091094	2.173307	3.820204	5.316075	0.000000
11	H	1.090693	2.169779	2.676852	4.919995	1.785296
12	H	2.168222	1.096648	2.984306	4.991591	3.071049
13	H	2.160574	1.096055	4.112053	5.517949	2.460975
14	Br	3.841457	4.342777	6.126089	6.491857	2.986436
15	H	2.794729	3.586696	4.246331	4.292127	2.472875
16	C	4.881487	5.627803	4.632213	2.873229	4.983562
17	C	6.029472	6.743444	5.263668	2.895628	6.229449
18	H	5.010182	5.734159	5.332403	3.904150	4.891997
19	H	6.951206	7.646703	6.340118	3.950066	7.053298
20	H	6.251955	6.948504	4.971925	2.312720	6.611672
21	O	2.406455	1.404305	4.477103	6.656165	2.744770
22	H	2.867110	1.962306	5.275149	7.266211	2.852463
23	C	4.942058	4.352997	7.641371	8.976750	4.345167
24	C	5.094789	4.687569	7.886972	9.517315	4.434781
25	O	4.290843	3.539032	6.921767	8.637194	3.891526
26	H	4.482995	4.104172	7.161782	8.240490	3.796070
27	H	5.839240	5.070108	8.426973	9.687443	5.326354
28	H	6.063786	5.552641	8.808619	10.539399	5.459186
29	C	4.783939	4.837905	7.613336	9.230724	3.944753
30	H	4.808161	4.911299	7.521634	9.385636	4.083755
31	H	5.731873	5.878326	8.559348	10.042637	4.811103
32	H	4.004458	4.279782	6.836825	8.280207	3.055868

		11	12	13	14	15
11	H	0.000000				
12	H	2.542010	0.000000			
13	H	3.064735	1.775506	0.000000		
14	Br	4.741038	5.260389	3.779049	0.000000	
15	H	3.707525	4.172589	3.224384	2.199834	0.000000

16	C	5.565724	5.738191	5.323535	4.704186	2.814615
17	C	6.625012	6.709961	6.475026	6.002319	4.138511
18	H	5.803284	6.022736	5.289376	3.986526	2.480581
19	H	7.594657	7.666650	7.286971	6.430480	4.801628
20	H	6.723354	6.759647	6.804179	6.800290	4.781778
21	O	2.612807	2.033083	2.083788	4.971829	4.697139
22	H	3.243460	2.797789	2.197490	4.573404	4.734887
23	C	5.643618	5.301792	3.805423	3.893116	5.288981
24	C	5.551067	5.678150	4.465362	4.523755	5.908451
25	O	4.805588	4.435618	3.300463	4.480910	5.407589
26	H	5.306093	5.090990	3.435595	2.849116	4.358153
27	H	6.574520	5.915279	4.418841	4.675089	6.073954
28	H	6.443143	6.478933	5.367014	5.574494	6.992494
29	C	5.099710	5.896590	4.800076	4.166503	5.570951
30	H	4.889721	5.904131	5.107484	4.945209	6.061165
31	H	6.053689	6.950939	5.775230	4.538699	6.202559
32	H	4.418967	5.369406	4.205804	3.179314	4.535922

		16	17	18	19	20
16	C	0.000000				
17	C	1.326527	0.000000			
18	H	1.082875	2.122825	0.000000		
19	H	2.079920	1.081096	2.446936	0.000000	
20	H	2.126367	1.082585	3.100436	1.847105	0.000000
21	O	6.960729	8.107740	7.000459	9.003215	8.319647
22	H	7.214361	8.426855	7.107771	9.252918	8.750755
23	C	7.940704	9.228021	7.428334	9.790439	9.851902
24	C	8.686795	10.000484	8.223955	10.623997	10.577342
25	O	8.070337	9.344478	7.734973	10.038609	9.831640
26	H	6.987146	8.278318	6.415162	8.796615	8.956007
27	H	8.596419	9.848348	8.059070	10.364341	10.486750
28	H	9.762675	11.073008	9.298052	11.695062	11.641514
29	C	8.382093	9.704191	7.916847	10.331317	10.285530
30	H	8.836755	10.139453	8.477031	10.838978	10.634157
31	H	8.983081	10.304518	8.423839	10.856604	10.952396
32	H	7.336324	8.657096	6.865513	9.275656	9.254999

		21	22	23	24	25
21	O	0.000000				
22	H	0.977184	0.000000			
23	C	3.962931	3.019725	0.000000		
24	C	3.952112	3.003696	1.468048	0.000000	
25	O	2.783266	1.808796	1.450347	1.447757	0.000000
26	H	4.051700	3.219966	1.087356	2.208322	2.145435
27	H	4.678815	3.753056	1.086553	2.216616	2.133432
28	H	4.654353	3.720022	2.191512	1.088918	2.108615

29	C	4.196569	3.413005	2.602094	1.503795	2.520288
30	H	4.068581	3.421434	3.428322	2.149508	2.906225
31	H	5.288664	4.493786	3.166394	2.135732	3.425870
32	H	3.931884	3.255761	2.717447	2.152160	2.743365

		26	27	28	29	30
26	H	0.000000				
27	H	1.852607	0.000000			
28	H	3.120400	2.503449	0.000000		
29	C	2.812541	3.541074	2.208009	0.000000	
30	H	3.741228	4.339181	2.583464	1.094291	0.000000
31	H	3.336366	3.958103	2.530755	1.094417	1.769848
32	H	2.505138	3.772456	3.099818	1.091786	1.786797

		31	32
31	H	0.000000	
32	H	1.767803	0.000000

Stoichiometry C10H17BrN2O2
Framework group C1[X(C10H17BrN2O2)]
Deg. of freedom 90
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.716652	2.112378	-0.446355
2	6	0	-3.794579	1.347418	-0.137569
3	7	0	-3.325544	0.049454	0.039503
4	6	0	-1.993160	0.040577	-0.160765
5	7	0	-1.608122	1.279798	-0.460715
6	6	0	-0.205585	1.678812	-0.699455
7	6	0	0.455791	2.231868	0.575095
8	1	0	-2.644048	3.164572	-0.661605
9	1	0	-4.831284	1.611605	-0.036231
10	1	0	0.323030	0.788927	-1.044646
11	1	0	-0.201826	2.438249	-1.482303
12	1	0	-0.159425	3.040937	0.986864
13	1	0	0.513649	1.432701	1.322973
14	35	0	0.527926	-2.050605	-0.142493
15	1	0	-1.297257	-0.823309	-0.100997
16	6	0	-4.056117	-1.125473	0.367456
17	6	0	-5.366942	-1.169564	0.566120
18	1	0	-3.415708	-1.995817	0.438146

19	1	0	-5.831049	-2.114595	0.811661
20	1	0	-6.013064	-0.303755	0.496182
21	8	0	1.718404	2.759773	0.260137
22	1	0	2.405704	2.082291	0.413510
23	6	0	3.810626	-0.465010	1.223567
24	6	0	4.550093	0.011000	0.048080
25	8	0	3.735978	0.926061	0.820014
26	1	0	2.894702	-1.031300	1.072764
27	1	0	4.335682	-0.620121	2.162105
28	1	0	5.612613	0.212015	0.176091
29	6	0	4.104310	-0.290905	-1.356032
30	1	0	4.284513	0.566800	-2.011273
31	1	0	4.674518	-1.139218	-1.747154
32	1	0	3.045738	-0.556850	-1.382393

Rotational constants (GHZ): 0.6034828 0.2205929 0.1722645

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.

475 basis functions, 751 primitive gaussians, 492 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1307.4692723884 Hartrees.

NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 475 RedAO= T EigKep= 3.81D-06 NBF= 475

NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000740 0.000172 0.000061 Ang= 0.09 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3225.52370721 A.U. after 10 cycles
NFock= 10 Conv=0.28D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000007459	0.000034140	-0.000060979
2	6	-0.000007407	0.000020636	-0.000045193
3	7	-0.000003120	-0.000027812	0.000027054
4	6	-0.000064768	0.000049890	0.000023879
5	7	0.000042294	-0.000088470	0.000062059
6	6	-0.000051849	-0.000040537	-0.000026699
7	6	-0.000043060	-0.000018321	-0.000008173
8	1	-0.000004087	-0.000010825	0.000035901
9	1	-0.000004609	-0.000000536	0.000012597
10	1	0.000023237	0.000025317	-0.000001444
11	1	0.000011670	-0.000000149	0.000033994
12	1	-0.000010657	0.000002778	-0.000003527
13	1	-0.000004256	0.000010305	0.000012665
14	35	0.000008346	0.000020909	-0.000014130
15	1	0.000035645	0.000081314	0.000000456
16	6	0.000012918	-0.000022443	0.000001575
17	6	-0.000007222	0.000006726	-0.000002883
18	1	-0.000003544	0.000010042	-0.000007577
19	1	0.000001610	0.000008403	-0.000008043
20	1	-0.000003644	0.000001157	-0.000002481
21	8	0.000127784	-0.000047100	-0.000001076
22	1	-0.000030155	-0.000025556	-0.000047367
23	6	-0.000025163	0.000005970	0.000040718
24	6	0.000090523	0.000011921	-0.000014513
25	8	-0.000107422	-0.000073478	0.000007556
26	1	-0.000009281	0.000038830	-0.000020404
27	1	0.000000076	0.000000193	-0.000010108
28	1	0.000017548	-0.000000799	-0.000004544
29	6	0.000008925	0.000011972	0.000052701
30	1	-0.000000598	-0.000000788	-0.000016196

```
      31        1             0.000000339       0.000008378       0.000000612
      32        1            -0.000007535       0.000007934      -0.000016428
 ---------------------------------------------------------------------
 Cartesian Forces:  Max        0.000127784 RMS        0.000033476

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 GSVD:  received Info=                1 from GESDD.
 Internal  Forces:  Max        0.000106220 RMS        0.000020861
 Search for a local minimum.
 Step number   29 out of a maximum of   177
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swapping is turned off.
 Update second derivatives using D2CorX and points     25     26     27     28     29
 DE= -6.53D-06 DEPred=-2.79D-06 R= 2.34D+00
 TightC=F SS=  1.41D+00  RLast= 1.57D-01 DXNew= 3.2661D+00 4.7178D-01
 Trust test= 2.34D+00 RLast= 1.57D-01 DXMaxT set to 1.94D+00
 ITU=  1  1  1  1  1  1  1  1  1  1  1  1 -1  1  1  1  1  1  1  1
 ITU=  1  1  1  1  0  1  0  1  0
      Eigenvalues ---    0.00004    0.00129    0.00230    0.00237    0.00280
      Eigenvalues ---    0.00440    0.00647    0.01074    0.01246    0.01397
      Eigenvalues ---    0.01485    0.01753    0.01907    0.02015    0.02101
      Eigenvalues ---    0.02178    0.02315    0.02371    0.02499    0.02989
      Eigenvalues ---    0.03062    0.03085    0.03442    0.03546    0.04097
      Eigenvalues ---    0.04613    0.04994    0.05191    0.05434    0.05651
      Eigenvalues ---    0.05809    0.05922    0.06631    0.09365    0.09655
      Eigenvalues ---    0.10535    0.11200    0.11502    0.11701    0.13090
      Eigenvalues ---    0.14029    0.14216    0.15069    0.15946    0.15991
      Eigenvalues ---    0.16000    0.16001    0.16003    0.16015    0.16046
      Eigenvalues ---    0.16501    0.17106    0.19270    0.21472    0.22053
      Eigenvalues ---    0.22898    0.23358    0.23952    0.24267    0.25044
      Eigenvalues ---    0.27670    0.28537    0.30818    0.32261    0.33104
      Eigenvalues ---    0.33309    0.34043    0.34154    0.34489    0.34831
      Eigenvalues ---    0.35041    0.35685    0.35689    0.35856    0.36166
      Eigenvalues ---    0.36436    0.36672    0.37223    0.37246    0.37718
      Eigenvalues ---    0.38578    0.42158    0.42621    0.44604    0.45646
      Eigenvalues ---    0.49315    0.53959    0.55080    0.56270    0.60399
 Eigenvalue     1 is      3.69D-05 Eigenvector:
                              D52       D55       D54       D53       D47
   1                      -0.50140   0.50057   0.49647   0.49532   0.03018
                              D46       D41       D35       D38       D39
```

1 0.02878 -0.01701 -0.01701 -0.01673 -0.01673

En-DIIS/RFO-DIIS IScMMF= 0 using points: 29 28 27 26 25

RFO step: Lambda=-2.07466868D-07.

DidBck=F Rises=F RFO-DIIS coefs: 1.18054 -0.08011 -0.27691 0.13370 0.04278

Iteration 1 RMS(Cart)= 0.00339587 RMS(Int)= 0.00002047

Iteration 2 RMS(Cart)= 0.00003516 RMS(Int)= 0.00001534

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001534

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56505	0.00000	-0.00004	0.00001	-0.00003	2.56502
R2	2.62001	0.00000	0.00007	-0.00004	0.00002	2.62003
R3	2.03417	0.00000	0.00002	-0.00001	0.00001	2.03418
R4	2.62941	-0.00001	-0.00003	-0.00002	-0.00005	2.62936
R5	2.03075	0.00000	0.00002	0.00000	0.00001	2.03076
R6	2.54618	0.00001	0.00008	-0.00005	0.00003	2.54621
R7	2.68696	-0.00001	-0.00004	0.00000	-0.00004	2.68693
R8	2.51688	0.00011	0.00029	-0.00003	0.00026	2.51714
R9	2.09934	0.00008	0.00047	-0.00007	0.00039	2.09973
R10	2.79227	0.00001	0.00003	-0.00004	-0.00002	2.79225
R11	2.90783	0.00002	0.00018	-0.00006	0.00011	2.90793
R12	2.06187	0.00002	0.00010	0.00000	0.00011	2.06197
R13	2.06111	0.00001	0.00006	-0.00003	0.00004	2.06115
R14	2.07236	0.00001	0.00008	-0.00005	0.00003	2.07239
R15	2.07124	0.00001	0.00014	-0.00003	0.00010	2.07135
R16	2.65375	0.00007	-0.00034	0.00034	0.00000	2.65375
R17	4.15708	0.00000	-0.00152	0.00066	-0.00087	4.15621
R18	8.46769	0.00000	0.00010	0.00130	0.00141	8.46910
R19	2.50677	0.00001	0.00003	-0.00001	0.00002	2.50679
R20	2.04634	0.00000	0.00001	0.00000	0.00001	2.04635
R21	2.04298	0.00000	0.00001	0.00000	0.00001	2.04298
R22	2.04579	0.00000	0.00001	0.00000	0.00001	2.04580
R23	1.84661	-0.00002	0.00018	-0.00016	0.00002	1.84663
R24	3.41813	0.00001	-0.00084	0.00073	-0.00010	3.41803
R25	2.77421	0.00002	0.00009	-0.00012	-0.00006	2.77415
R26	2.74076	0.00006	0.00018	0.00012	0.00031	2.74107
R27	2.05480	0.00002	0.00011	-0.00008	0.00004	2.05484
R28	2.05329	0.00001	0.00003	-0.00003	0.00000	2.05328
R29	2.73586	0.00007	0.00028	-0.00005	0.00025	2.73611
R30	2.05776	0.00002	0.00009	-0.00005	0.00004	2.05780
R31	2.84176	0.00002	0.00006	0.00004	0.00010	2.84186
R32	2.06791	0.00000	-0.00002	-0.00001	-0.00003	2.06788
R33	2.06815	0.00000	0.00003	-0.00003	-0.00001	2.06814
R34	2.06318	0.00001	0.00005	-0.00004	0.00001	2.06319

A1	1.87431	0.00002	0.00005	0.00001	0.00006	1.87437
A2	2.27828	-0.00001	-0.00003	-0.00004	-0.00006	2.27822
A3	2.13056	-0.00001	-0.00002	0.00002	0.00000	2.13057
A4	1.86185	0.00001	0.00002	-0.00004	-0.00002	1.86184
A5	2.27708	0.00000	-0.00003	0.00003	0.00001	2.27709
A6	2.14423	0.00000	0.00000	0.00000	0.00001	2.14424
A7	1.89713	0.00002	0.00008	0.00002	0.00011	1.89724
A8	2.24845	-0.00002	-0.00008	-0.00001	-0.00009	2.24837
A9	2.13759	0.00000	0.00000	-0.00002	-0.00002	2.13757
A10	1.88938	-0.00003	-0.00011	0.00000	-0.00011	1.88926
A11	2.23518	0.00001	0.00003	-0.00006	-0.00004	2.23514
A12	2.15862	0.00001	0.00009	0.00006	0.00015	2.15877
A13	1.90208	-0.00002	-0.00003	0.00000	-0.00004	1.90205
A14	2.21235	-0.00002	-0.00012	-0.00001	-0.00013	2.21221
A15	2.16766	0.00003	0.00011	0.00000	0.00012	2.16778
A16	1.95110	-0.00001	0.00007	-0.00007	0.00000	1.95110
A17	1.86580	0.00000	-0.00008	-0.00005	-0.00012	1.86567
A18	1.88312	0.00001	0.00013	0.00011	0.00022	1.88334
A19	1.92512	-0.00002	-0.00044	0.00013	-0.00032	1.92479
A20	1.92066	0.00001	0.00025	0.00001	0.00026	1.92093
A21	1.91680	0.00000	0.00009	-0.00013	-0.00004	1.91676
A22	1.91246	0.00001	0.00016	0.00008	0.00025	1.91271
A23	1.90266	-0.00003	-0.00034	-0.00006	-0.00039	1.90227
A24	1.91324	0.00002	0.00001	0.00018	0.00018	1.91341
A25	1.88740	0.00000	-0.00028	0.00007	-0.00021	1.88718
A26	1.88732	0.00001	0.00025	-0.00007	0.00018	1.88750
A27	1.96023	-0.00001	0.00019	-0.00021	0.00000	1.96024
A28	1.79193	-0.00001	-0.00051	-0.00053	-0.00099	1.79094
A29	2.83234	-0.00002	0.00004	0.00012	0.00019	2.83252
A30	2.17698	0.00001	0.00004	0.00001	0.00005	2.17703
A31	1.95555	0.00000	0.00002	0.00001	0.00003	1.95558
A32	2.15065	-0.00001	-0.00005	-0.00003	-0.00008	2.15058
A33	2.07977	0.00000	0.00002	-0.00005	-0.00003	2.07974
A34	2.15737	0.00000	-0.00004	0.00006	0.00002	2.15739
A35	2.04605	0.00000	0.00003	-0.00001	0.00001	2.04606
A36	1.91405	-0.00005	0.00006	-0.00031	-0.00017	1.91388
A37	3.04910	-0.00002	0.00091	0.00034	0.00123	3.05033
A38	2.07386	0.00003	0.00016	0.00018	0.00033	2.07419
A39	2.08808	-0.00002	0.00007	-0.00017	-0.00010	2.08798
A40	2.00156	0.00002	0.00002	0.00021	0.00023	2.00179
A41	1.98464	-0.00001	-0.00001	-0.00002	-0.00003	1.98461
A42	2.04036	-0.00002	-0.00019	-0.00009	-0.00028	2.04008
A43	2.04567	0.00000	-0.00003	0.00004	0.00001	2.04567
A44	2.13320	0.00000	0.00005	-0.00013	-0.00008	2.13312

A45	1.94909	0.00000	-0.00029	0.00032	0.00002	1.94912
A46	2.04659	0.00000	0.00010	-0.00011	-0.00002	2.04658
A47	2.02203	0.00000	0.00007	-0.00006	0.00002	2.02205
A48	1.42006	0.00006	0.00059	0.00065	0.00124	1.42130
A49	0.99973	-0.00004	-0.00120	-0.00044	-0.00176	0.99797
A50	2.36526	0.00002	-0.00076	0.00009	-0.00061	2.36465
A51	2.34306	0.00003	0.00113	0.00090	0.00201	2.34507
A52	1.93148	-0.00002	0.00000	-0.00016	-0.00016	1.93133
A53	1.91225	0.00001	-0.00001	0.00008	0.00007	1.91232
A54	1.93785	-0.00002	-0.00014	-0.00011	-0.00025	1.93760
A55	1.88363	0.00001	0.00013	0.00010	0.00023	1.88386
A56	1.91360	0.00002	-0.00003	0.00003	0.00000	1.91360
A57	1.88360	0.00001	0.00006	0.00007	0.00013	1.88373
A58	3.76312	0.00009	0.00172	0.00156	0.00325	3.76637
A59	5.05301	-0.00003	-0.00067	-0.00057	-0.00127	5.05175
D1	0.00443	-0.00001	-0.00034	0.00002	-0.00031	0.00412
D2	-3.13159	0.00001	-0.00004	0.00026	0.00023	-3.13136
D3	3.13761	-0.00002	-0.00030	-0.00042	-0.00072	3.13688
D4	0.00159	0.00000	-0.00001	-0.00018	-0.00018	0.00141
D5	-0.00678	0.00000	0.00025	-0.00022	0.00002	-0.00675
D6	-3.09940	0.00001	0.00111	0.00008	0.00118	-3.09821
D7	-3.14082	0.00001	0.00022	0.00017	0.00039	-3.14043
D8	0.04975	0.00002	0.00108	0.00047	0.00155	0.05130
D9	-0.00065	0.00001	0.00031	0.00019	0.00050	-0.00015
D10	-3.13572	0.00000	-0.00006	0.00002	-0.00005	-3.13577
D11	3.13589	0.00000	0.00004	-0.00003	0.00001	3.13590
D12	0.00082	-0.00001	-0.00033	-0.00020	-0.00053	0.00029
D13	-0.00357	-0.00002	-0.00016	-0.00033	-0.00049	-0.00406
D14	3.14150	-0.00003	-0.00037	-0.00064	-0.00102	3.14048
D15	3.13200	-0.00001	0.00019	-0.00017	0.00001	3.13202
D16	-0.00611	-0.00002	-0.00003	-0.00049	-0.00052	-0.00663
D17	-0.00007	0.00000	0.00048	0.00020	0.00068	0.00061
D18	3.14087	0.00001	0.00050	0.00029	0.00079	-3.14152
D19	-3.13434	-0.00001	0.00006	0.00001	0.00006	-3.13428
D20	0.00660	-0.00001	0.00008	0.00010	0.00018	0.00678
D21	0.00637	0.00001	-0.00005	0.00034	0.00029	0.00666
D22	3.10053	0.00000	-0.00089	0.00005	-0.00084	3.09969
D23	-3.13851	0.00002	0.00015	0.00064	0.00079	-3.13772
D24	-0.04436	0.00001	-0.00069	0.00034	-0.00034	-0.04470
D25	-3.14102	0.00001	0.00117	0.00152	0.00270	-3.13831
D26	0.00455	0.00000	0.00093	0.00116	0.00209	0.00664
D27	1.43203	0.00000	-0.00270	-0.00237	-0.00506	1.42697
D28	-2.74285	-0.00003	-0.00325	-0.00229	-0.00553	-2.74839
D29	-0.68210	-0.00002	-0.00313	-0.00241	-0.00553	-0.68764

D30	-1.65357	0.00001	-0.00171	-0.00202	-0.00373	-1.65729
D31	0.45473	-0.00001	-0.00227	-0.00194	-0.00420	0.45053
D32	2.51549	-0.00001	-0.00214	-0.00206	-0.00420	2.51128
D33	-0.93672	0.00000	-0.00105	-0.00003	-0.00108	-0.93780
D34	1.12569	-0.00001	-0.00149	0.00006	-0.00142	1.12427
D35	-3.00531	-0.00002	-0.00146	-0.00011	-0.00156	-3.00687
D36	-3.01015	0.00001	-0.00071	-0.00001	-0.00071	-3.01087
D37	-0.94774	0.00000	-0.00115	0.00009	-0.00106	-0.94880
D38	1.20444	-0.00001	-0.00111	-0.00009	-0.00119	1.20325
D39	1.15550	0.00002	-0.00068	0.00006	-0.00062	1.15488
D40	-3.06527	0.00001	-0.00113	0.00016	-0.00096	-3.06623
D41	-0.91309	-0.00001	-0.00109	-0.00001	-0.00110	-0.91419
D42	-1.64993	0.00002	0.00097	0.00062	0.00159	-1.64834
D43	2.54915	-0.00001	0.00062	0.00045	0.00108	2.55023
D44	0.46793	-0.00001	0.00068	0.00054	0.00122	0.46915
D45	0.46447	0.00000	-0.00031	-0.00121	-0.00152	0.46295
D46	-0.26998	-0.00002	-0.00018	-0.00048	-0.00071	-0.27069
D47	2.57172	-0.00001	-0.00037	-0.00083	-0.00121	2.57050
D48	3.14128	0.00000	0.00005	0.00011	0.00016	3.14144
D49	0.00028	0.00000	0.00005	0.00004	0.00009	0.00037
D50	0.00041	0.00000	0.00003	0.00001	0.00004	0.00045
D51	-3.14059	0.00000	0.00003	-0.00006	-0.00003	-3.14062
D52	-1.99029	0.00000	-0.01220	0.00034	-0.01187	-2.00216
D53	2.49389	-0.00002	0.01343	0.00039	0.01381	2.50770
D54	2.13127	0.00000	0.01384	0.00004	0.01386	2.14513
D55	-2.55912	0.00002	0.01409	0.00096	0.01508	-2.54404
D56	-2.72947	0.00002	-0.00036	0.00058	0.00022	-2.72925
D57	-0.03045	0.00001	-0.00012	0.00021	0.00009	-0.03036
D58	-0.02182	-0.00001	-0.00032	0.00035	0.00003	-0.02179
D59	2.67719	-0.00001	-0.00008	-0.00001	-0.00009	2.67710
D60	-0.17258	0.00000	0.00137	0.00053	0.00187	-0.17070
D61	0.25739	-0.00001	0.00128	0.00113	0.00243	0.25982
D62	-2.58502	0.00001	0.00167	0.00044	0.00208	-2.58294
D63	-2.15505	0.00001	0.00158	0.00104	0.00264	-2.15242
D64	2.15713	-0.00001	0.00092	-0.00002	0.00089	2.15802
D65	-0.23592	-0.00002	0.00104	-0.00019	0.00085	-0.23507
D66	2.48791	0.00000	0.00009	-0.00021	-0.00012	2.48779
D67	-1.72028	0.00000	0.00024	-0.00014	0.00011	-1.72017
D68	0.35862	0.00001	0.00022	-0.00007	0.00016	0.35878
D69	1.27156	-0.00001	0.00003	-0.00022	-0.00020	1.27135
D70	-2.93663	0.00000	0.00018	-0.00015	0.00003	-2.93660
D71	-0.85773	0.00000	0.00016	-0.00008	0.00008	-0.85765
D72	-1.09072	-0.00001	0.00030	-0.00055	-0.00025	-1.09096
D73	0.98429	0.00000	0.00046	-0.00048	-0.00002	0.98427

D74	3.06319	0.00000	0.00044	-0.00041	0.00003	3.06322

Item	Value	Threshold	Converged?
Maximum Force	0.000106	0.000450	YES
RMS Force	0.000021	0.000300	YES
Maximum Displacement	0.015032	0.001800	NO
RMS Displacement	0.003430	0.001200	NO

Predicted change in Energy=-6.036185D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.378847	-1.913561	-0.244982
2	6	0	-2.510846	-1.173884	-0.127288
3	7	0	-2.113034	0.110827	0.229441
4	6	0	-0.769132	0.136691	0.322895
5	7	0	-0.308145	-1.081509	0.044079
6	6	0	1.125476	-1.435793	-0.005889
7	6	0	1.683095	-1.359718	-1.438095
8	1	0	-1.244234	-2.950751	-0.499627
9	1	0	-3.541053	-1.449591	-0.259549
10	1	0	1.649094	-0.730880	0.641823
11	1	0	1.234538	-2.448284	0.384776
12	1	0	1.064545	-1.970756	-2.106450
13	1	0	1.635880	-0.320880	-1.784562
14	35	0	1.652526	2.230853	1.014206
15	1	0	-0.117126	0.997170	0.585722
16	6	0	-2.917852	1.256023	0.479403
17	6	0	-4.242286	1.279168	0.408386
18	1	0	-2.322450	2.122441	0.739105
19	1	0	-4.764966	2.202168	0.617324
20	1	0	-4.843711	0.416801	0.150293
21	8	0	2.990710	-1.871174	-1.463048
22	1	0	3.631599	-1.139974	-1.365478
23	6	0	4.846714	1.613336	-1.120777
24	6	0	5.717474	0.750143	-0.313469
25	8	0	4.868584	0.179371	-1.338158
26	1	0	3.928057	1.991877	-0.679011
27	1	0	5.269726	2.186151	-1.941469
28	1	0	6.769399	0.704701	-0.591283
29	6	0	5.400912	0.403407	1.115212
30	1	0	5.679449	-0.632408	1.331878

31	1	0	5.972178	1.053271	1.785341
32	1	0	4.340193	0.550382	1.328006

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357348	0.000000			
3	N	2.205052	1.391399	0.000000		
4	C	2.213090	2.225722	1.347396	0.000000	
5	N	1.386460	2.211287	2.171094	1.332012	0.000000
6	C	2.560677	3.647763	3.596577	2.484018	1.477594
7	C	3.332530	4.397942	4.399293	3.369532	2.497855
8	H	1.076443	2.213639	3.264906	3.230257	2.160080
9	H	2.211474	1.074632	2.171003	3.246395	3.267931
10	H	3.369508	4.253573	3.877131	2.588863	2.076300
11	H	2.740859	3.989262	4.216565	3.271180	2.089024
12	H	3.072215	4.163593	4.459416	3.702084	2.701817
13	H	3.741059	4.546373	4.277492	3.230299	2.775197
14	Br	5.286866	5.498083	4.392018	3.275341	3.969524
15	H	3.279385	3.309343	2.212734	1.111132	2.156564
16	C	3.597156	2.537356	1.421860	2.427838	3.530458
17	C	4.338167	3.049967	2.435314	3.657235	4.602497
18	H	4.260061	3.413486	2.085714	2.555236	3.847828
19	H	5.398944	4.127134	3.399544	4.507724	5.565464
20	H	4.194295	2.837180	2.748905	4.087842	4.777821
21	O	4.536355	5.704172	5.730711	4.621420	3.711798
22	H	5.192159	6.266090	6.091722	4.883329	4.184716
23	C	7.208581	7.930278	7.246981	5.983511	5.932255
24	C	7.580091	8.452324	7.875299	6.546551	6.308001
25	O	6.678757	7.599571	7.155771	5.877479	5.504445
26	H	6.603337	7.196243	6.392059	5.148700	5.283367
27	H	7.993075	8.667087	7.970256	6.767233	6.762592
28	H	8.565579	9.479838	8.940017	7.614972	7.327064
29	C	7.292709	8.162571	7.571631	6.226423	5.995468
30	H	7.344889	8.336864	7.905097	6.572196	6.140961
31	H	8.183023	8.976639	8.287320	6.958744	6.857968
32	H	6.422829	7.213023	6.560808	5.223656	5.091030

		6	7	8	9	10
6	C	0.000000				
7	C	1.538811	0.000000			
8	H	2.855592	3.461411	0.000000		
9	H	4.673439	5.356191	2.754360	0.000000	
10	H	1.091150	2.173166	3.821267	5.316639	0.000000
11	H	1.090711	2.170031	2.679357	4.921262	1.785330

12	H	2.168468	1.096663	2.978714	4.989408	3.071155
13	H	2.160375	1.096109	4.106378	5.513647	2.460816
14	Br	3.842223	4.348209	6.126332	6.491640	2.985054
15	H	2.795241	3.590481	4.246697	4.292365	2.471606
16	C	4.881587	5.629176	4.632110	2.873113	4.983088
17	C	6.029554	6.744136	5.263556	2.895513	6.229217
18	H	5.010413	5.736726	5.332381	3.904064	4.891223
19	H	6.951292	7.647828	6.340008	3.949963	7.052910
20	H	6.252016	6.948252	4.971824	2.312640	6.611754
21	O	2.406650	1.404302	4.475312	6.655079	2.744209
22	H	2.866468	1.962199	5.272795	7.264013	2.850778
23	C	4.938398	4.352956	7.636516	8.970947	4.338996
24	C	5.095033	4.689617	7.886486	9.516410	4.433703
25	O	4.288886	3.539226	6.918623	8.633592	3.887672
26	H	4.478445	4.104784	7.156420	8.234516	3.788361
27	H	5.834360	5.068579	8.420116	9.678704	5.318970
28	H	6.064509	5.554224	8.808465	10.538333	5.458843
29	C	4.787367	4.842535	7.616827	9.234843	3.948018
30	H	4.813909	4.916561	7.527717	9.392449	4.090188
31	H	5.735369	5.882965	8.563286	10.047261	4.814549
32	H	4.007315	4.284853	6.839883	8.284580	3.058512

		11	12	13	14	15
11	H	0.000000				
12	H	2.542270	0.000000			
13	H	3.064792	1.775423	0.000000		
14	Br	4.739749	5.266663	3.787443	0.000000	
15	H	3.706552	4.177645	3.229324	2.199373	0.000000
16	C	5.565357	5.740926	5.324344	4.703687	2.814672
17	C	6.624958	6.711846	6.474722	6.001795	4.138589
18	H	5.802520	6.026872	5.292173	3.985959	2.480568
19	H	7.594395	7.669122	7.287363	6.429817	4.801608
20	H	6.723750	6.760238	6.802422	6.799871	4.781949
21	O	2.613742	2.033222	2.083830	4.975355	4.699308
22	H	3.243603	2.798036	2.197598	4.576254	4.735768
23	C	5.640147	5.303025	3.806738	3.891314	5.285027
24	C	5.551053	5.680477	4.468849	4.525375	5.908648
25	O	4.804098	4.436669	3.301500	4.481654	5.406238
26	H	5.301105	5.093108	3.438773	2.846424	4.353446
27	H	6.570551	5.915289	4.417540	4.671418	6.067829
28	H	6.444276	6.480676	5.369241	5.575762	6.992503
29	C	5.101407	5.900834	4.807156	4.171350	5.575093
30	H	4.894041	5.908521	5.114655	4.951291	6.067335
31	H	6.055385	6.955259	5.782385	4.543208	6.206597
32	H	4.418911	5.374151	4.214319	3.185279	4.540737

		16	17	18	19	20
16	C	0.000000				
17	C	1.326538	0.000000			
18	H	1.082880	2.122794	0.000000		
19	H	2.079914	1.081100	2.446849	0.000000	
20	H	2.126392	1.082591	3.100430	1.847120	0.000000
21	O	6.961579	8.108215	7.002007	9.003920	8.319607
22	H	7.213854	8.425966	7.107975	9.252227	8.749399
23	C	7.935789	9.222795	7.423966	9.785301	9.846404
24	C	8.686393	9.999888	8.223836	10.623384	10.576617
25	O	8.067918	9.341730	7.733144	10.035980	9.828557
26	H	6.982111	8.273143	6.410689	8.791664	8.950560
27	H	8.588492	9.839859	8.051750	10.355807	10.477962
28	H	9.761822	11.071882	9.297399	11.693790	11.640325
29	C	8.386480	9.708648	7.921291	10.335788	10.289974
30	H	8.843443	10.146319	8.483570	10.845792	10.641141
31	H	8.987726	10.309331	8.428439	10.861422	10.957277
32	H	7.341476	8.662319	6.870879	9.281023	9.260073

		21	22	23	24	25
21	O	0.000000				
22	H	0.977196	0.000000			
23	C	3.962791	3.019453	0.000000		
24	C	3.953236	3.005019	1.468016	0.000000	
25	O	2.783297	1.808742	1.450513	1.447889	0.000000
26	H	4.051728	3.219878	1.087375	2.208515	2.145751
27	H	4.678108	3.752110	1.086550	2.216525	2.133557
28	H	4.655492	3.721290	2.191506	1.088941	2.108766
29	C	4.198836	3.415599	2.602059	1.503850	2.520434
30	H	4.071299	3.424477	3.428167	2.149432	2.906128
31	H	5.290894	4.496253	3.166365	2.135828	3.426057
32	H	3.933831	3.257954	2.717163	2.152033	2.743224

		26	27	28	29	30
26	H	0.000000				
27	H	1.852463	0.000000			
28	H	3.120536	2.503341	0.000000		
29	C	2.812788	3.541000	2.208089	0.000000	
30	H	3.741380	4.339003	2.583486	1.094276	0.000000
31	H	3.336532	3.958026	2.530890	1.094413	1.769981
32	H	2.505171	3.772166	3.099762	1.091792	1.786789

		31	32
31	H	0.000000	
32	H	1.767888	0.000000

Stoichiometry C10H17BrN2O2

Framework group C1[X(C10H17BrN2O2)]

Deg. of freedom 90

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.715512	2.112530	-0.445800
2	6	0	-3.793461	1.348033	-0.136022
3	7	0	-3.324952	0.049704	0.039568
4	6	0	-1.992737	0.040148	-0.161901
5	7	0	-1.607385	1.279423	-0.461833
6	6	0	-0.204841	1.678258	-0.700759
7	6	0	0.455231	2.236026	0.572481
8	1	0	-2.642722	3.164718	-0.661047
9	1	0	-4.829938	1.612692	-0.033515
10	1	0	0.324499	0.787203	-1.041976
11	1	0	-0.200483	2.434671	-1.486552
12	1	0	-0.159967	3.047007	0.980540
13	1	0	0.511318	1.439547	1.323434
14	35	0	0.527086	-2.052221	-0.143547
15	1	0	-1.297093	-0.824242	-0.102553
16	6	0	-4.055846	-1.124914	0.367825
17	6	0	-5.366532	-1.168444	0.567604
18	1	0	-3.415836	-1.995610	0.437857
19	1	0	-5.830822	-2.113313	0.813436
20	1	0	-6.012338	-0.302334	0.498380
21	8	0	1.718754	2.761649	0.257370
22	1	0	2.405012	2.083658	0.413224
23	6	0	3.805877	-0.465034	1.224914
24	6	0	4.550239	0.010514	0.052374
25	8	0	3.733778	0.926301	0.821210
26	1	0	2.890142	-1.030789	1.070856
27	1	0	4.327265	-0.620617	2.165414
28	1	0	5.612440	0.210670	0.184505
29	6	0	4.109619	-0.291071	-1.353494
30	1	0	4.292882	0.566637	-2.007857
31	1	0	4.680610	-1.139841	-1.742466
32	1	0	3.050909	-0.556087	-1.383669

Rotational constants (GHZ): 0.6028350 0.2206469 0.1722443

Standard basis: 6-311++G(d,p) (5D, 7F)

```
 There are     492 symmetry adapted cartesian basis functions of A     symmetry.
 There are     475 symmetry adapted basis functions of A     symmetry.
   475 basis functions,     751 primitive gaussians,     492 cartesian basis functions
    71 alpha electrons        71 beta electrons
         nuclear repulsion energy       1307.3523244152 Hartrees.
 NAtoms=      32 NActive=      32 NUniq=      32 SFac= 1.00D+00 NAtFMM=      60 NAOKFM=F
Big=F
 Integral buffers will be       131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=     475 RedAO= T EigKep=    3.80D-06    NBF=     475
 NBsUse=     475 1.00D-06 EigRej= -1.00D+00 NBFU=     475
 Initial guess from the checkpoint file:    "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"
 B after Tr=          0.000000        0.000000        0.000000
             Rot=       1.000000        0.000140        0.000128        0.000057 Ang=      0.02 deg.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                    energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3225.52370852         A.U. after        9 cycles
                  NFock=    9    Conv=0.37D-08         -V/T= 2.0018
 Calling FoFJK, ICntrl=            2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center         Atomic                         Forces (Hartrees/Bohr)
 Number         Number                      X                      Y                      Z
 -------------------------------------------------------------------
       1              6                 0.000020546       0.000013042      -0.000053967
       2              6                -0.000007517      -0.000002985       0.000016811
       3              7                 0.000011504       0.000011583      -0.000020748
       4              6                -0.000008266      -0.000008780       0.000037618
       5              7                 0.000007822       0.000005234       0.000021727
       6              6                -0.000011269      -0.000007019      -0.000000601
       7              6                -0.000075191       0.000035775       0.000007887
       8              1                -0.000002977      -0.000003593       0.000018264
       9              1                -0.000000201       0.000000545       0.000013383
      10              1                 0.000000764      -0.000000826       0.000005691
      11              1                 0.000007051       0.000003372       0.000023660
      12              1                 0.000015835      -0.000008138       0.000012771
      13              1                 0.000008337      -0.000008919      -0.000004622
      14             35                 0.000010801       0.000019567      -0.000007789
      15              1                -0.000008891      -0.000005108      -0.000010634
```

16	6	0.000000525	0.000002652	-0.000002588
17	6	0.000001423	0.000001895	-0.000005851
18	1	-0.000001498	0.000004758	-0.000005574
19	1	0.000000986	0.000004518	-0.000005083
20	1	-0.000001862	0.000004357	-0.000000965
21	8	0.000081087	-0.000026647	-0.000023542
22	1	-0.000005357	-0.000057960	-0.000006805
23	6	-0.000004788	-0.000015476	-0.000001551
24	6	0.000056169	-0.000002326	-0.000019031
25	8	-0.000084507	0.000030164	0.000052819
26	1	-0.000004428	0.000013214	-0.000011489
27	1	0.000007801	-0.000006835	-0.000020204
28	1	-0.000001046	-0.000009848	-0.000002220
29	6	-0.000014093	0.000010561	-0.000013011
30	1	-0.000000167	0.000000244	0.000007957
31	1	-0.000000499	0.000001477	-0.000001369
32	1	0.000001906	0.000001502	-0.000000943

Cartesian Forces: Max 0.000084507 RMS 0.000021419

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000049504 RMS 0.000010285
Search for a local minimum.
Step number 30 out of a maximum of 177
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 25 26 27 28 29
30
DE= -1.31D-06 DEPred=-6.04D-07 R= 2.17D+00
TightC=F SS= 1.41D+00 RLast= 3.13D-02 DXNew= 3.2661D+00 9.3893D-02
Trust test= 2.17D+00 RLast= 3.13D-02 DXMaxT set to 1.94D+00
ITU= 1 1 1 1 1 1 1 1 1 1 1 1 1 -1 1 1 1 1 1 1
ITU= 1 1 1 1 1 0 1 0 1 0

Eigenvalues ---	0.00004	0.00120	0.00194	0.00234	0.00283
Eigenvalues ---	0.00357	0.00632	0.01057	0.01220	0.01402
Eigenvalues ---	0.01448	0.01751	0.01906	0.01974	0.02111
Eigenvalues ---	0.02191	0.02315	0.02380	0.02663	0.02984
Eigenvalues ---	0.03063	0.03087	0.03447	0.03535	0.04113
Eigenvalues ---	0.04608	0.04885	0.05239	0.05437	0.05603

Eigenvalues --- 0.05702 0.05932 0.06786 0.09226 0.09386
Eigenvalues --- 0.10595 0.11096 0.11531 0.11768 0.12901
Eigenvalues --- 0.13864 0.14136 0.14718 0.15946 0.15992
Eigenvalues --- 0.15994 0.16001 0.16003 0.16014 0.16050
Eigenvalues --- 0.16499 0.17233 0.19028 0.21339 0.22043
Eigenvalues --- 0.22889 0.23331 0.23896 0.24235 0.25050
Eigenvalues --- 0.27676 0.28552 0.30754 0.32261 0.33107
Eigenvalues --- 0.33304 0.34020 0.34139 0.34502 0.34821
Eigenvalues --- 0.35009 0.35685 0.35689 0.35856 0.36209
Eigenvalues --- 0.36436 0.36675 0.37196 0.37251 0.37586
Eigenvalues --- 0.38485 0.42152 0.42564 0.44113 0.45728
Eigenvalues --- 0.49391 0.53989 0.55076 0.56346 0.60393
Eigenvalue 1 is 3.78D-05 Eigenvector:

	D52	D55	D53	D54	D46
1	-0.50675	0.49809	0.49587	0.49301	0.03286
	D47	D44	D42	D43	D39
1	0.03190	0.01791	0.01710	0.01682	-0.01589

En-DIIS/RFO-DIIS IScMMF= 0 using points: 30 29 28 27 26
RFO step: Lambda=-6.76922125D-08.
DidBck=F Rises=F RFO-DIIS coefs: 1.41696 -0.34195 -0.16607 0.15407 -0.06301
Iteration 1 RMS(Cart)= 0.00220956 RMS(Int)= 0.00000421
Iteration 2 RMS(Cart)= 0.00000284 RMS(Int)= 0.00000377
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000377

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56502	0.00001	-0.00002	0.00001	0.00000	2.56501
R2	2.62003	-0.00001	0.00001	0.00000	0.00001	2.62004
R3	2.03418	0.00000	0.00001	0.00000	0.00001	2.03419
R4	2.62936	0.00000	-0.00002	0.00001	-0.00001	2.62935
R5	2.03076	0.00000	0.00000	0.00000	0.00000	2.03076
R6	2.54621	-0.00001	0.00001	0.00000	0.00001	2.54622
R7	2.68693	0.00000	-0.00002	0.00001	-0.00001	2.68692
R8	2.51714	0.00000	0.00012	0.00001	0.00014	2.51728
R9	2.09973	-0.00001	0.00018	-0.00004	0.00015	2.09988
R10	2.79225	-0.00001	-0.00002	-0.00001	-0.00003	2.79222
R11	2.90793	0.00000	0.00006	-0.00002	0.00004	2.90797
R12	2.06197	0.00000	0.00005	0.00001	0.00006	2.06203
R13	2.06115	0.00000	0.00002	0.00003	0.00004	2.06119
R14	2.07239	-0.00001	0.00001	-0.00003	-0.00002	2.07237
R15	2.07135	0.00000	0.00005	0.00000	0.00005	2.07139
R16	2.65375	0.00005	-0.00001	0.00006	0.00005	2.65379
R17	4.15621	0.00001	-0.00032	-0.00005	-0.00038	4.15584
R18	8.46910	0.00000	0.00029	0.00038	0.00067	8.46976

R19	2.50679	0.00000	0.00001	0.00000	0.00001	2.50681
R20	2.04635	0.00000	0.00000	0.00000	0.00000	2.04635
R21	2.04298	0.00000	0.00000	0.00000	0.00001	2.04299
R22	2.04580	0.00000	0.00001	0.00000	0.00000	2.04580
R23	1.84663	-0.00004	0.00000	-0.00003	-0.00003	1.84660
R24	3.41803	0.00000	0.00002	-0.00003	-0.00002	3.41801
R25	2.77415	0.00000	-0.00001	0.00008	0.00007	2.77422
R26	2.74107	0.00001	0.00012	-0.00004	0.00008	2.74115
R27	2.05484	0.00001	0.00001	0.00003	0.00004	2.05488
R28	2.05328	0.00001	-0.00001	0.00004	0.00003	2.05332
R29	2.73611	0.00001	0.00012	-0.00003	0.00009	2.73621
R30	2.05780	0.00000	0.00002	0.00001	0.00002	2.05782
R31	2.84186	0.00000	0.00008	-0.00004	0.00004	2.84190
R32	2.06788	0.00000	-0.00001	0.00002	0.00001	2.06789
R33	2.06814	0.00000	-0.00001	0.00001	0.00000	2.06815
R34	2.06319	0.00000	0.00001	0.00000	0.00001	2.06320
A1	1.87437	0.00000	0.00002	0.00000	0.00002	1.87439
A2	2.27822	0.00000	-0.00003	-0.00002	-0.00004	2.27817
A3	2.13057	0.00000	0.00000	0.00001	0.00001	2.13058
A4	1.86184	0.00000	-0.00001	0.00001	0.00000	1.86184
A5	2.27709	0.00000	0.00000	0.00000	0.00001	2.27710
A6	2.14424	0.00000	0.00000	-0.00002	-0.00001	2.14423
A7	1.89724	0.00000	0.00006	-0.00003	0.00004	1.89727
A8	2.24837	0.00000	-0.00005	0.00001	-0.00004	2.24833
A9	2.13757	0.00000	-0.00001	0.00002	0.00000	2.13757
A10	1.88926	0.00000	-0.00007	0.00003	-0.00004	1.88923
A11	2.23514	-0.00001	0.00000	-0.00007	-0.00008	2.23507
A12	2.15877	0.00001	0.00007	0.00004	0.00012	2.15889
A13	1.90205	0.00000	0.00000	-0.00002	-0.00002	1.90202
A14	2.21221	-0.00002	-0.00008	-0.00008	-0.00016	2.21205
A15	2.16778	0.00002	0.00006	0.00009	0.00015	2.16793
A16	1.95110	-0.00002	-0.00002	-0.00007	-0.00009	1.95102
A17	1.86567	0.00000	-0.00004	-0.00002	-0.00006	1.86561
A18	1.88334	0.00001	0.00008	0.00006	0.00014	1.88348
A19	1.92479	0.00001	-0.00014	0.00007	-0.00007	1.92472
A20	1.92093	0.00001	0.00014	0.00001	0.00015	1.92108
A21	1.91676	-0.00001	-0.00002	-0.00005	-0.00007	1.91668
A22	1.91271	0.00001	0.00014	0.00000	0.00014	1.91285
A23	1.90227	0.00001	-0.00017	0.00007	-0.00010	1.90217
A24	1.91341	0.00000	0.00007	0.00003	0.00011	1.91352
A25	1.88718	0.00000	-0.00007	0.00000	-0.00006	1.88712
A26	1.88750	-0.00001	0.00003	-0.00011	-0.00007	1.88743
A27	1.96024	-0.00001	0.00000	0.00000	0.00000	1.96023
A28	1.79094	-0.00003	-0.00033	-0.00024	-0.00058	1.79036

A29	2.83252	0.00000	-0.00003	-0.00009	-0.00012	2.83241
A30	2.17703	0.00000	0.00002	0.00002	0.00004	2.17707
A31	1.95558	0.00000	0.00002	0.00000	0.00002	1.95560
A32	2.15058	0.00000	-0.00004	-0.00002	-0.00006	2.15052
A33	2.07974	0.00000	-0.00002	-0.00001	-0.00003	2.07971
A34	2.15739	0.00000	0.00001	0.00001	0.00003	2.15741
A35	2.04606	0.00000	0.00001	-0.00001	0.00000	2.04606
A36	1.91388	-0.00004	-0.00016	-0.00013	-0.00032	1.91356
A37	3.05033	-0.00001	0.00037	0.00001	0.00040	3.05073
A38	2.07419	0.00001	0.00021	0.00001	0.00022	2.07441
A39	2.08798	0.00000	-0.00001	-0.00006	-0.00007	2.08791
A40	2.00179	0.00000	0.00003	0.00015	0.00018	2.00197
A41	1.98461	0.00000	-0.00006	-0.00007	-0.00013	1.98448
A42	2.04008	0.00000	-0.00014	0.00001	-0.00014	2.03994
A43	2.04567	-0.00001	0.00002	0.00005	0.00007	2.04574
A44	2.13312	0.00000	-0.00001	-0.00005	-0.00007	2.13306
A45	1.94912	0.00000	0.00003	-0.00011	-0.00008	1.94904
A46	2.04658	-0.00001	-0.00008	-0.00002	-0.00010	2.04648
A47	2.02205	0.00001	0.00001	0.00006	0.00008	2.02213
A48	1.42130	0.00003	0.00054	0.00062	0.00114	1.42244
A49	0.99797	0.00000	-0.00063	0.00005	-0.00056	0.99741
A50	2.36465	0.00003	-0.00023	0.00034	0.00010	2.36475
A51	2.34507	0.00000	0.00100	0.00075	0.00176	2.34683
A52	1.93133	0.00001	-0.00007	0.00006	-0.00001	1.93132
A53	1.91232	0.00000	0.00001	0.00005	0.00005	1.91237
A54	1.93760	0.00000	-0.00011	0.00001	-0.00011	1.93749
A55	1.88386	-0.00001	0.00010	-0.00005	0.00005	1.88391
A56	1.91360	0.00000	0.00000	-0.00003	-0.00003	1.91357
A57	1.88373	0.00000	0.00008	-0.00004	0.00005	1.88377
A58	3.76637	0.00004	0.00154	0.00137	0.00290	3.76927
A59	5.05175	-0.00002	-0.00034	-0.00010	-0.00044	5.05131
D1	0.00412	0.00001	-0.00014	0.00021	0.00007	0.00418
D2	-3.13136	0.00001	0.00016	0.00012	0.00028	-3.13108
D3	3.13688	0.00000	-0.00039	-0.00003	-0.00043	3.13646
D4	0.00141	-0.00001	-0.00009	-0.00013	-0.00022	0.00119
D5	-0.00675	-0.00001	-0.00003	0.00000	-0.00002	-0.00678
D6	-3.09821	-0.00001	0.00055	0.00011	0.00066	-3.09755
D7	-3.14043	0.00000	0.00020	0.00022	0.00042	-3.14001
D8	0.05130	0.00001	0.00077	0.00033	0.00110	0.05240
D9	-0.00015	-0.00001	0.00026	-0.00035	-0.00008	-0.00023
D10	-3.13577	-0.00001	0.00000	-0.00024	-0.00024	-3.13601
D11	3.13590	-0.00001	-0.00001	-0.00027	-0.00027	3.13563
D12	0.00029	0.00000	-0.00027	-0.00016	-0.00043	-0.00014
D13	-0.00406	0.00000	-0.00028	0.00035	0.00007	-0.00399

D14	3.14048	-0.00001	-0.00054	-0.00036	-0.00089	3.13959
D15	3.13202	0.00000	-0.00004	0.00025	0.00021	3.13223
D16	-0.00663	-0.00001	-0.00029	-0.00046	-0.00075	-0.00738
D17	0.00061	0.00000	0.00024	-0.00012	0.00012	0.00073
D18	-3.14152	0.00000	0.00030	-0.00015	0.00015	-3.14137
D19	-3.13428	0.00000	-0.00005	0.00000	-0.00005	-3.13433
D20	0.00678	0.00000	0.00001	-0.00003	-0.00002	0.00676
D21	0.00666	0.00001	0.00019	-0.00022	-0.00003	0.00663
D22	3.09969	0.00000	-0.00037	-0.00033	-0.00070	3.09899
D23	-3.13772	0.00002	0.00043	0.00045	0.00088	-3.13684
D24	-0.04470	0.00001	-0.00013	0.00034	0.00021	-0.04449
D25	-3.13831	0.00002	0.00107	0.00204	0.00311	-3.13521
D26	0.00664	0.00000	0.00079	0.00123	0.00201	0.00866
D27	1.42697	-0.00001	-0.00213	-0.00162	-0.00375	1.42322
D28	-2.74839	-0.00001	-0.00234	-0.00159	-0.00393	-2.75232
D29	-0.68764	-0.00001	-0.00235	-0.00163	-0.00398	-0.69161
D30	-1.65729	0.00000	-0.00148	-0.00148	-0.00296	-1.66026
D31	0.45053	0.00000	-0.00169	-0.00146	-0.00314	0.44739
D32	2.51128	-0.00001	-0.00169	-0.00150	-0.00319	2.50810
D33	-0.93780	-0.00001	-0.00031	0.00003	-0.00029	-0.93809
D34	1.12427	0.00000	-0.00042	0.00007	-0.00035	1.12393
D35	-3.00687	0.00000	-0.00048	0.00014	-0.00034	-3.00722
D36	-3.01087	0.00000	-0.00016	0.00005	-0.00010	-3.01097
D37	-0.94880	0.00000	-0.00026	0.00010	-0.00016	-0.94896
D38	1.20325	0.00000	-0.00032	0.00017	-0.00016	1.20309
D39	1.15488	0.00000	-0.00013	0.00007	-0.00007	1.15482
D40	-3.06623	0.00000	-0.00024	0.00011	-0.00012	-3.06636
D41	-0.91419	0.00000	-0.00030	0.00018	-0.00012	-0.91431
D42	-1.64834	0.00001	0.00079	0.00072	0.00151	-1.64682
D43	2.55023	0.00000	0.00057	0.00077	0.00133	2.55156
D44	0.46915	0.00001	0.00063	0.00083	0.00146	0.47062
D45	0.46295	0.00000	-0.00061	-0.00146	-0.00206	0.46088
D46	-0.27069	-0.00001	-0.00022	-0.00042	-0.00064	-0.27133
D47	2.57050	-0.00001	-0.00072	-0.00121	-0.00193	2.56857
D48	3.14144	0.00000	0.00008	-0.00008	0.00000	3.14144
D49	0.00037	0.00000	0.00004	-0.00002	0.00001	0.00039
D50	0.00045	0.00000	0.00002	-0.00005	-0.00003	0.00042
D51	-3.14062	0.00000	-0.00003	0.00001	-0.00002	-3.14064
D52	-2.00216	0.00000	-0.00488	0.00725	0.00238	-1.99978
D53	2.50770	0.00000	0.00549	-0.00695	-0.00145	2.50625
D54	2.14513	-0.00001	0.00512	-0.00806	-0.00294	2.14219
D55	-2.54404	0.00001	0.00583	-0.00685	-0.00102	-2.54506
D56	-2.72925	0.00001	-0.00002	0.00001	-0.00001	-2.72926
D57	-0.03036	0.00001	0.00002	0.00019	0.00022	-0.03015

D58	-0.02179	0.00000	0.00009	-0.00010	0.00000	-0.02179
D59	2.67710	0.00001	0.00013	0.00009	0.00022	2.67732
D60	-0.17070	-0.00001	0.00046	-0.00018	0.00028	-0.17043
D61	0.25982	0.00000	0.00113	0.00119	0.00232	0.26214
D62	-2.58294	-0.00001	0.00073	-0.00029	0.00044	-2.58249
D63	-2.15242	0.00000	0.00140	0.00109	0.00249	-2.14993
D64	2.15802	-0.00003	0.00033	-0.00065	-0.00032	2.15770
D65	-0.23507	-0.00003	0.00037	-0.00061	-0.00024	-0.23531
D66	2.48779	0.00000	0.00007	-0.00004	0.00002	2.48781
D67	-1.72017	0.00000	0.00015	-0.00004	0.00012	-1.72005
D68	0.35878	0.00000	0.00019	-0.00005	0.00014	0.35892
D69	1.27135	0.00000	0.00008	0.00002	0.00009	1.27145
D70	-2.93660	0.00000	0.00016	0.00002	0.00019	-2.93641
D71	-0.85765	0.00000	0.00020	0.00001	0.00021	-0.85744
D72	-1.09096	0.00000	0.00011	0.00014	0.00025	-1.09072
D73	0.98427	0.00000	0.00019	0.00014	0.00034	0.98461
D74	3.06322	0.00000	0.00023	0.00013	0.00036	3.06358

Item	Value	Threshold	Converged?
Maximum Force	0.000050	0.000450	YES
RMS Force	0.000010	0.000300	YES
Maximum Displacement	0.009167	0.001800	NO
RMS Displacement	0.002211	0.001200	NO

Predicted change in Energy=-2.544681D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.378471	-1.912575	-0.247197
2	6	0	-2.510429	-1.172826	-0.129593
3	7	0	-2.112723	0.111240	0.229542
4	6	0	-0.768919	0.136680	0.324610
5	7	0	-0.307877	-1.081255	0.044384
6	6	0	1.125668	-1.435817	-0.005369
7	6	0	1.682856	-1.361973	-1.437882
8	1	0	-1.243880	-2.949498	-0.502960
9	1	0	-3.540569	-1.448129	-0.263226
10	1	0	1.649513	-0.729822	0.641029
11	1	0	1.234859	-2.447651	0.387021
12	1	0	1.064283	-1.974130	-2.105175
13	1	0	1.635294	-0.323656	-1.785944
14	35	0	1.652481	2.230199	1.018065

15	1	0	-0.117015	0.996926	0.588773
16	6	0	-2.917586	1.256262	0.480127
17	6	0	-4.241934	1.279853	0.407544
18	1	0	-2.322323	2.122204	0.741739
19	1	0	-4.764604	2.202711	0.617147
20	1	0	-4.843295	0.418015	0.147529
21	8	0	2.990591	-1.873202	-1.462539
22	1	0	3.631082	-1.141675	-1.364987
23	6	0	4.843832	1.612782	-1.120345
24	6	0	5.716932	0.750891	-0.314105
25	8	0	4.866933	0.178709	-1.337157
26	1	0	3.925479	1.990704	-0.677359
27	1	0	5.264875	2.185603	-1.942068
28	1	0	6.768440	0.706357	-0.593689
29	6	0	5.403007	0.404374	1.115231
30	1	0	5.683100	-0.631027	1.331885
31	1	0	5.974464	1.055223	1.784244
32	1	0	4.342404	0.550118	1.329483

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357347	0.000000			
3	N	2.205048	1.391392	0.000000		
4	C	2.213134	2.225750	1.347403	0.000000	
5	N	1.386465	2.211310	2.171129	1.332086	0.000000
6	C	2.560565	3.647712	3.596630	2.484168	1.477579
7	C	3.330558	4.396708	4.399668	3.370985	2.497785
8	H	1.076447	2.213620	3.264899	3.230317	2.160096
9	H	2.211478	1.074634	2.170990	3.246416	3.267953
10	H	3.369947	4.253849	3.877000	2.588390	2.076263
11	H	2.741903	3.989894	4.216519	3.270747	2.089132
12	H	3.069678	4.162161	4.460162	3.704052	2.701972
13	H	3.738340	4.544404	4.277727	3.232118	2.774882
14	Br	5.286788	5.497955	4.391869	3.275191	3.969482
15	H	3.279530	3.309426	2.212767	1.111209	2.156763
16	C	3.597138	2.537322	1.421855	2.427842	3.530501
17	C	4.338168	3.049960	2.435340	3.657261	4.602556
18	H	4.260081	3.413476	2.085726	2.555262	3.847914
19	H	5.398941	4.127126	3.399553	4.507722	5.565510
20	H	4.194337	2.837223	2.748974	4.087915	4.777915
21	O	4.535119	5.703376	5.731053	4.622493	3.711857
22	H	5.190315	6.264610	6.091274	4.883538	4.183943
23	C	7.204692	7.926308	7.243651	5.980781	5.929126

24	C	7.579134	8.451284	7.874529	6.546103	6.307423
25	O	6.675819	7.596732	7.153649	5.875888	5.502256
26	H	6.599433	7.192280	6.388642	5.145748	5.280071
27	H	7.987597	8.661378	7.965415	6.763327	6.758248
28	H	8.564521	9.478614	8.939068	7.614433	7.326456
29	C	7.294718	8.164534	7.573412	6.228115	5.997333
30	H	7.348581	8.340466	7.908285	6.575144	6.144279
31	H	8.185367	8.978885	8.289198	6.960422	6.859990
32	H	6.424888	7.215176	6.562861	5.225545	5.092934

		6	7	8	9	10
6	C	0.000000				
7	C	1.538833	0.000000			
8	H	2.855448	3.458337	0.000000		
9	H	4.673373	5.354569	2.754335	0.000000	
10	H	1.091180	2.173154	3.821962	5.317010	0.000000
11	H	1.090734	2.170178	2.681057	4.922050	1.785328
12	H	2.168580	1.096654	2.974231	4.987396	3.071227
13	H	2.160340	1.096134	4.102528	5.511140	2.460767
14	Br	3.842475	4.351585	6.126310	6.491500	2.983938
15	H	2.795622	3.593226	4.246877	4.292426	2.470832
16	C	4.881690	5.630095	4.632080	2.873050	4.982852
17	C	6.029636	6.744477	5.263530	2.895468	6.229162
18	H	5.010621	5.738614	5.332398	3.904018	4.890774
19	H	6.951382	7.648519	6.339983	3.949931	7.052746
20	H	6.252087	6.947844	4.971828	2.312642	6.611931
21	O	2.406780	1.404327	4.473248	6.653953	2.744232
22	H	2.865690	1.961996	5.270348	7.262257	2.849621
23	C	4.935774	4.352214	7.632548	8.966717	4.335194
24	C	5.094773	4.690505	7.885521	9.515230	4.432683
25	O	4.286889	3.538671	6.915461	8.630528	3.884641
26	H	4.475663	4.104656	7.152502	8.230368	3.784102
27	H	5.830825	5.066592	8.414522	9.672558	5.314408
28	H	6.064314	5.554621	8.807427	10.536920	5.458072
29	C	4.789329	4.845399	7.618930	9.236853	3.949681
30	H	4.817273	4.920147	7.531601	9.396175	4.093514
31	H	5.737492	5.885816	8.565838	10.049615	4.816484
32	H	4.009134	4.288076	6.841910	8.286795	3.060045

		11	12	13	14	15
11	H	0.000000				
12	H	2.542511	0.000000			
13	H	3.064879	1.775395	0.000000		
14	Br	4.738660	5.270387	3.792748	0.000000	
15	H	3.705857	4.180909	3.233235	2.199174	0.000000
16	C	5.565109	5.742342	5.325404	4.703556	2.814650

17	C	6.624950	6.712533	6.474908	6.001668	4.138580
18	H	5.801977	6.029425	5.294728	3.985860	2.480530
19	H	7.594233	7.670265	7.288077	6.429655	4.801542
20	H	6.724088	6.759920	6.801508	6.799775	4.782003
21	O	2.614088	2.033182	2.083870	4.978135	4.701354
22	H	3.242991	2.798092	2.197620	4.578573	4.736985
23	C	5.637726	5.302906	3.806249	3.890851	5.283026
24	C	5.550786	5.681620	4.469981	4.525792	5.908524
25	O	4.802345	4.436746	3.301102	4.482006	5.405407
26	H	5.298239	5.093625	3.439502	2.845759	4.351143
27	H	6.567551	5.913963	4.415271	4.670521	6.064887
28	H	6.444383	6.481281	5.369506	5.576099	6.992292
29	C	5.102724	5.903628	4.810666	4.172472	5.576640
30	H	4.896911	5.911918	5.118600	4.952876	6.069908
31	H	6.056914	6.958049	5.785841	4.543912	6.207952
32	H	4.419467	5.377247	4.218746	3.186744	4.542544

		16	17	18	19	20
16	C	0.000000				
17	C	1.326546	0.000000			
18	H	1.082882	2.122769	0.000000		
19	H	2.079908	1.081103	2.446782	0.000000	
20	H	2.126414	1.082593	3.100427	1.847125	0.000000
21	O	6.962330	8.108537	7.003511	9.004510	8.319361
22	H	7.213848	8.425559	7.108743	9.252098	8.748452
23	C	7.932731	9.219351	7.421633	9.782072	9.842530
24	C	8.685683	9.998979	8.223437	10.622504	10.575552
25	O	8.066125	9.339591	7.732036	10.034061	9.825990
26	H	6.979020	8.269762	6.408288	8.788529	8.946798
27	H	8.583902	9.834657	8.048131	10.350861	10.472148
28	H	9.760869	11.070668	9.296771	11.692575	11.638941
29	C	8.388166	9.710415	7.922824	10.337428	10.291906
30	H	8.846420	10.149491	8.486185	10.848753	10.644631
31	H	8.989420	10.311185	8.429824	10.863076	10.959415
32	H	7.343534	8.664487	6.872807	9.283107	9.262372

		21	22	23	24	25
21	O	0.000000				
22	H	0.977178	0.000000			
23	C	3.962788	3.019544	0.000000		
24	C	3.954453	3.006148	1.468054	0.000000	
25	O	2.783293	1.808734	1.450553	1.447938	0.000000
26	H	4.052197	3.220451	1.087397	2.208708	2.145925
27	H	4.677202	3.751411	1.086568	2.216532	2.133517
28	H	4.656304	3.721980	2.191595	1.088954	2.108764
29	C	4.201429	3.417817	2.602063	1.503870	2.520419

30	H	4.074483	3.427048	3.428190	2.149448	2.906129
31	H	5.293465	4.498384	3.166361	2.135887	3.426083
32	H	3.936403	3.260110	2.717047	2.151980	2.742999

		26	27	28	29	30
26	H	0.000000				
27	H	1.852419	0.000000			
28	H	3.120733	2.503397	0.000000		
29	C	2.812990	3.541036	2.208169	0.000000	
30	H	3.741626	4.339018	2.583485	1.094279	0.000000
31	H	3.336608	3.958115	2.531141	1.094416	1.770017
32	H	2.505300	3.772109	3.099783	1.091798	1.786778

		31	32
31	H	0.000000	
32	H	1.767925	0.000000

Stoichiometry C10H17BrN2O2
Framework group C1[X(C10H17BrN2O2)]
Deg. of freedom 90
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.714540	2.112514	-0.445265
2	6	0	-3.792557	1.348350	-0.134909
3	7	0	-3.324481	0.049731	0.039638
4	6	0	-1.992458	0.039606	-0.163107
5	7	0	-1.606790	1.278926	-0.462772
6	6	0	-0.204276	1.677610	-0.702032
7	6	0	0.454922	2.238721	0.570217
8	1	0	-2.641563	3.164716	-0.660398
9	1	0	-4.828852	1.613381	-0.031523
10	1	0	0.325504	0.785780	-1.040625
11	1	0	-0.199619	2.431936	-1.489860
12	1	0	-0.160518	3.050696	0.975900
13	1	0	0.510501	1.444107	1.323218
14	35	0	0.526797	-2.053210	-0.144243
15	1	0	-1.297086	-0.825121	-0.104030
16	6	0	-4.055622	-1.124635	0.368224
17	6	0	-5.366134	-1.167638	0.569304
18	1	0	-3.415983	-1.995678	0.437360
19	1	0	-5.830583	-2.112396	0.815279

20	1	0	-6.011639	-0.301228	0.501020
21	8	0	1.718669	2.763645	0.254732
22	1	0	2.404483	2.085467	0.411615
23	6	0	3.802744	-0.463611	1.226912
24	6	0	4.549932	0.010117	0.055386
25	8	0	3.731999	0.927237	0.821154
26	1	0	2.887191	-1.029412	1.071783
27	1	0	4.321997	-0.617949	2.168817
28	1	0	5.611887	0.210257	0.189611
29	6	0	4.112249	-0.293191	-1.351051
30	1	0	4.297305	0.563559	-2.006169
31	1	0	4.683638	-1.142783	-1.737644
32	1	0	3.053455	-0.557678	-1.383080

Rotational constants (GHZ): 0.6023882 0.2207079 0.1722443

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.

475 basis functions, 751 primitive gaussians, 492 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1307.3069266681 Hartrees.

NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 475 RedAO= T EigKep= 3.80D-06 NBF= 475

NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000224 0.000078 0.000025 Ang= 0.03 deg.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3225.52370947 A.U. after 8 cycles

NFock= 8 Conv=0.95D-08 -V/T= 2.0018

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z

1	6	0.000012312	0.000003664	-0.000025623
2	6	-0.000005121	-0.000010267	0.000023628
3	7	0.000016360	0.000012316	-0.000014227
4	6	0.000022274	-0.000030671	-0.000001410
5	7	-0.000020839	0.000055737	0.000011655
6	6	0.000006063	0.000011750	0.000016478
7	6	-0.000072909	0.000029561	0.000019126
8	1	-0.000002081	0.000001765	0.000007384
9	1	0.000001326	0.000000768	0.000008659
10	1	-0.000010408	-0.000009633	0.000007157
11	1	0.000003306	0.000009230	0.000009260
12	1	0.000016133	-0.000009825	0.000016564
13	1	0.000011309	-0.000018081	-0.000009894
14	35	0.000013305	0.000022517	-0.000007189
15	1	-0.000020279	-0.000047527	-0.000005510
16	6	-0.000005340	0.000011291	0.000003170
17	6	0.000006320	-0.000000420	-0.000004947
18	1	0.000000825	0.000001673	-0.000006483
19	1	0.000001421	0.000002468	-0.000006764
20	1	-0.000000160	0.000004991	-0.000000828
21	8	0.000043320	-0.000001382	-0.000027815
22	1	0.000027802	-0.000068347	0.000007255
23	6	0.000028454	-0.000024331	-0.000029903
24	6	0.000018705	-0.000014810	-0.000030958
25	8	-0.000088568	0.000062836	0.000065608
26	1	0.000008387	-0.000008314	-0.000002542
27	1	0.000009503	-0.000006177	-0.000009121
28	1	-0.000010530	0.000000964	0.000005265
29	6	-0.000018167	0.000012288	-0.000028034
30	1	0.000000845	0.000004481	0.000009273
31	1	-0.000002850	-0.000000332	-0.000004199
32	1	0.000009280	0.000001820	0.000004965

Cartesian Forces: Max 0.000088568 RMS 0.000022794

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000058234 RMS 0.000011178
Search for a local minimum.
Step number 31 out of a maximum of 177

All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 25 26 27 28 29
30 31
DE= -9.53D-07 DEPred=-2.54D-07 R= 3.74D+00
Trust test= 3.74D+00 RLast= 1.24D-02 DXMaxT set to 1.94D+00
ITU= 0 1 1 1 1 1 1 1 1 1 1 1 1 -1 1 1 1 1 1
ITU= 1 1 1 1 1 1 0 1 0 1 0

Eigenvalues ---	0.00003	0.00126	0.00132	0.00233	0.00289
Eigenvalues ---	0.00318	0.00628	0.01046	0.01242	0.01417
Eigenvalues ---	0.01443	0.01753	0.01899	0.01912	0.02112
Eigenvalues ---	0.02193	0.02316	0.02385	0.02680	0.02931
Eigenvalues ---	0.03063	0.03077	0.03418	0.03545	0.04068
Eigenvalues ---	0.04504	0.04635	0.05229	0.05444	0.05572
Eigenvalues ---	0.05682	0.05933	0.06739	0.09010	0.09391
Eigenvalues ---	0.10601	0.11037	0.11541	0.11809	0.12970
Eigenvalues ---	0.13854	0.14135	0.14860	0.15956	0.15992
Eigenvalues ---	0.15997	0.16001	0.16003	0.16011	0.16046
Eigenvalues ---	0.16577	0.17863	0.19128	0.21648	0.22058
Eigenvalues ---	0.22965	0.23509	0.23977	0.24220	0.25072
Eigenvalues ---	0.27690	0.28567	0.30769	0.32499	0.33107
Eigenvalues ---	0.33414	0.34049	0.34259	0.34483	0.34857
Eigenvalues ---	0.35111	0.35685	0.35689	0.35856	0.36172
Eigenvalues ---	0.36438	0.36673	0.37225	0.37262	0.37740
Eigenvalues ---	0.39322	0.42150	0.42840	0.44007	0.45927
Eigenvalues ---	0.49526	0.53838	0.55031	0.58546	0.60486

Eigenvalue 1 is 3.32D-05 Eigenvector:

	D52	D53	D55	D54	D46
1	-0.51164	0.49645	0.49499	0.48958	0.03713
	D47	D44	D43	D42	D25
1	0.03210	0.02092	0.01971	0.01952	-0.01842

En-DIIS/RFO-DIIS IScMMF= 0 using points: 31 30 29 28 27
RFO step: Lambda=-6.41796090D-08.
DidBck=F Rises=F RFO-DIIS coefs: 2.36850 -1.39102 -0.13734 0.20208 -0.04222
Iteration 1 RMS(Cart)= 0.00331993 RMS(Int)= 0.00000363
Iteration 2 RMS(Cart)= 0.00000787 RMS(Int)= 0.00000112
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000112

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56501	0.00000	0.00002	-0.00002	-0.00001	2.56501
R2	2.62004	0.00000	-0.00001	0.00003	0.00001	2.62005
R3	2.03419	0.00000	0.00000	0.00000	0.00000	2.03419

R4	2.62935	0.00000	-0.00001	0.00001	0.00001	2.62936
R5	2.03076	0.00000	0.00000	0.00000	0.00000	2.03076
R6	2.54622	-0.00001	-0.00001	-0.00001	-0.00002	2.54620
R7	2.68692	0.00000	0.00001	-0.00001	-0.00001	2.68691
R8	2.51728	-0.00006	0.00007	-0.00007	0.00000	2.51727
R9	2.09988	-0.00003	0.00003	-0.00004	-0.00001	2.09987
R10	2.79222	-0.00001	-0.00004	-0.00002	-0.00006	2.79216
R11	2.90797	0.00000	-0.00003	-0.00003	-0.00005	2.90792
R12	2.06203	-0.00001	0.00003	0.00000	0.00003	2.06206
R13	2.06119	-0.00001	0.00003	-0.00001	0.00002	2.06121
R14	2.07237	-0.00001	-0.00004	-0.00001	-0.00005	2.07232
R15	2.07139	-0.00001	0.00001	0.00000	0.00001	2.07140
R16	2.65379	0.00004	0.00021	-0.00002	0.00019	2.65398
R17	4.15584	0.00001	-0.00006	0.00029	0.00023	4.15607
R18	8.46976	0.00000	0.00124	-0.00189	-0.00065	8.46912
R19	2.50681	-0.00001	0.00001	-0.00001	0.00000	2.50681
R20	2.04635	0.00000	0.00000	0.00000	0.00000	2.04635
R21	2.04299	0.00000	0.00001	0.00000	0.00000	2.04299
R22	2.04580	0.00000	0.00000	0.00000	0.00000	2.04580
R23	1.84660	-0.00003	-0.00010	0.00001	-0.00009	1.84651
R24	3.41801	0.00000	0.00017	-0.00008	0.00009	3.41810
R25	2.77422	-0.00003	0.00004	-0.00002	0.00002	2.77424
R26	2.74115	-0.00001	0.00005	-0.00007	-0.00003	2.74112
R27	2.05488	-0.00001	0.00002	-0.00003	-0.00001	2.05487
R28	2.05332	0.00001	0.00004	-0.00002	0.00002	2.05334
R29	2.73621	-0.00001	0.00004	-0.00002	0.00002	2.73623
R30	2.05782	-0.00001	0.00000	-0.00002	-0.00002	2.05781
R31	2.84190	-0.00001	0.00001	0.00002	0.00003	2.84193
R32	2.06789	0.00000	0.00001	-0.00001	0.00000	2.06789
R33	2.06815	-0.00001	0.00000	-0.00001	-0.00001	2.06814
R34	2.06320	-0.00001	-0.00001	0.00000	-0.00001	2.06319
A1	1.87439	-0.00001	0.00002	-0.00002	0.00000	1.87439
A2	2.27817	0.00000	-0.00005	0.00000	-0.00005	2.27812
A3	2.13058	0.00000	0.00002	0.00002	0.00005	2.13063
A4	1.86184	-0.00001	0.00000	-0.00002	-0.00002	1.86182
A5	2.27710	0.00001	0.00002	0.00000	0.00002	2.27713
A6	2.14423	0.00000	-0.00002	0.00002	-0.00001	2.14422
A7	1.89727	0.00000	0.00001	0.00003	0.00003	1.89730
A8	2.24833	0.00001	-0.00001	0.00000	-0.00002	2.24831
A9	2.13757	0.00000	0.00001	-0.00002	-0.00001	2.13756
A10	1.88923	0.00001	0.00001	-0.00003	-0.00002	1.88921
A11	2.23507	-0.00001	-0.00013	0.00002	-0.00011	2.23496
A12	2.15889	0.00000	0.00013	0.00001	0.00013	2.15902
A13	1.90202	0.00001	-0.00003	0.00004	0.00001	1.90203

A14	2.21205	-0.00001	-0.00014	0.00002	-0.00012	2.21193
A15	2.16793	0.00000	0.00014	-0.00006	0.00008	2.16801
A16	1.95102	-0.00001	-0.00012	-0.00002	-0.00014	1.95087
A17	1.86561	0.00000	-0.00005	-0.00003	-0.00008	1.86553
A18	1.88348	0.00001	0.00017	-0.00001	0.00016	1.88364
A19	1.92472	0.00002	0.00005	0.00004	0.00009	1.92481
A20	1.92108	0.00000	0.00010	-0.00001	0.00009	1.92117
A21	1.91668	-0.00001	-0.00014	0.00002	-0.00013	1.91656
A22	1.91285	0.00000	0.00010	0.00006	0.00015	1.91300
A23	1.90217	0.00002	-0.00002	0.00006	0.00004	1.90221
A24	1.91352	0.00001	0.00010	0.00001	0.00012	1.91364
A25	1.88712	0.00000	0.00001	-0.00002	-0.00001	1.88710
A26	1.88743	-0.00001	-0.00008	-0.00009	-0.00017	1.88725
A27	1.96023	-0.00001	-0.00010	-0.00002	-0.00012	1.96011
A28	1.79036	-0.00003	-0.00082	0.00008	-0.00075	1.78961
A29	2.83241	0.00003	0.00010	-0.00010	-0.00001	2.83240
A30	2.17707	0.00000	0.00004	-0.00002	0.00002	2.17708
A31	1.95560	0.00000	0.00002	0.00000	0.00002	1.95562
A32	2.15052	0.00000	-0.00005	0.00002	-0.00003	2.15048
A33	2.07971	0.00000	-0.00004	0.00000	-0.00003	2.07968
A34	2.15741	0.00000	0.00005	0.00000	0.00004	2.15746
A35	2.04606	0.00000	-0.00001	0.00000	-0.00001	2.04605
A36	1.91356	-0.00002	-0.00045	0.00001	-0.00045	1.91311
A37	3.05073	0.00000	0.00026	-0.00014	0.00011	3.05084
A38	2.07441	-0.00001	0.00019	-0.00001	0.00018	2.07459
A39	2.08791	0.00000	-0.00015	0.00002	-0.00012	2.08779
A40	2.00197	-0.00001	0.00030	-0.00016	0.00014	2.00211
A41	1.98448	0.00001	-0.00015	0.00007	-0.00008	1.98440
A42	2.03994	0.00001	-0.00010	0.00003	-0.00007	2.03987
A43	2.04574	-0.00002	0.00011	-0.00010	0.00002	2.04576
A44	2.13306	0.00001	-0.00014	0.00003	-0.00010	2.13295
A45	1.94904	0.00001	-0.00001	0.00016	0.00014	1.94918
A46	2.04648	-0.00001	-0.00011	-0.00005	-0.00017	2.04631
A47	2.02213	0.00000	0.00008	0.00001	0.00008	2.02221
A48	1.42244	0.00001	0.00130	0.00060	0.00191	1.42435
A49	0.99741	0.00002	-0.00039	0.00027	-0.00011	0.99729
A50	2.36475	0.00004	0.00067	0.00064	0.00131	2.36606
A51	2.34683	0.00000	0.00106	0.00073	0.00180	2.34862
A52	1.93132	0.00001	-0.00001	0.00000	-0.00001	1.93131
A53	1.91237	0.00000	0.00010	-0.00004	0.00005	1.91243
A54	1.93749	0.00001	-0.00010	0.00006	-0.00004	1.93745
A55	1.88391	-0.00001	0.00002	-0.00001	0.00001	1.88392
A56	1.91357	-0.00001	-0.00002	0.00000	-0.00002	1.91355
A57	1.88377	-0.00001	0.00002	0.00000	0.00002	1.88379

A58	3.76927	0.00001	0.00236	0.00134	0.00370	3.77297
A59	5.05131	-0.00001	-0.00094	-0.00051	-0.00145	5.04986
D1	0.00418	0.00001	0.00022	-0.00011	0.00011	0.00429
D2	-3.13108	0.00001	0.00036	0.00000	0.00036	-3.13073
D3	3.13646	0.00000	-0.00041	-0.00010	-0.00051	3.13594
D4	0.00119	0.00000	-0.00028	0.00001	-0.00027	0.00092
D5	-0.00678	-0.00001	-0.00010	-0.00006	-0.00016	-0.00694
D6	-3.09755	-0.00001	0.00051	-0.00008	0.00043	-3.09713
D7	-3.14001	0.00000	0.00047	-0.00007	0.00040	-3.13961
D8	0.05240	0.00000	0.00108	-0.00009	0.00099	0.05338
D9	-0.00023	-0.00001	-0.00027	0.00025	-0.00002	-0.00026
D10	-3.13601	0.00000	-0.00033	0.00009	-0.00024	-3.13625
D11	3.13563	0.00000	-0.00039	0.00014	-0.00025	3.13538
D12	-0.00014	0.00000	-0.00045	-0.00001	-0.00047	-0.00061
D13	-0.00399	0.00000	0.00021	-0.00029	-0.00007	-0.00406
D14	3.13959	0.00000	-0.00108	-0.00030	-0.00138	3.13821
D15	3.13223	0.00000	0.00027	-0.00014	0.00013	3.13235
D16	-0.00738	0.00000	-0.00102	-0.00016	-0.00118	-0.00856
D17	0.00073	0.00000	-0.00001	-0.00008	-0.00009	0.00064
D18	-3.14137	0.00000	0.00003	0.00003	0.00006	-3.14131
D19	-3.13433	0.00000	-0.00008	-0.00026	-0.00034	-3.13466
D20	0.00676	0.00000	-0.00004	-0.00014	-0.00019	0.00657
D21	0.00663	0.00001	-0.00007	0.00022	0.00014	0.00678
D22	3.09899	0.00001	-0.00067	0.00024	-0.00043	3.09855
D23	-3.13684	0.00001	0.00115	0.00023	0.00138	-3.13546
D24	-0.04449	0.00001	0.00055	0.00025	0.00080	-0.04368
D25	-3.13521	0.00001	0.00440	0.00190	0.00630	-3.12891
D26	0.00866	0.00000	0.00292	0.00188	0.00481	0.01346
D27	1.42322	-0.00001	-0.00395	-0.00130	-0.00525	1.41797
D28	-2.75232	0.00000	-0.00400	-0.00127	-0.00527	-2.75759
D29	-0.69161	0.00000	-0.00410	-0.00128	-0.00538	-0.69699
D30	-1.66026	-0.00001	-0.00325	-0.00133	-0.00458	-1.66483
D31	0.44739	0.00000	-0.00330	-0.00130	-0.00460	0.44279
D32	2.50810	0.00000	-0.00340	-0.00130	-0.00471	2.50339
D33	-0.93809	0.00000	-0.00022	-0.00005	-0.00027	-0.93836
D34	1.12393	0.00000	-0.00017	0.00000	-0.00017	1.12375
D35	-3.00722	0.00000	-0.00024	0.00002	-0.00022	-3.00744
D36	-3.01097	-0.00001	-0.00011	-0.00003	-0.00014	-3.01111
D37	-0.94896	0.00000	-0.00005	0.00002	-0.00004	-0.94900
D38	1.20309	0.00000	-0.00013	0.00004	-0.00009	1.20300
D39	1.15482	-0.00001	-0.00003	-0.00007	-0.00010	1.15472
D40	-3.06636	0.00000	0.00003	-0.00003	0.00000	-3.06636
D41	-0.91431	0.00000	-0.00005	-0.00001	-0.00005	-0.91436
D42	-1.64682	0.00000	0.00076	0.00103	0.00179	-1.64503

D43	2.55156	0.00000	0.00063	0.00101	0.00164	2.55320
D44	0.47062	0.00002	0.00073	0.00111	0.00184	0.47246
D45	0.46088	0.00000	-0.00278	-0.00224	-0.00502	0.45586
D46	-0.27133	-0.00001	-0.00162	-0.00004	-0.00165	-0.27298
D47	2.56857	0.00000	-0.00217	-0.00053	-0.00270	2.56587
D48	3.14144	0.00000	-0.00002	0.00012	0.00010	3.14154
D49	0.00039	0.00000	0.00000	0.00003	0.00003	0.00042
D50	0.00042	0.00000	-0.00006	0.00000	-0.00007	0.00035
D51	-3.14064	0.00000	-0.00004	-0.00010	-0.00014	-3.14078
D52	-1.99978	0.00000	0.01180	0.00656	0.01836	-1.98142
D53	2.50625	0.00000	-0.01025	-0.00652	-0.01676	2.48949
D54	2.14219	-0.00002	-0.01109	-0.00743	-0.01852	2.12367
D55	-2.54506	0.00001	-0.00930	-0.00600	-0.01531	-2.56037
D56	-2.72926	0.00001	0.00020	0.00004	0.00025	-2.72901
D57	-0.03015	0.00001	0.00036	-0.00010	0.00026	-0.02989
D58	-0.02179	0.00000	0.00004	0.00015	0.00019	-0.02160
D59	2.67732	0.00001	0.00019	0.00002	0.00021	2.67753
D60	-0.17043	-0.00001	0.00022	-0.00005	0.00016	-0.17026
D61	0.26214	0.00000	0.00145	0.00102	0.00247	0.26460
D62	-2.58249	-0.00002	0.00021	0.00001	0.00021	-2.58228
D63	-2.14993	0.00000	0.00144	0.00108	0.00251	-2.14741
D64	2.15770	-0.00002	-0.00112	-0.00074	-0.00186	2.15585
D65	-0.23531	-0.00003	-0.00109	-0.00088	-0.00197	-0.23728
D66	2.48781	0.00000	-0.00010	0.00033	0.00023	2.48804
D67	-1.72005	0.00000	-0.00003	0.00029	0.00027	-1.71978
D68	0.35892	0.00000	0.00000	0.00030	0.00029	0.35922
D69	1.27145	0.00000	-0.00001	0.00037	0.00036	1.27181
D70	-2.93641	0.00000	0.00007	0.00033	0.00040	-2.93601
D71	-0.85744	0.00000	0.00009	0.00034	0.00043	-0.85701
D72	-1.09072	0.00000	0.00006	0.00017	0.00023	-1.09049
D73	0.98461	0.00000	0.00013	0.00013	0.00026	0.98487
D74	3.06358	0.00000	0.00016	0.00014	0.00029	3.06387

Item	Value	Threshold	Converged?
Maximum Force	0.000058	0.000450	YES
RMS Force	0.000011	0.000300	YES
Maximum Displacement	0.011953	0.001800	NO
RMS Displacement	0.003322	0.001200	NO

Predicted change in Energy=-2.626672D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-1.378217	-1.911133	-0.251316
2	6	0	-2.510024	-1.171185	-0.133543
3	7	0	-2.112290	0.111707	0.229744
4	6	0	-0.768646	0.136270	0.327109
5	7	0	-0.307724	-1.081138	0.044422
6	6	0	1.125685	-1.436245	-0.004437
7	6	0	1.682890	-1.365295	-1.437058
8	1	0	-1.243763	-2.947527	-0.509285
9	1	0	-3.540090	-1.445672	-0.269408
10	1	0	1.649595	-0.729100	0.640676
11	1	0	1.234687	-2.447304	0.390034
12	1	0	1.064414	-1.978700	-2.103251
13	1	0	1.635494	-0.327666	-1.787201
14	35	0	1.652846	2.228898	1.023466
15	1	0	-0.116813	0.995865	0.593539
16	6	0	-2.917013	1.256481	0.481879
17	6	0	-4.241205	1.281013	0.406810
18	1	0	-2.321793	2.121433	0.746844
19	1	0	-4.763727	2.203634	0.617823
20	1	0	-4.842583	0.420240	0.143330
21	8	0	2.990680	-1.876701	-1.460844
22	1	0	3.630829	-1.144964	-1.363115
23	6	0	4.840051	1.612125	-1.120427
24	6	0	5.715927	0.751987	-0.315303
25	8	0	4.864145	0.177865	-1.335798
26	1	0	3.922333	1.989709	-0.675852
27	1	0	5.258709	2.184454	-1.943723
28	1	0	6.766856	0.708370	-0.597166
29	6	0	5.405432	0.406546	1.115059
30	1	0	5.687355	-0.628258	1.332199
31	1	0	5.977356	1.058849	1.782247
32	1	0	4.345069	0.551055	1.331301

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357344	0.000000			
3	N	2.205031	1.391395	0.000000		
4	C	2.213145	2.225767	1.347390	0.000000	
5	N	1.386472	2.211313	2.171101	1.332083	0.000000
6	C	2.560467	3.647644	3.596592	2.484193	1.477548
7	C	3.327807	4.395152	4.400358	3.372983	2.497614
8	H	1.076447	2.213592	3.264875	3.230340	2.160131

9	H	2.211487	1.074633	2.170989	3.246425	3.267960
10	H	3.370534	4.254091	3.876545	2.587486	2.076186
11	H	2.743370	3.990674	4.216217	3.269887	2.089232
12	H	3.066052	4.160341	4.461402	3.706731	2.702013
13	H	3.734804	4.542183	4.278668	3.235032	2.774645
14	Br	5.286991	5.498066	4.391895	3.275306	3.969724
15	H	3.279566	3.309412	2.212692	1.111204	2.156830
16	C	3.597116	2.537311	1.421851	2.427819	3.530471
17	C	4.338159	3.049957	2.435346	3.657247	4.602538
18	H	4.260076	3.413480	2.085733	2.555252	3.847900
19	H	5.398924	4.127121	3.399542	4.507680	5.565472
20	H	4.194386	2.837273	2.749029	4.087955	4.777956
21	O	4.533365	5.702388	5.731679	4.623998	3.711901
22	H	5.187837	6.262796	6.090964	4.884036	4.182994
23	C	7.199691	7.921134	7.239424	5.977541	5.925380
24	C	7.577809	8.449728	7.873247	6.545342	6.306673
25	O	6.671364	7.592347	7.150241	5.873273	5.498939
26	H	6.594894	7.187529	6.384643	5.142612	5.276579
27	H	7.980405	8.653917	7.959389	6.758754	6.752925
28	H	8.562921	9.476718	8.937506	7.613500	7.325549
29	C	7.297705	8.167171	7.575411	6.230020	5.999968
30	H	7.353611	8.345070	7.911853	6.578348	6.148532
31	H	8.189055	8.982145	8.291545	6.962552	6.863077
32	H	6.428300	7.218323	6.565358	5.227861	5.095939

		6	7	8	9	10
6	C	0.000000				
7	C	1.538804	0.000000			
8	H	2.855368	3.453914	0.000000		
9	H	4.673302	5.352512	2.754310	0.000000	
10	H	1.091195	2.173208	3.823003	5.317383	0.000000
11	H	1.090747	2.170229	2.683601	4.923071	1.785272
12	H	2.168647	1.096626	2.967665	4.984832	3.071331
13	H	2.160347	1.096138	4.097177	5.508203	2.460881
14	Br	3.842884	4.355836	6.126585	6.491577	2.982665
15	H	2.795806	3.596850	4.246948	4.292389	2.469397
16	C	4.881668	5.631620	4.632046	2.873028	4.982134
17	C	6.029604	6.745198	5.263500	2.895452	6.228706
18	H	5.010649	5.741445	5.332388	3.904005	4.889656
19	H	6.951338	7.649749	6.339951	3.949924	7.052103
20	H	6.252087	6.947486	4.971847	2.312675	6.611862
21	O	2.406934	1.404427	4.470194	6.652537	2.744428
22	H	2.864717	1.961754	5.266869	7.260076	2.848405
23	C	4.933002	4.351201	7.627366	8.961089	4.331492
24	C	5.094637	4.691120	7.884245	9.513447	4.431994

25	O	4.284153	3.537228	6.910698	8.625788	3.881027
26	H	4.473165	4.104947	7.147908	8.225254	3.780279
27	H	5.826850	5.063981	8.406960	9.664368	5.309767
28	H	6.064117	5.554477	8.805869	10.534726	5.457558
29	C	4.792221	4.848716	7.622342	9.239579	3.952346
30	H	4.821646	4.924200	7.537272	9.401013	4.097789
31	H	5.740771	5.889214	8.570107	10.053044	4.819695
32	H	4.012230	4.292250	6.845646	8.290049	3.062897

		11	12	13	14	15
11	H	0.000000				
12	H	2.542646	0.000000			
13	H	3.064941	1.775368	0.000000		
14	Br	4.737400	5.275082	3.799496	0.000000	
15	H	3.704508	4.185213	3.238863	2.199296	0.000000
16	C	5.564448	5.744654	5.327623	4.703459	2.814518
17	C	6.624653	6.713846	6.475887	6.001549	4.138452
18	H	5.800795	6.033285	5.299018	3.985703	2.480392
19	H	7.593687	7.672248	7.289832	6.429432	4.801365
20	H	6.724350	6.759782	6.800867	6.799742	4.781938
21	O	2.614354	2.033123	2.083878	4.981721	4.704108
22	H	3.242085	2.798107	2.197541	4.581608	4.738825
23	C	5.635522	5.302395	3.804809	3.890368	5.280905
24	C	5.551079	5.682428	4.470132	4.525726	5.908158
25	O	4.800310	4.435956	3.299018	4.481663	5.403833
26	H	5.295908	5.094451	3.440198	2.845253	4.348998
27	H	6.564477	5.911802	4.411682	4.669950	6.061905
28	H	6.444978	6.481240	5.368467	5.575980	6.991805
29	C	5.105412	5.906890	4.814002	4.172679	5.578035
30	H	4.901311	5.915876	5.122362	4.953375	6.072213
31	H	6.060056	6.961379	5.789228	4.543804	6.209340
32	H	4.421608	5.381310	4.223625	3.187159	4.544286

		16	17	18	19	20
16	C	0.000000				
17	C	1.326545	0.000000			
18	H	1.082883	2.122751	0.000000		
19	H	2.079887	1.081104	2.446721	0.000000	
20	H	2.126437	1.082593	3.100431	1.847122	0.000000
21	O	6.963608	8.109220	7.005807	9.005599	8.319214
22	H	7.214235	8.425374	7.110203	9.252340	8.747454
23	C	7.928803	9.214733	7.418768	9.777727	9.837229
24	C	8.684335	9.997290	8.222438	10.620789	10.573672
25	O	8.063113	9.336007	7.729978	10.030767	9.821769
26	H	6.975287	8.265456	6.405508	8.784475	8.941927
27	H	8.578294	9.828000	8.044075	10.344617	10.464433

28	H	9.759206	11.068573	9.295518	11.690439	11.636599
29	C	8.389660	9.712050	7.923789	10.338692	10.293991
30	H	8.849319	10.152732	8.488221	10.851500	10.648585
31	H	8.991097	10.313107	8.430719	10.864497	10.961978
32	H	7.345541	8.666696	6.874207	9.284946	9.265060

		21	22	23	24	25
21	O	0.000000				
22	H	0.977129	0.000000			
23	C	3.963327	3.020373	0.000000		
24	C	3.955912	3.007319	1.468066	0.000000	
25	O	2.783299	1.808782	1.450540	1.447950	0.000000
26	H	4.053803	3.222341	1.087393	2.208831	2.146000
27	H	4.676549	3.751283	1.086578	2.216475	2.133460
28	H	4.657042	3.722390	2.191609	1.088945	2.108867
29	C	4.204703	3.420197	2.602013	1.503886	2.520315
30	H	4.078205	3.429432	3.428208	2.149455	2.906152
31	H	5.296729	4.500699	3.166243	2.135937	3.426015
32	H	3.940107	3.262898	2.716955	2.151960	2.742651

		26	27	28	29	30
26	H	0.000000				
27	H	1.852383	0.000000			
28	H	3.120791	2.503307	0.000000		
29	C	2.813068	3.540994	2.208233	0.000000	
30	H	3.741835	4.338981	2.583476	1.094281	0.000000
31	H	3.336447	3.958067	2.531355	1.094412	1.770022
32	H	2.505414	3.772071	3.099805	1.091794	1.786761

		31	32
31	H	0.000000	
32	H	1.767928	0.000000

Stoichiometry C10H17BrN2O2
Framework group C1[X(C10H17BrN2O2)]
Deg. of freedom 90
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.713566	2.112584	-0.443459
2	6	0	-3.791545	1.348629	-0.132468
3	7	0	-3.323897	0.049549	0.039802
4	6	0	-1.992193	0.038929	-0.164922

5	7	0	-1.606315	1.278384	-0.463740
6	6	0	-0.203954	1.676818	-0.704124
7	6	0	0.454647	2.242359	0.566437
8	1	0	-2.640444	3.164936	-0.657811
9	1	0	-4.827579	1.614034	-0.027439
10	1	0	0.326161	0.784013	-1.039661
11	1	0	-0.199299	2.428450	-1.494538
12	1	0	-0.160984	3.055577	0.969258
13	1	0	0.510223	1.450310	1.322141
14	35	0	0.526841	-2.054326	-0.145315
15	1	0	-1.297133	-0.826102	-0.106723
16	6	0	-4.055154	-1.124772	0.368275
17	6	0	-5.365333	-1.167260	0.571614
18	1	0	-3.415902	-1.996257	0.435398
19	1	0	-5.829848	-2.112043	0.817371
20	1	0	-6.010497	-0.300428	0.505484
21	8	0	1.718487	2.766611	0.249763
22	1	0	2.403901	2.088363	0.407778
23	6	0	3.798675	-0.461290	1.230294
24	6	0	4.549224	0.009784	0.059830
25	8	0	3.728961	0.928589	0.821096
26	1	0	2.883658	-1.027634	1.074022
27	1	0	4.315317	-0.613301	2.174024
28	1	0	5.610789	0.210207	0.196618
29	6	0	4.115415	-0.296756	-1.347123
30	1	0	4.302532	0.558401	-2.003739
31	1	0	4.687615	-1.147420	-1.730129
32	1	0	3.056634	-0.560986	-1.381465

Rotational constants (GHZ): 0.6018059 0.2208022 0.1722490

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.

475 basis functions, 751 primitive gaussians, 492 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1307.2676636064 Hartrees.

NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 475 RedAO= T EigKep= 3.79D-06 NBF= 475

NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 0.000324 0.000096 -0.000001 Ang= 0.04 deg.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3225.52371082 A.U. after 9 cycles
NFock= 9 Conv=0.52D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000001728	-0.000011656	0.000017347
2	6	0.000004250	-0.000008921	0.000034969
3	7	-0.000000164	0.000021319	-0.000017763
4	6	0.000022453	-0.000030140	-0.000017793
5	7	-0.000022234	0.000063358	-0.000017886
6	6	0.000017058	0.000012467	0.000026152
7	6	-0.000004430	0.000004415	0.000023260
8	1	0.000000907	0.000005187	-0.000003741
9	1	0.000001977	0.000001448	0.000003122
10	1	-0.000013590	-0.000006718	0.000005779
11	1	0.000000330	0.000005270	-0.000001048
12	1	0.000009693	-0.000011178	0.000014146
13	1	0.000003761	-0.000015701	-0.000014251
14	35	0.000004137	0.000018552	-0.000007783
15	1	-0.000011237	-0.000059388	0.000013674
16	6	-0.000007471	0.000015798	-0.000003413
17	6	0.000003842	0.000003030	-0.000004798
18	1	0.000002556	0.000000488	-0.000005802
19	1	0.000000084	0.000001173	-0.000005351
20	1	0.000001830	0.000003339	0.000000113
21	8	-0.000035108	0.000013443	-0.000021456
22	1	0.000059809	-0.000052654	0.000008103
23	6	0.000052532	-0.000015285	-0.000053070
24	6	-0.000029170	-0.000013841	-0.000005981
25	8	-0.000066847	0.000066423	0.000054763
26	1	0.000006232	-0.000019903	0.000008195
27	1	0.000007517	-0.000004168	-0.000006383
28	1	-0.000008437	-0.000006967	-0.000000543

29	6	-0.000007512	0.000011188	-0.000034885
30	1	0.000000957	0.000005665	0.000010522
31	1	-0.000000843	0.000001517	-0.000004173
32	1	0.000008845	0.000002439	0.000005974

Cartesian Forces: Max 0.000066847 RMS 0.000021942

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000057955 RMS 0.000011054
Search for a local minimum.
Step number 32 out of a maximum of 177
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 25 26 27 28 29
30 31 32
DE= -1.34D-06 DEPred=-2.63D-07 R= 5.12D+00
TightC=F SS= 1.41D+00 RLast= 3.88D-02 DXNew= 3.2661D+00 1.1646D-01
Trust test= 5.12D+00 RLast= 3.88D-02 DXMaxT set to 1.94D+00
ITU= 1 0 1 1 1 1 1 1 1 1 1 1 1 1 -1 1 1 1 1
ITU= 1 1 1 1 1 1 1 0 1 0 1 0

Eigenvalues ---	0.00003	0.00087	0.00131	0.00234	0.00278
Eigenvalues ---	0.00327	0.00634	0.01059	0.01260	0.01366
Eigenvalues ---	0.01482	0.01761	0.01821	0.01924	0.02125
Eigenvalues ---	0.02206	0.02317	0.02376	0.02425	0.02976
Eigenvalues ---	0.03061	0.03084	0.03417	0.03565	0.03879
Eigenvalues ---	0.04422	0.04630	0.05204	0.05443	0.05561
Eigenvalues ---	0.05678	0.05928	0.06512	0.09304	0.09433
Eigenvalues ---	0.10526	0.11071	0.11544	0.11743	0.13079
Eigenvalues ---	0.13853	0.14138	0.15131	0.15955	0.15993
Eigenvalues ---	0.16000	0.16001	0.16006	0.16015	0.16045
Eigenvalues ---	0.16637	0.17994	0.19335	0.21706	0.22083
Eigenvalues ---	0.23035	0.23667	0.23918	0.24263	0.25045
Eigenvalues ---	0.27800	0.28580	0.30769	0.32418	0.33103
Eigenvalues ---	0.33341	0.34053	0.34181	0.34470	0.34851
Eigenvalues ---	0.35104	0.35686	0.35690	0.35858	0.36166
Eigenvalues ---	0.36438	0.36671	0.37234	0.37258	0.37800
Eigenvalues ---	0.38559	0.42157	0.42665	0.45224	0.45973
Eigenvalues ---	0.49343	0.53877	0.55064	0.57458	0.60420

Eigenvalue 1 is 3.19D-05 Eigenvector:

	D52	D53	D54	D55	D46
1	0.51101	-0.49548	-0.49396	-0.49156	-0.03559
	D47	D25	D26	D44	D43
1	-0.03345	0.02951	0.02218	-0.01469	-0.01409

En-DIIS/RFO-DIIS IScMMF= 0 using points: 32 31 30 29 28

RFO step: Lambda=-5.94704012D-08.

DidBck=F Rises=F RFO-DIIS coefs: 2.09954 -1.06025 -0.38004 0.32262 0.01813

Iteration 1 RMS(Cart)= 0.00338053 RMS(Int)= 0.00001369

Iteration 2 RMS(Cart)= 0.00001202 RMS(Int)= 0.00000313

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000313

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56501	0.00000	0.00001	0.00000	0.00001	2.56501
R2	2.62005	0.00000	0.00001	0.00002	0.00002	2.62007
R3	2.03419	0.00000	0.00000	0.00000	0.00000	2.03419
R4	2.62936	0.00000	0.00002	-0.00001	0.00002	2.62937
R5	2.03076	0.00000	-0.00001	0.00000	-0.00001	2.03076
R6	2.54620	0.00000	-0.00004	0.00002	-0.00002	2.54618
R7	2.68691	0.00001	0.00001	0.00001	0.00002	2.68693
R8	2.51727	-0.00006	-0.00010	0.00001	-0.00009	2.51718
R9	2.09987	-0.00004	-0.00015	0.00002	-0.00014	2.09973
R10	2.79216	0.00000	-0.00006	0.00005	0.00000	2.79216
R11	2.90792	0.00000	-0.00010	0.00003	-0.00007	2.90785
R12	2.06206	-0.00001	-0.00001	0.00001	0.00000	2.06206
R13	2.06121	-0.00001	0.00001	0.00000	0.00002	2.06123
R14	2.07232	-0.00001	-0.00007	0.00001	-0.00006	2.07226
R15	2.07140	-0.00001	-0.00003	0.00002	-0.00001	2.07139
R16	2.65398	-0.00001	0.00023	-0.00008	0.00016	2.65414
R17	4.15607	0.00001	0.00058	-0.00006	0.00052	4.15659
R18	8.46912	0.00000	-0.00113	-0.00018	-0.00130	8.46781
R19	2.50681	0.00000	-0.00001	0.00000	-0.00001	2.50680
R20	2.04635	0.00000	0.00000	0.00000	0.00000	2.04635
R21	2.04299	0.00000	0.00000	0.00000	0.00000	2.04299
R22	2.04580	0.00000	0.00000	0.00000	0.00000	2.04580
R23	1.84651	0.00000	-0.00012	0.00003	-0.00008	1.84642
R24	3.41810	0.00000	0.00016	0.00010	0.00026	3.41836
R25	2.77424	-0.00003	0.00004	-0.00003	0.00001	2.77425
R26	2.74112	-0.00002	-0.00014	0.00001	-0.00013	2.74100
R27	2.05487	0.00000	-0.00002	0.00001	-0.00001	2.05486
R28	2.05334	0.00000	0.00002	0.00000	0.00003	2.05336
R29	2.73623	-0.00002	-0.00006	0.00000	-0.00006	2.73617
R30	2.05781	-0.00001	-0.00004	0.00001	-0.00003	2.05778
R31	2.84193	-0.00002	0.00000	-0.00005	-0.00005	2.84188

R32	2.06789	0.00000	0.00001	0.00000	0.00001	2.06790
R33	2.06814	0.00000	-0.00001	0.00001	0.00000	2.06814
R34	2.06319	-0.00001	-0.00002	0.00000	-0.00002	2.06317
A1	1.87439	-0.00001	-0.00002	0.00000	-0.00002	1.87437
A2	2.27812	0.00000	-0.00003	0.00001	-0.00003	2.27810
A3	2.13063	0.00000	0.00005	-0.00001	0.00005	2.13067
A4	1.86182	0.00000	-0.00002	0.00003	0.00001	1.86183
A5	2.27713	0.00000	0.00003	-0.00002	0.00001	2.27713
A6	2.14422	0.00000	-0.00001	-0.00001	-0.00002	2.14420
A7	1.89730	-0.00001	-0.00001	-0.00004	-0.00005	1.89725
A8	2.24831	0.00001	0.00001	0.00002	0.00003	2.24835
A9	2.13756	0.00000	-0.00001	0.00002	0.00001	2.13757
A10	1.88921	0.00002	0.00002	0.00004	0.00006	1.88927
A11	2.23496	-0.00001	-0.00011	-0.00006	-0.00017	2.23479
A12	2.15902	-0.00001	0.00009	0.00002	0.00011	2.15913
A13	1.90203	0.00001	0.00002	-0.00003	-0.00001	1.90202
A14	2.21193	0.00001	-0.00009	0.00001	-0.00007	2.21186
A15	2.16801	-0.00001	0.00005	0.00003	0.00008	2.16809
A16	1.95087	0.00000	-0.00017	0.00006	-0.00011	1.95076
A17	1.86553	-0.00001	-0.00004	-0.00008	-0.00013	1.86540
A18	1.88364	0.00000	0.00010	0.00004	0.00015	1.88379
A19	1.92481	0.00002	0.00022	0.00000	0.00023	1.92504
A20	1.92117	-0.00001	0.00001	-0.00006	-0.00005	1.92112
A21	1.91656	0.00000	-0.00013	0.00004	-0.00010	1.91646
A22	1.91300	-0.00001	0.00008	0.00000	0.00007	1.91307
A23	1.90221	0.00002	0.00018	0.00001	0.00019	1.90240
A24	1.91364	0.00001	0.00006	0.00009	0.00015	1.91379
A25	1.88710	0.00000	0.00007	-0.00009	-0.00001	1.88709
A26	1.88725	-0.00001	-0.00025	-0.00004	-0.00029	1.88696
A27	1.96011	-0.00001	-0.00015	0.00004	-0.00012	1.96000
A28	1.78961	-0.00002	-0.00052	-0.00011	-0.00063	1.78898
A29	2.83240	0.00004	-0.00003	0.00015	0.00011	2.83251
A30	2.17708	0.00000	0.00000	0.00000	0.00000	2.17708
A31	1.95562	0.00000	0.00001	-0.00001	0.00000	1.95561
A32	2.15048	0.00000	-0.00001	0.00001	0.00000	2.15049
A33	2.07968	0.00000	-0.00003	0.00002	-0.00001	2.07967
A34	2.15746	0.00000	0.00004	-0.00002	0.00002	2.15747
A35	2.04605	0.00000	-0.00001	0.00000	-0.00001	2.04604
A36	1.91311	0.00000	-0.00046	0.00008	-0.00037	1.91274
A37	3.05084	0.00001	-0.00034	0.00012	-0.00024	3.05060
A38	2.07459	-0.00003	0.00009	-0.00014	-0.00005	2.07454
A39	2.08779	0.00001	-0.00011	0.00002	-0.00009	2.08770
A40	2.00211	-0.00001	0.00008	0.00001	0.00009	2.00220
A41	1.98440	0.00001	-0.00008	0.00009	0.00001	1.98441

A42	2.03987	0.00001	0.00002	0.00004	0.00006	2.03993
A43	2.04576	-0.00002	0.00002	0.00000	0.00002	2.04578
A44	2.13295	0.00002	-0.00010	0.00001	-0.00008	2.13287
A45	1.94918	0.00000	0.00016	-0.00010	0.00006	1.94924
A46	2.04631	0.00000	-0.00018	0.00012	-0.00006	2.04625
A47	2.02221	0.00000	0.00009	-0.00003	0.00006	2.02227
A48	1.42435	0.00000	0.00169	0.00051	0.00220	1.42655
A49	0.99729	0.00004	0.00051	0.00021	0.00071	0.99800
A50	2.36606	0.00004	0.00175	0.00067	0.00242	2.36847
A51	2.34862	-0.00001	0.00112	0.00036	0.00147	2.35010
A52	1.93131	0.00001	0.00004	0.00001	0.00005	1.93135
A53	1.91243	0.00000	0.00004	0.00000	0.00004	1.91246
A54	1.93745	0.00001	0.00004	0.00000	0.00004	1.93749
A55	1.88392	-0.00001	-0.00007	0.00000	-0.00007	1.88385
A56	1.91355	-0.00001	-0.00002	-0.00001	-0.00003	1.91352
A57	1.88379	-0.00001	-0.00003	0.00000	-0.00003	1.88376
A58	3.77297	-0.00001	0.00281	0.00087	0.00368	3.77665
A59	5.04986	0.00000	-0.00127	-0.00071	-0.00198	5.04787
D1	0.00429	0.00001	0.00025	-0.00002	0.00022	0.00451
D2	-3.13073	0.00000	0.00033	-0.00019	0.00014	-3.13059
D3	3.13594	0.00001	-0.00033	0.00022	-0.00011	3.13583
D4	0.00092	0.00000	-0.00024	0.00004	-0.00019	0.00073
D5	-0.00694	0.00000	-0.00019	0.00016	-0.00004	-0.00697
D6	-3.09713	-0.00001	0.00006	-0.00017	-0.00010	-3.09723
D7	-3.13961	0.00000	0.00032	-0.00006	0.00026	-3.13935
D8	0.05338	-0.00001	0.00058	-0.00038	0.00020	0.05358
D9	-0.00026	-0.00001	-0.00022	-0.00012	-0.00033	-0.00059
D10	-3.13625	0.00000	-0.00026	-0.00006	-0.00032	-3.13657
D11	3.13538	0.00000	-0.00030	0.00004	-0.00026	3.13512
D12	-0.00061	0.00000	-0.00034	0.00010	-0.00025	-0.00086
D13	-0.00406	0.00001	0.00010	0.00022	0.00031	-0.00375
D14	3.13821	0.00001	-0.00121	0.00018	-0.00103	3.13718
D15	3.13235	0.00000	0.00014	0.00016	0.00031	3.13266
D16	-0.00856	0.00000	-0.00117	0.00013	-0.00104	-0.00959
D17	0.00064	0.00000	-0.00035	0.00006	-0.00029	0.00035
D18	-3.14131	0.00000	-0.00022	0.00003	-0.00019	-3.14151
D19	-3.13466	0.00000	-0.00041	0.00013	-0.00028	-3.13494
D20	0.00657	0.00000	-0.00028	0.00009	-0.00018	0.00639
D21	0.00678	0.00000	0.00006	-0.00023	-0.00017	0.00660
D22	3.09855	0.00000	-0.00020	0.00008	-0.00011	3.09844
D23	-3.13546	0.00000	0.00130	-0.00020	0.00110	-3.13437
D24	-0.04368	0.00000	0.00104	0.00012	0.00116	-0.04253
D25	-3.12891	0.00000	0.00622	0.00238	0.00860	-3.12031
D26	0.01346	0.00000	0.00472	0.00234	0.00707	0.02053

D27	1.41797	-0.00001	-0.00405	-0.00093	-0.00498	1.41299
D28	-2.75759	0.00001	-0.00390	-0.00094	-0.00485	-2.76244
D29	-0.69699	0.00000	-0.00403	-0.00092	-0.00495	-0.70194
D30	-1.66483	-0.00001	-0.00376	-0.00129	-0.00505	-1.66989
D31	0.44279	0.00000	-0.00361	-0.00131	-0.00492	0.43787
D32	2.50339	0.00000	-0.00374	-0.00129	-0.00502	2.49836
D33	-0.93836	0.00000	0.00008	-0.00027	-0.00019	-0.93855
D34	1.12375	0.00000	0.00032	-0.00037	-0.00005	1.12370
D35	-3.00744	0.00000	0.00029	-0.00026	0.00003	-3.00741
D36	-3.01111	0.00000	0.00009	-0.00021	-0.00011	-3.01122
D37	-0.94900	0.00000	0.00033	-0.00031	0.00002	-0.94897
D38	1.20300	0.00000	0.00030	-0.00020	0.00010	1.20310
D39	1.15472	-0.00001	0.00011	-0.00022	-0.00011	1.15460
D40	-3.06636	0.00000	0.00034	-0.00032	0.00002	-3.06633
D41	-0.91436	0.00000	0.00032	-0.00021	0.00010	-0.91426
D42	-1.64503	0.00000	0.00124	0.00072	0.00195	-1.64308
D43	2.55320	0.00000	0.00125	0.00070	0.00195	2.55515
D44	0.47246	0.00002	0.00141	0.00081	0.00222	0.47468
D45	0.45586	0.00000	-0.00508	-0.00265	-0.00773	0.44813
D46	-0.27298	0.00000	-0.00179	0.00015	-0.00163	-0.27461
D47	2.56587	0.00001	-0.00258	0.00015	-0.00242	2.56345
D48	3.14154	0.00000	0.00005	-0.00006	0.00000	3.14154
D49	0.00042	0.00000	0.00000	0.00001	0.00001	0.00043
D50	0.00035	0.00000	-0.00009	-0.00002	-0.00011	0.00024
D51	-3.14078	0.00000	-0.00014	0.00004	-0.00010	-3.14088
D52	-1.98142	0.00000	0.02583	0.00321	0.02905	-1.95237
D53	2.48949	0.00001	-0.02460	-0.00302	-0.02762	2.46187
D54	2.12367	-0.00002	-0.02637	-0.00334	-0.02972	2.09395
D55	-2.56037	0.00001	-0.02333	-0.00231	-0.02563	-2.58600
D56	-2.72901	0.00000	0.00022	-0.00004	0.00018	-2.72883
D57	-0.02989	0.00000	0.00027	-0.00008	0.00019	-0.02969
D58	-0.02160	0.00000	0.00021	-0.00021	0.00000	-0.02160
D59	2.67753	0.00000	0.00027	-0.00025	0.00001	2.67754
D60	-0.17026	-0.00001	-0.00047	0.00034	-0.00014	-0.17040
D61	0.26460	0.00001	0.00165	0.00070	0.00235	0.26695
D62	-2.58228	-0.00002	-0.00050	0.00016	-0.00034	-2.58262
D63	-2.14741	0.00000	0.00162	0.00052	0.00214	-2.14527
D64	2.15585	-0.00003	-0.00249	-0.00099	-0.00348	2.15236
D65	-0.23728	-0.00003	-0.00261	-0.00097	-0.00358	-0.24086
D66	2.48804	0.00001	0.00028	0.00004	0.00032	2.48836
D67	-1.71978	0.00000	0.00024	0.00004	0.00028	-1.71950
D68	0.35922	0.00000	0.00026	0.00004	0.00030	0.35952
D69	1.27181	0.00000	0.00047	-0.00004	0.00043	1.27224
D70	-2.93601	0.00000	0.00043	-0.00004	0.00039	-2.93562

D71	-0.85701	-0.00001	0.00044	-0.00004	0.00041	-0.85660
D72	-1.09049	0.00000	0.00032	0.00001	0.00033	-1.09016
D73	0.98487	0.00000	0.00028	0.00001	0.00029	0.98516
D74	3.06387	0.00000	0.00030	0.00001	0.00031	3.06418

Item	Value	Threshold	Converged?
Maximum Force	0.000058	0.000450	YES
RMS Force	0.000011	0.000300	YES
Maximum Displacement	0.014068	0.001800	NO
RMS Displacement	0.003378	0.001200	NO

Predicted change in Energy=-2.624381D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.378073	-1.909681	-0.255960
2	6	0	-2.509694	-1.169547	-0.137533
3	7	0	-2.111867	0.112088	0.230093
4	6	0	-0.768383	0.135574	0.329753
5	7	0	-0.307622	-1.081122	0.043977
6	6	0	1.125658	-1.436885	-0.003785
7	6	0	1.683194	-1.368638	-1.436369
8	1	0	-1.243791	-2.945394	-0.516730
9	1	0	-3.539698	-1.443116	-0.275672
10	1	0	1.649505	-0.728836	0.640391
11	1	0	1.234281	-2.447303	0.392452
12	1	0	1.064808	-1.983080	-2.101636
13	1	0	1.636306	-0.331675	-1.788526
14	35	0	1.653305	2.227491	1.028632
15	1	0	-0.116619	0.994293	0.598857
16	6	0	-2.916355	1.256607	0.484185
17	6	0	-4.240384	1.282204	0.406695
18	1	0	-2.321086	2.120398	0.752801
19	1	0	-4.762717	2.204514	0.619526
20	1	0	-4.841820	0.422626	0.139481
21	8	0	2.990868	-1.880609	-1.459198
22	1	0	3.630938	-1.148946	-1.360844
23	6	0	4.837079	1.611441	-1.121207
24	6	0	5.714748	0.752863	-0.316367
25	8	0	4.861217	0.176913	-1.334322
26	1	0	3.920163	1.989524	-0.675417
27	1	0	5.254100	2.182591	-1.946172

28	1	0	6.765155	0.709140	-0.600099
29	6	0	5.406927	0.409625	1.115076
30	1	0	5.689856	-0.624640	1.333509
31	1	0	5.979600	1.063356	1.780224
32	1	0	4.346866	0.553839	1.332942

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357347	0.000000			
3	N	2.205051	1.391403	0.000000		
4	C	2.213108	2.225727	1.347380	0.000000	
5	N	1.386484	2.211308	2.171103	1.332035	0.000000
6	C	2.560429	3.647622	3.596607	2.484203	1.477546
7	C	3.325274	4.393964	4.401378	3.375214	2.497487
8	H	1.076445	2.213579	3.264888	3.230311	2.160166
9	H	2.211491	1.074630	2.170981	3.246381	3.267955
10	H	3.371064	4.254213	3.876005	2.586481	2.076093
11	H	2.744789	3.991352	4.215868	3.268921	2.089342
12	H	3.062610	4.158918	4.462954	3.709574	2.701990
13	H	3.731667	4.540608	4.280250	3.238511	2.774634
14	Br	5.287307	5.498214	4.391937	3.275533	3.970100
15	H	3.279489	3.309272	2.212529	1.111131	2.156785
16	C	3.597153	2.537347	1.421861	2.427828	3.530474
17	C	4.338210	3.050009	2.435353	3.657250	4.602553
18	H	4.260096	3.413504	2.085739	2.555267	3.847883
19	H	5.398972	4.127171	3.399546	4.507681	5.565477
20	H	4.194469	2.837351	2.749052	4.087969	4.778005
21	O	4.531697	5.701631	5.732578	4.625722	3.711975
22	H	5.185526	6.261332	6.091067	4.884888	4.182150
23	C	7.195489	7.916854	7.236153	5.975338	5.922457
24	C	7.576338	8.448023	7.871792	6.544426	6.305735
25	O	6.666744	7.587857	7.146712	5.870540	5.495385
26	H	6.591741	7.184157	6.382014	5.141008	5.274520
27	H	7.974285	8.647803	7.954909	6.755769	6.748724
28	H	8.560889	9.474505	8.935726	7.612345	7.324210
29	C	7.300353	8.169192	7.576542	6.231075	6.002138
30	H	7.357538	8.348264	7.913733	6.579841	6.151505
31	H	8.192700	8.985085	8.293349	6.964188	6.866039
32	H	6.431832	7.221133	6.567088	5.229446	5.098900

		6	7	8	9	10
6	C	0.000000				
7	C	1.538766	0.000000			
8	H	2.855346	3.449513	0.000000		

9	H	4.673276	5.350828	2.754294	0.000000	
10	H	1.091198	2.173342	3.824032	5.317631	0.000000
11	H	1.090755	2.170168	2.686178	4.923988	1.785221
12	H	2.168643	1.096595	2.961015	4.982688	3.071435
13	H	2.160452	1.096132	4.091937	5.505910	2.461209
14	Br	3.843429	4.359962	6.126993	6.491674	2.981713
15	H	2.795901	3.600683	4.246903	4.292229	2.467812
16	C	4.881689	5.633497	4.632074	2.873055	4.981311
17	C	6.029623	6.746305	5.263541	2.895506	6.228137
18	H	5.010662	5.744572	5.332403	3.904024	4.888391
19	H	6.951350	7.651398	6.339990	3.949983	7.051352
20	H	6.252128	6.947498	4.971919	2.312762	6.611662
21	O	2.407099	1.404510	4.467030	6.651348	2.744834
22	H	2.863729	1.961549	5.263339	7.258247	2.847369
23	C	4.931081	4.350539	7.622802	8.956318	4.329059
24	C	5.094355	4.691333	7.882799	9.511506	4.431368
25	O	4.281246	3.535388	6.905677	8.620939	3.877495
26	H	4.472206	4.106134	7.144580	8.221456	3.778455
27	H	5.823874	5.061867	8.400127	9.657495	5.306583
28	H	6.063410	5.553633	8.803737	10.532210	5.456781
29	C	4.794863	4.851627	7.625681	9.241695	3.954699
30	H	4.824935	4.927383	7.542198	9.404469	4.100696
31	H	5.744096	5.892382	8.574582	10.056149	4.822954
32	H	4.015719	4.296528	6.849917	8.292970	3.066046

		11	12	13	14	15
11	H	0.000000				
12	H	2.542578	0.000000			
13	H	3.064991	1.775327	0.000000		
14	Br	4.736455	5.279566	3.806047	0.000000	
15	H	3.702988	4.189653	3.245079	2.199571	0.000000
16	C	5.563734	5.747322	5.330532	4.703278	2.814334
17	C	6.624302	6.715570	6.477583	6.001328	4.138267
18	H	5.799516	6.037436	5.303957	3.985390	2.480219
19	H	7.593086	7.674681	7.292356	6.429092	4.801175
20	H	6.724544	6.760051	6.800904	6.799615	4.781773
21	O	2.614450	2.032962	2.083865	4.985465	4.707137
22	H	3.240948	2.798138	2.197590	4.584861	4.741106
23	C	5.634245	5.302061	3.803415	3.890725	5.280021
24	C	5.551403	5.682826	4.469583	4.525359	5.907688
25	O	4.798220	4.434756	3.296212	4.480973	5.402235
26	H	5.295257	5.095953	3.441363	2.845885	4.348549
27	H	6.562319	5.909920	4.408495	4.670888	6.060846
28	H	6.445064	6.480480	5.366633	5.575766	6.991253
29	C	5.108346	5.909846	4.816432	4.171546	5.578341

30	H	4.905083	5.919177	5.124862	4.951904	6.072546
31	H	6.063719	6.964538	5.791916	4.542789	6.210015
32	H	4.424879	5.385554	4.227864	3.185748	4.544841

		16	17	18	19	20
16	C	0.000000				
17	C	1.326542	0.000000			
18	H	1.082883	2.122749	0.000000		
19	H	2.079879	1.081104	2.446711	0.000000	
20	H	2.126443	1.082590	3.100434	1.847113	0.000000
21	O	6.965210	8.110238	7.008414	9.007076	8.319355
22	H	7.215113	8.425699	7.112152	9.253162	8.746910
23	C	7.925839	9.211038	7.416891	9.774352	9.832787
24	C	8.682775	9.995383	8.221187	10.618873	10.571565
25	O	8.059983	9.332307	7.727787	10.027402	9.817402
26	H	6.972792	8.262312	6.403916	8.781543	8.938209
27	H	8.574405	9.823030	8.041876	10.340208	10.458251
28	H	9.757408	11.066342	9.294179	11.688261	11.634042
29	C	8.390020	9.712560	7.923395	10.338707	10.295085
30	H	8.850272	10.154049	8.488089	10.852197	10.650759
31	H	8.991945	10.314192	8.430559	10.864936	10.963836
32	H	7.346336	8.667717	6.874028	9.285375	9.266796

		21	22	23	24	25
21	O	0.000000				
22	H	0.977084	0.000000			
23	C	3.964485	3.021909	0.000000		
24	C	3.957368	3.008334	1.468069	0.000000	
25	O	2.783378	1.808920	1.450473	1.447918	0.000000
26	H	4.056579	3.225439	1.087387	2.208797	2.145996
27	H	4.676426	3.751853	1.086594	2.216435	2.133416
28	H	4.657262	3.722168	2.191615	1.088930	2.108869
29	C	4.208254	3.422493	2.601932	1.503860	2.520219
30	H	4.081814	3.431265	3.428253	2.149471	2.906278
31	H	5.300311	4.502976	3.166078	2.135941	3.425924
32	H	3.944783	3.266268	2.716924	2.151960	2.742431

		26	27	28	29	30
26	H	0.000000				
27	H	1.852425	0.000000			
28	H	3.120742	2.503249	0.000000		
29	C	2.812902	3.540904	2.208238	0.000000	
30	H	3.741852	4.338979	2.583423	1.094288	0.000000
31	H	3.336052	3.957911	2.531502	1.094413	1.769982
32	H	2.505349	3.772068	3.099820	1.091784	1.786739

		31	32
31	H	0.000000	

32 H 1.767905 0.000000

Stoichiometry C10H17BrN2O2

Framework group C1[X(C10H17BrN2O2)]

Deg. of freedom 90

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.712727	2.112745	-0.441171
2	6	0	-3.790641	1.348816	-0.129878
3	7	0	-3.323353	0.049277	0.039961
4	6	0	-1.991993	0.038337	-0.166903
5	7	0	-1.605918	1.278014	-0.464329
6	6	0	-0.203742	1.676204	-0.706177
7	6	0	0.454649	2.246037	0.562528
8	1	0	-2.639465	3.165351	-0.654212
9	1	0	-4.826413	1.614524	-0.023079
10	1	0	0.326522	0.782484	-1.039037
11	1	0	-0.199322	2.425334	-1.498977
12	1	0	-0.161133	3.060397	0.962717
13	1	0	0.510611	1.456571	1.320893
14	35	0	0.526982	-2.055334	-0.146164
15	1	0	-1.297276	-0.826965	-0.110032
16	6	0	-4.054628	-1.125148	0.368062
17	6	0	-5.364453	-1.167253	0.573732
18	1	0	-3.415694	-1.997043	0.432840
19	1	0	-5.829002	-2.112157	0.818959
20	1	0	-6.009300	-0.300006	0.510044
21	8	0	1.718356	2.769913	0.244333
22	1	0	2.403593	2.091687	0.402932
23	6	0	3.795519	-0.458577	1.233973
24	6	0	4.548303	0.009559	0.063763
25	8	0	3.725795	0.929987	0.820573
26	1	0	2.881289	-1.026077	1.077325
27	1	0	4.310307	-0.607503	2.179225
28	1	0	5.609435	0.211041	0.202230
29	6	0	4.117615	-0.301380	-1.343155
30	1	0	4.305867	0.551816	-2.002007
31	1	0	4.690901	-1.153001	-1.722396
32	1	0	3.059008	-0.566062	-1.379009

```
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.6012140           0.2209025           0.1722528
 Standard basis: 6-311++G(d,p) (5D, 7F)
 There are     492 symmetry adapted cartesian basis functions of A      symmetry.
 There are     475 symmetry adapted basis functions of A      symmetry.
    475 basis functions,      751 primitive gaussians,      492 cartesian basis functions
     71 alpha electrons              71 beta electrons
          nuclear repulsion energy           1307.2283037544 Hartrees.
 NAtoms=       32 NActive=       32 NUniq=       32 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      475 RedAO= T EigKep=    3.78D-06    NBF=      475
 NBsUse=      475 1.00D-06 EigRej= -1.00D+00 NBFU=      475
 Initial guess from the checkpoint file:    "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"
 B after Tr=          0.000000        0.000000        0.000000
              Rot=        1.000000        0.000361        0.000073      -0.000009 Ang=      0.04 deg.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                    energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3225.52371215         A.U. after        9 cycles
                  NFock=    9    Conv=0.85D-08         -V/T= 2.0018
 Calling FoFJK, ICntrl=              2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center         Atomic                             Forces (Hartrees/Bohr)
 Number         Number                       X                   Y                   Z
 -------------------------------------------------------------------
        1              6              -0.000018737      -0.000016835       0.000048116
        2              6               0.000006855      -0.000002074       0.000011438
        3              7              -0.000006045       0.000000497       0.000009207
        4              6               0.000010778       0.000009875      -0.000047937
        5              7              -0.000017534       0.000031280      -0.000020057
        6              6               0.000014605       0.000008912       0.000027086
        7              6               0.000057426      -0.000023694       0.000013732
        8              1               0.000001342       0.000004518      -0.000005926
        9              1               0.000000374       0.000000525      -0.000002588
       10              1              -0.000006036       0.000001856       0.000001597
       11              1              -0.000004098       0.000001068      -0.000002113
       12              1              -0.000003301      -0.000009316       0.000007377
```

13	1	-0.000005466	-0.000006481	-0.000009941
14	35	-0.000005256	0.000012764	-0.000009328
15	1	0.000015158	-0.000040890	0.000025730
16	6	-0.000003067	0.000010123	-0.000002152
17	6	0.000001353	0.000003337	-0.000001870
18	1	0.000003764	0.000001629	-0.000007286
19	1	0.000000205	0.000002301	-0.000007096
20	1	0.000002171	0.000000844	-0.000000235
21	8	-0.000083037	0.000018916	0.000000762
22	1	0.000064066	-0.000025349	-0.000006014
23	6	0.000069408	0.000009265	-0.000053498
24	6	-0.000037521	-0.000011235	0.000010196
25	8	-0.000060434	0.000041138	0.000034735
26	1	-0.000003093	-0.000026453	0.000002845
27	1	-0.000002569	-0.000005908	-0.000002974
28	1	0.000000790	-0.000006818	-0.000004341
29	6	0.000003786	0.000001524	-0.000011505
30	1	0.000000930	0.000006405	0.000005543
31	1	0.000001553	0.000004862	-0.000006604
32	1	0.000001632	0.000003414	0.000003101

Cartesian Forces: Max 0.000083037 RMS 0.000021705

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000048012 RMS 0.000009622
Search for a local minimum.
Step number 33 out of a maximum of 177
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 24 25 26 27 28
29 30 31 32 33
DE= -1.33D-06 DEPred=-2.62D-07 R= 5.07D+00
TightC=F SS= 1.41D+00 RLast= 5.98D-02 DXNew= 3.2661D+00 1.7938D-01
Trust test= 5.07D+00 RLast= 5.98D-02 DXMaxT set to 1.94D+00
ITU= 1 1 0 1 1 1 1 1 1 1 1 1 1 1 1 -1 1 1 1
ITU= 1 1 1 1 1 1 1 1 0 1 0 1 0
Eigenvalues --- 0.00003 0.00072 0.00124 0.00234 0.00267
Eigenvalues --- 0.00332 0.00635 0.01081 0.01217 0.01297
Eigenvalues --- 0.01463 0.01722 0.01817 0.01956 0.02127

Eigenvalues --- 0.02180 0.02220 0.02320 0.02396 0.03004
Eigenvalues --- 0.03061 0.03097 0.03420 0.03580 0.03841
Eigenvalues --- 0.04407 0.04633 0.05187 0.05444 0.05561
Eigenvalues --- 0.05679 0.05918 0.06436 0.09359 0.09608
Eigenvalues --- 0.10383 0.11155 0.11535 0.11678 0.13048
Eigenvalues --- 0.13822 0.14135 0.15112 0.15950 0.15994
Eigenvalues --- 0.16000 0.16001 0.16005 0.16024 0.16045
Eigenvalues --- 0.16666 0.17650 0.19167 0.21434 0.22069
Eigenvalues --- 0.22913 0.23418 0.23968 0.24210 0.25029
Eigenvalues --- 0.27782 0.28592 0.30814 0.31946 0.33103
Eigenvalues --- 0.33266 0.34045 0.34154 0.34491 0.34832
Eigenvalues --- 0.35025 0.35685 0.35690 0.35858 0.36261
Eigenvalues --- 0.36436 0.36677 0.37192 0.37243 0.37550
Eigenvalues --- 0.38160 0.42174 0.42509 0.45556 0.46265
Eigenvalues --- 0.49318 0.54325 0.55275 0.55932 0.60389
Eigenvalue 1 is 3.33D-05 Eigenvector:

	D52	D54	D53	D55	D25
1	0.50845	-0.49799	-0.49499	-0.48941	0.03755
	D26	D46	D47	D45	A48
1	0.03127	-0.03107	-0.03095	-0.02441	0.01536

En-DIIS/RFO-DIIS IScMMF= 0 using points: 33 32 31 30 29
RFO step: Lambda=-3.51578345D-08.
DidBck=F Rises=F RFO-DIIS coefs: 1.82299 -0.94550 -0.37405 0.58680 -0.09024
Iteration 1 RMS(Cart)= 0.00181763 RMS(Int)= 0.00000670
Iteration 2 RMS(Cart)= 0.00000498 RMS(Int)= 0.00000194
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000194

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56501	-0.00001	0.00000	-0.00001	-0.00001	2.56501
R2	2.62007	0.00001	0.00001	0.00002	0.00003	2.62011
R3	2.03419	0.00000	-0.00001	0.00000	-0.00001	2.03418
R4	2.62937	0.00000	0.00001	0.00000	0.00001	2.62938
R5	2.03076	0.00000	0.00000	0.00000	0.00000	2.03076
R6	2.54618	0.00000	-0.00002	0.00001	-0.00001	2.54617
R7	2.68693	0.00000	0.00002	-0.00001	0.00001	2.68694
R8	2.51718	-0.00003	-0.00012	0.00003	-0.00010	2.51709
R9	2.09973	-0.00001	-0.00015	0.00004	-0.00011	2.09962
R10	2.79216	0.00001	0.00002	0.00001	0.00003	2.79218
R11	2.90785	0.00000	-0.00006	0.00004	-0.00003	2.90782
R12	2.06206	0.00000	-0.00002	0.00001	-0.00001	2.06206
R13	2.06123	0.00000	-0.00001	0.00001	0.00000	2.06123
R14	2.07226	0.00000	-0.00003	0.00001	-0.00002	2.07224
R15	2.07139	0.00000	-0.00003	0.00003	0.00000	2.07139

R16	2.65414	-0.00005	0.00008	-0.00010	-0.00002	2.65412
R17	4.15659	0.00000	0.00051	-0.00020	0.00031	4.15690
R18	8.46781	0.00000	-0.00120	-0.00060	-0.00180	8.46601
R19	2.50680	0.00000	-0.00001	0.00000	-0.00001	2.50679
R20	2.04635	0.00000	0.00000	0.00000	0.00000	2.04635
R21	2.04299	0.00000	0.00000	0.00000	0.00000	2.04299
R22	2.04580	0.00000	0.00000	0.00000	0.00000	2.04580
R23	1.84642	0.00002	-0.00004	0.00002	-0.00002	1.84640
R24	3.41836	0.00000	0.00020	-0.00008	0.00013	3.41849
R25	2.77425	-0.00001	-0.00004	0.00005	0.00001	2.77426
R26	2.74100	-0.00001	-0.00011	-0.00001	-0.00012	2.74088
R27	2.05486	0.00000	-0.00003	0.00002	-0.00001	2.05486
R28	2.05336	0.00000	0.00000	0.00000	0.00000	2.05336
R29	2.73617	0.00000	-0.00008	0.00002	-0.00006	2.73611
R30	2.05778	0.00000	-0.00003	0.00002	-0.00001	2.05777
R31	2.84188	0.00000	-0.00005	0.00003	-0.00003	2.84185
R32	2.06790	0.00000	0.00001	0.00000	0.00001	2.06791
R33	2.06814	0.00000	0.00000	0.00000	0.00000	2.06814
R34	2.06317	0.00000	-0.00002	0.00002	0.00000	2.06317
A1	1.87437	0.00000	-0.00002	0.00000	-0.00003	1.87435
A2	2.27810	0.00000	0.00000	0.00000	0.00000	2.27809
A3	2.13067	0.00000	0.00002	0.00000	0.00003	2.13070
A4	1.86183	0.00000	0.00001	0.00000	0.00001	1.86184
A5	2.27713	0.00000	0.00000	-0.00001	-0.00001	2.27712
A6	2.14420	0.00000	-0.00001	0.00001	0.00000	2.14420
A7	1.89725	0.00000	-0.00005	0.00003	-0.00002	1.89723
A8	2.24835	0.00000	0.00004	-0.00001	0.00003	2.24838
A9	2.13757	0.00000	0.00001	-0.00002	-0.00001	2.13757
A10	1.88927	0.00000	0.00006	-0.00003	0.00003	1.88930
A11	2.23479	0.00000	-0.00009	0.00000	-0.00009	2.23470
A12	2.15913	-0.00001	0.00003	0.00003	0.00006	2.15918
A13	1.90202	0.00000	0.00000	0.00001	0.00001	1.90203
A14	2.21186	0.00001	0.00002	0.00000	0.00003	2.21189
A15	2.16809	-0.00002	-0.00001	-0.00001	-0.00002	2.16808
A16	1.95076	0.00001	-0.00003	0.00001	-0.00002	1.95075
A17	1.86540	-0.00001	-0.00007	0.00000	-0.00007	1.86533
A18	1.88379	0.00000	0.00005	-0.00001	0.00004	1.88383
A19	1.92504	0.00000	0.00018	-0.00005	0.00014	1.92518
A20	1.92112	-0.00001	-0.00010	0.00003	-0.00007	1.92105
A21	1.91646	0.00000	-0.00003	0.00002	-0.00001	1.91645
A22	1.91307	-0.00001	-0.00001	0.00001	0.00000	1.91307
A23	1.90240	0.00001	0.00017	-0.00002	0.00015	1.90255
A24	1.91379	0.00001	0.00008	0.00000	0.00008	1.91387
A25	1.88709	0.00000	0.00000	-0.00004	-0.00004	1.88705

A26	1.88696	0.00000	-0.00016	-0.00002	-0.00018	1.88678
A27	1.96000	0.00000	-0.00008	0.00007	-0.00001	1.95999
A28	1.78898	-0.00002	-0.00023	-0.00006	-0.00029	1.78869
A29	2.83251	0.00003	0.00017	0.00013	0.00029	2.83280
A30	2.17708	-0.00001	-0.00001	-0.00001	-0.00002	2.17706
A31	1.95561	0.00000	-0.00001	0.00000	-0.00001	1.95560
A32	2.15049	0.00001	0.00003	0.00001	0.00004	2.15052
A33	2.07967	0.00000	0.00001	0.00001	0.00001	2.07968
A34	2.15747	0.00000	0.00000	-0.00001	-0.00001	2.15746
A35	2.04604	0.00000	-0.00001	0.00001	0.00000	2.04604
A36	1.91274	0.00001	-0.00011	0.00000	-0.00010	1.91264
A37	3.05060	0.00002	-0.00030	0.00013	-0.00018	3.05042
A38	2.07454	-0.00002	-0.00014	0.00001	-0.00013	2.07441
A39	2.08770	0.00002	-0.00003	0.00009	0.00005	2.08776
A40	2.00220	-0.00002	-0.00001	-0.00014	-0.00016	2.00204
A41	1.98441	0.00001	0.00008	-0.00002	0.00006	1.98447
A42	2.03993	0.00001	0.00010	0.00000	0.00010	2.04003
A43	2.04578	-0.00002	-0.00002	-0.00001	-0.00002	2.04576
A44	2.13287	0.00002	-0.00003	0.00006	0.00003	2.13290
A45	1.94924	0.00000	0.00007	-0.00005	0.00002	1.94927
A46	2.04625	0.00000	0.00002	0.00002	0.00004	2.04629
A47	2.02227	-0.00001	0.00000	-0.00002	-0.00002	2.02226
A48	1.42655	0.00000	0.00112	0.00044	0.00157	1.42812
A49	0.99800	0.00003	0.00072	0.00015	0.00087	0.99887
A50	2.36847	0.00003	0.00172	0.00044	0.00217	2.37064
A51	2.35010	-0.00001	0.00030	0.00030	0.00060	2.35069
A52	1.93135	0.00001	0.00003	0.00002	0.00005	1.93141
A53	1.91246	-0.00001	0.00000	-0.00004	-0.00004	1.91243
A54	1.93749	0.00001	0.00007	0.00001	0.00008	1.93757
A55	1.88385	0.00000	-0.00006	0.00000	-0.00007	1.88378
A56	1.91352	0.00000	-0.00001	-0.00001	-0.00001	1.91350
A57	1.88376	0.00000	-0.00003	0.00002	-0.00002	1.88375
A58	3.77665	-0.00001	0.00143	0.00073	0.00216	3.77881
A59	5.04787	0.00000	-0.00135	-0.00024	-0.00159	5.04628
D1	0.00451	0.00000	0.00011	-0.00010	0.00001	0.00452
D2	-3.13059	-0.00001	-0.00005	-0.00012	-0.00017	-3.13076
D3	3.13583	0.00001	0.00012	0.00007	0.00019	3.13603
D4	0.00073	0.00000	-0.00004	0.00005	0.00002	0.00075
D5	-0.00697	0.00000	0.00000	0.00001	0.00001	-0.00696
D6	-3.09723	0.00000	-0.00036	-0.00009	-0.00044	-3.09767
D7	-3.13935	-0.00001	0.00000	-0.00015	-0.00015	-3.13950
D8	0.05358	-0.00001	-0.00037	-0.00024	-0.00061	0.05297
D9	-0.00059	0.00000	-0.00018	0.00016	-0.00002	-0.00062
D10	-3.13657	0.00000	-0.00012	0.00004	-0.00008	-3.13665

D11	3.13512	0.00001	-0.00004	0.00018	0.00013	3.13526
D12	-0.00086	0.00001	0.00002	0.00006	0.00008	-0.00078
D13	-0.00375	0.00000	0.00019	-0.00016	0.00003	-0.00372
D14	3.13718	0.00001	-0.00033	0.00011	-0.00021	3.13697
D15	3.13266	0.00000	0.00013	-0.00005	0.00009	3.13275
D16	-0.00959	0.00001	-0.00038	0.00022	-0.00016	-0.00975
D17	0.00035	0.00000	-0.00023	0.00018	-0.00005	0.00030
D18	-3.14151	0.00000	-0.00017	0.00022	0.00005	-3.14146
D19	-3.13494	0.00000	-0.00016	0.00005	-0.00011	-3.13506
D20	0.00639	0.00000	-0.00010	0.00008	-0.00002	0.00637
D21	0.00660	0.00000	-0.00012	0.00009	-0.00003	0.00657
D22	3.09844	0.00001	0.00023	0.00018	0.00042	3.09885
D23	-3.13437	-0.00001	0.00037	-0.00016	0.00021	-3.13416
D24	-0.04253	-0.00001	0.00072	-0.00007	0.00065	-0.04188
D25	-3.12031	-0.00001	0.00501	0.00111	0.00611	-3.11420
D26	0.02053	0.00001	0.00442	0.00141	0.00583	0.02636
D27	1.41299	0.00000	-0.00205	-0.00042	-0.00247	1.41052
D28	-2.76244	0.00000	-0.00189	-0.00047	-0.00236	-2.76480
D29	-0.70194	0.00001	-0.00194	-0.00045	-0.00239	-0.70434
D30	-1.66989	-0.00001	-0.00246	-0.00052	-0.00299	-1.67287
D31	0.43787	0.00000	-0.00230	-0.00058	-0.00288	0.43499
D32	2.49836	0.00000	-0.00235	-0.00056	-0.00291	2.49545
D33	-0.93855	0.00000	-0.00008	0.00002	-0.00006	-0.93860
D34	1.12370	0.00000	0.00002	-0.00004	-0.00002	1.12368
D35	-3.00741	0.00000	0.00008	0.00004	0.00012	-3.00729
D36	-3.01122	0.00000	-0.00009	0.00005	-0.00004	-3.01126
D37	-0.94897	0.00000	0.00001	-0.00001	0.00000	-0.94898
D38	1.20310	0.00000	0.00007	0.00006	0.00013	1.20324
D39	1.15460	0.00000	-0.00010	0.00004	-0.00007	1.15454
D40	-3.06633	-0.00001	0.00000	-0.00002	-0.00003	-3.06636
D41	-0.91426	0.00000	0.00005	0.00006	0.00011	-0.91415
D42	-1.64308	0.00000	0.00078	0.00077	0.00154	-1.64154
D43	2.55515	0.00000	0.00084	0.00077	0.00160	2.55675
D44	0.47468	0.00001	0.00099	0.00079	0.00178	0.47646
D45	0.44813	0.00000	-0.00486	-0.00186	-0.00672	0.44142
D46	-0.27461	0.00001	-0.00088	0.00074	-0.00014	-0.27475
D47	2.56345	0.00001	-0.00081	0.00045	-0.00036	2.56309
D48	3.14154	0.00000	0.00000	0.00006	0.00006	-3.14158
D49	0.00043	0.00000	0.00000	0.00003	0.00003	0.00046
D50	0.00024	0.00000	-0.00006	0.00002	-0.00005	0.00020
D51	-3.14088	0.00000	-0.00006	-0.00001	-0.00007	-3.14095
D52	-1.95237	0.00000	0.01940	0.00044	0.01985	-1.93252
D53	2.46187	0.00001	-0.01871	-0.00083	-0.01953	2.44234
D54	2.09395	-0.00001	-0.01948	-0.00139	-0.02087	2.07307

D55	-2.58600	0.00001	-0.01735	-0.00059	-0.01794	-2.60395
D56	-2.72883	0.00000	0.00014	-0.00025	-0.00011	-2.72894
D57	-0.02969	-0.00001	0.00003	-0.00017	-0.00015	-0.02984
D58	-0.02160	0.00000	-0.00002	0.00000	-0.00002	-0.02162
D59	2.67754	0.00000	-0.00014	0.00008	-0.00006	2.67748
D60	-0.17040	-0.00001	-0.00010	-0.00029	-0.00039	-0.17079
D61	0.26695	0.00001	0.00070	0.00038	0.00108	0.26804
D62	-2.58262	-0.00001	-0.00034	-0.00010	-0.00044	-2.58306
D63	-2.14527	0.00000	0.00046	0.00057	0.00103	-2.14423
D64	2.15236	-0.00002	-0.00240	-0.00067	-0.00307	2.14929
D65	-0.24086	-0.00001	-0.00251	-0.00060	-0.00311	-0.24398
D66	2.48836	0.00001	0.00021	0.00014	0.00036	2.48871
D67	-1.71950	0.00000	0.00015	0.00013	0.00028	-1.71922
D68	0.35952	0.00000	0.00016	0.00013	0.00028	0.35980
D69	1.27224	0.00000	0.00024	0.00014	0.00038	1.27262
D70	-2.93562	0.00000	0.00018	0.00012	0.00031	-2.93531
D71	-0.85660	0.00000	0.00018	0.00012	0.00031	-0.85629
D72	-1.09016	0.00000	0.00010	0.00022	0.00032	-1.08985
D73	0.98516	0.00000	0.00004	0.00020	0.00024	0.98540
D74	3.06418	0.00000	0.00004	0.00021	0.00024	3.06442

Item	Value	Threshold	Converged?
Maximum Force	0.000048	0.000450	YES
RMS Force	0.000010	0.000300	YES
Maximum Displacement	0.008270	0.001800	NO
RMS Displacement	0.001816	0.001200	NO

Predicted change in Energy=-1.385009D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.377887	-1.908891	-0.258573
2	6	0	-2.509401	-1.168713	-0.139450
3	7	0	-2.111475	0.112253	0.230420
4	6	0	-0.768038	0.135265	0.330731
5	7	0	-0.307404	-1.081007	0.043189
6	6	0	1.125833	-1.437081	-0.003991
7	6	0	1.683539	-1.370529	-1.436573
8	1	0	-1.243701	-2.944168	-0.521106
9	1	0	-3.539389	-1.441816	-0.278624
10	1	0	1.649636	-0.728441	0.639565
11	1	0	1.234259	-2.447103	0.393312

12	1	0	1.065164	-1.985643	-2.101209
13	1	0	1.636922	-0.333999	-1.790042
14	35	0	1.653566	2.227452	1.029887
15	1	0	-0.116301	0.993457	0.601328
16	6	0	-2.915804	1.256576	0.485923
17	6	0	-4.239780	1.282617	0.407742
18	1	0	-2.320437	2.119791	0.756170
19	1	0	-4.762017	2.204714	0.621718
20	1	0	-4.841263	0.423602	0.138834
21	8	0	2.991067	-1.882877	-1.458819
22	1	0	3.631216	-1.151388	-1.359792
23	6	0	4.836311	1.611056	-1.121967
24	6	0	5.713807	0.752982	-0.316387
25	8	0	4.859600	0.176319	-1.333327
26	1	0	3.919730	1.990009	-0.676236
27	1	0	5.253302	2.181030	-1.947760
28	1	0	6.764084	0.708382	-0.600441
29	6	0	5.406354	0.411654	1.115575
30	1	0	5.689124	-0.622384	1.335308
31	1	0	5.979435	1.066094	1.779674
32	1	0	4.346415	0.556404	1.333676

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357342	0.000000			
3	N	2.205060	1.391410	0.000000		
4	C	2.213091	2.225708	1.347374	0.000000	
5	N	1.386502	2.211299	2.171082	1.331984	0.000000
6	C	2.560475	3.647643	3.596603	2.484162	1.477560
7	C	3.324131	4.393632	4.402231	3.376538	2.497473
8	H	1.076442	2.213571	3.264893	3.230292	2.160197
9	H	2.211482	1.074630	2.170989	3.246365	3.267947
10	H	3.371352	4.254209	3.875581	2.585829	2.076047
11	H	2.745530	3.991630	4.215540	3.268292	2.089385
12	H	3.060996	4.158531	4.464156	3.711227	2.701990
13	H	3.730249	4.540176	4.281575	3.240635	2.774736
14	Br	5.287643	5.498325	4.391896	3.275703	3.970501
15	H	3.279429	3.309179	2.212423	1.111070	2.156720
16	C	3.597172	2.537377	1.421866	2.427823	3.530448
17	C	4.338218	3.050025	2.435339	3.657232	4.602521
18	H	4.260092	3.413517	2.085734	2.555246	3.847824
19	H	5.398981	4.127187	3.399542	4.507679	5.565451
20	H	4.194452	2.837338	2.749012	4.087925	4.777958

21	O	4.530897	5.701396	5.733237	4.626690	3.711999
22	H	5.184362	6.260728	6.091311	4.885364	4.181631
23	C	7.193868	7.915298	7.235129	5.974698	5.921367
24	C	7.575027	8.446619	7.870487	6.543290	6.304585
25	O	6.664041	7.585291	7.144600	5.868653	5.493050
26	H	6.590950	7.183272	6.381492	5.140936	5.274218
27	H	7.972043	8.645827	7.953882	6.755235	6.747311
28	H	8.559129	9.472778	8.934274	7.611071	7.322712
29	C	7.300626	8.168955	7.575678	6.230207	6.002089
30	H	7.357867	8.348006	7.912637	6.578613	6.151280
31	H	8.193606	8.985419	8.292939	6.963783	6.866569
32	H	6.432774	7.221382	6.566490	5.228851	5.099461

		6	7	8	9	10
6	C	0.000000				
7	C	1.538752	0.000000			
8	H	2.855418	3.447194	0.000000		
9	H	4.673302	5.350225	2.754278	0.000000	
10	H	1.091195	2.173426	3.824658	5.317703	0.000000
11	H	1.090757	2.170102	2.687661	4.924411	1.785211
12	H	2.168622	1.096582	2.957423	4.981914	3.071483
13	H	2.160551	1.096133	4.089152	5.505074	2.461451
14	Br	3.843983	4.362315	6.127429	6.491726	2.981555
15	H	2.795858	3.602901	4.246855	4.292133	2.466765
16	C	4.881663	5.634859	4.632093	2.873101	4.980677
17	C	6.029601	6.747325	5.263550	2.895545	6.227626
18	H	5.010585	5.746501	5.332398	3.904060	4.887484
19	H	6.951329	7.652720	6.339999	3.950015	7.050746
20	H	6.252102	6.947939	4.971906	2.312775	6.611332
21	O	2.407147	1.404502	4.465300	6.650884	2.745064
22	H	2.862998	1.961470	5.261394	7.257469	2.846572
23	C	4.930381	4.350724	7.620869	8.954530	4.327948
24	C	5.093473	4.691181	7.881481	9.510006	4.430118
25	O	4.279160	3.534228	6.902711	8.618224	3.874889
26	H	4.472440	4.107540	7.143612	8.220340	3.778178
27	H	5.822797	5.061432	8.397263	9.655177	5.305250
28	H	6.062065	5.552741	8.801820	10.530360	5.455241
29	C	4.795217	4.852730	7.626499	9.241507	3.954659
30	H	4.825047	4.928262	7.543276	9.404345	4.100337
31	H	5.744981	5.893735	8.576100	10.056552	4.823626
32	H	4.016900	4.298636	6.851542	8.293269	3.066795

		11	12	13	14	15
11	H	0.000000				
12	H	2.542474	0.000000			
13	H	3.065026	1.775291	0.000000		

14	Br	4.736297	5.282059	3.809634	0.000000	
15	H	3.701991	4.192207	3.248782	2.199735	0.000000
16	C	5.563168	5.749203	5.332660	4.702939	2.814208
17	C	6.623906	6.717052	6.479146	6.000942	4.138136
18	H	5.798625	6.039991	5.307068	3.984872	2.480085
19	H	7.592556	7.676553	7.294386	6.428594	4.801067
20	H	6.724409	6.760778	6.801573	6.799313	4.781622
21	O	2.614405	2.032813	2.083852	4.987722	4.708847
22	H	3.240008	2.798268	2.197829	4.586745	4.742387
23	C	5.633782	5.302519	3.803374	3.891052	5.280107
24	C	5.550726	5.682916	4.469248	4.524608	5.906791
25	O	4.796532	4.434125	3.294643	4.480021	5.400944
26	H	5.295626	5.097539	3.442789	2.846531	4.349119
27	H	6.561473	5.909755	4.407771	4.671899	6.061420
28	H	6.443880	6.479797	5.365585	5.575208	6.990366
29	C	5.108867	5.911062	4.817388	4.169878	5.576976
30	H	4.905382	5.920231	5.125556	4.949806	6.070636
31	H	6.064755	6.965947	5.793148	4.541374	6.209008
32	H	4.426156	5.387676	4.229869	3.183729	4.543477

		16	17	18	19	20
16	C	0.000000				
17	C	1.326538	0.000000			
18	H	1.082883	2.122767	0.000000		
19	H	2.079882	1.081102	2.446754	0.000000	
20	H	2.126431	1.082590	3.100440	1.847111	0.000000
21	O	6.966299	8.111076	7.009964	9.008183	8.319720
22	H	7.215846	8.426217	7.113373	9.253982	8.746964
23	C	7.925039	9.209957	7.416552	9.773473	9.831333
24	C	8.681445	9.993937	8.219952	10.617460	10.570015
25	O	8.058135	9.330270	7.726320	10.025573	9.815048
26	H	6.972307	8.261539	6.403774	8.780861	8.937168
27	H	8.573898	9.822125	8.042170	10.339700	10.456704
28	H	9.756072	11.064864	9.293062	11.686903	11.632356
29	C	8.388603	9.711205	7.921502	10.337056	10.294067
30	H	8.848544	10.152465	8.485752	10.850256	10.649634
31	H	8.990849	10.313169	8.428862	10.863523	10.963242
32	H	7.344982	8.666458	6.872016	9.283715	9.265998

		21	22	23	24	25
21	O	0.000000				
22	H	0.977074	0.000000			
23	C	3.965597	3.023229	0.000000		
24	C	3.958057	3.008738	1.468077	0.000000	
25	O	2.783424	1.808987	1.450410	1.447887	0.000000
26	H	4.058830	3.227827	1.087383	2.208718	2.145833

27	H	4.676762	3.752583	1.086594	2.216475	2.133400
28	H	4.656940	3.721588	2.191603	1.088925	2.108856
29	C	4.210224	3.423690	2.601943	1.503844	2.520207
30	H	4.083565	3.431967	3.428374	2.149498	2.906485
31	H	5.302322	4.504177	3.165950	2.135901	3.425859
32	H	3.947796	3.268461	2.717070	2.152002	2.742395

		26	27	28	29	30
26	H	0.000000				
27	H	1.852478	0.000000			
28	H	3.120683	2.503283	0.000000		
29	C	2.812799	3.540923	2.208210	0.000000	
30	H	3.741880	4.339079	2.583332	1.094293	0.000000
31	H	3.335791	3.957792	2.531518	1.094414	1.769944
32	H	2.505400	3.772224	3.099843	1.091783	1.786732

		31	32
31	H	0.000000	
32	H	1.767895	0.000000

Stoichiometry C10H17BrN2O2
Framework group C1[X(C10H17BrN2O2)]
Deg. of freedom 90
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.712251	2.112979	-0.439538
2	6	0	-3.790130	1.348906	-0.128495
3	7	0	-3.322974	0.049111	0.039790
4	6	0	-1.991729	0.038186	-0.167775
5	7	0	-1.605594	1.278056	-0.464095
6	6	0	-0.203507	1.676124	-0.706739
7	6	0	0.454859	2.248203	0.560950
8	1	0	-2.638905	3.165817	-0.651386
9	1	0	-4.825783	1.614707	-0.020778
10	1	0	0.326809	0.781937	-1.038252
11	1	0	-0.199272	2.423986	-1.500738
12	1	0	-0.161020	3.063133	0.959791
13	1	0	0.511096	1.460125	1.320739
14	35	0	0.527137	-2.055867	-0.145838
15	1	0	-1.297195	-0.827251	-0.111942
16	6	0	-4.054236	-1.125539	0.367140

17	6	0	-5.363938	-1.167617	0.573565
18	1	0	-3.415373	-1.997574	0.430724
19	1	0	-5.828513	-2.112668	0.818166
20	1	0	-6.008660	-0.300187	0.511119
21	8	0	1.718376	2.771970	0.241861
22	1	0	2.403616	2.093700	0.400194
23	6	0	3.794703	-0.457240	1.235355
24	6	0	4.547375	0.009449	0.064486
25	8	0	3.724039	0.930500	0.819576
26	1	0	2.880879	-1.025566	1.079362
27	1	0	4.309373	-0.604223	2.180974
28	1	0	5.608328	0.211923	0.202832
29	6	0	4.117239	-0.304211	-1.341981
30	1	0	4.305308	0.547844	-2.002366
31	1	0	4.691069	-1.156233	-1.719502
32	1	0	3.058776	-0.569482	-1.377744

Rotational constants (GHZ): 0.6008827 0.2209802 0.1722610

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.

475 basis functions, 751 primitive gaussians, 492 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1307.2249257763 Hartrees.

NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 475 RedAO= T EigKep= 3.78D-06 NBF= 475

NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000191 0.000013 -0.000004 Ang= 0.02 deg.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3225.52371272 A.U. after 9 cycles

NFock= 9 Conv=0.41D-08 -V/T= 2.0018

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000013276	-0.000012054	0.000045104
2	6	0.000005459	0.000004215	0.000003067
3	7	-0.000009548	-0.000002306	0.000007834
4	6	-0.000014426	0.000021756	-0.000025590
5	7	-0.000000664	-0.000002664	-0.000016842
6	6	0.000001207	0.000003732	0.000013108
7	6	0.000062494	-0.000029993	0.000007830
8	1	0.000001126	0.000001534	0.000000264
9	1	-0.000000236	0.000000664	-0.000001140
10	1	-0.000000649	0.000005932	0.000000532
11	1	-0.000002926	-0.000001089	0.000000987
12	1	-0.000008152	-0.000007247	0.000004212
13	1	-0.000007640	-0.000001627	-0.000002739
14	35	-0.000012918	0.000008033	-0.000008206
15	1	0.000034414	-0.000013635	0.000018750
16	6	0.000000298	0.000005583	-0.000007517
17	6	-0.000001656	0.000004120	-0.000001188
18	1	0.000002481	0.000003310	-0.000007144
19	1	-0.000000006	0.000003350	-0.000006006
20	1	0.000001296	0.000000395	0.000000154
21	8	-0.000065128	0.000010261	0.000013813
22	1	0.000042354	-0.000007464	-0.000022110
23	6	0.000045265	0.000013662	-0.000033657
24	6	-0.000026446	-0.000006860	0.000013170
25	8	-0.000042553	0.000006566	0.000018311
26	1	-0.000002760	-0.000014651	-0.000001175
27	1	-0.000002684	-0.000005711	-0.000002451
28	1	0.000005194	-0.000006202	-0.000007042
29	6	0.000007830	0.000000010	0.000004191
30	1	0.000001627	0.000005824	-0.000001053
31	1	0.000001505	0.000006111	-0.000005570
32	1	-0.000000883	0.000006443	-0.000001900

Cartesian Forces: Max 0.000065128 RMS 0.000016370

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.000042918 RMS 0.000007277
Search for a local minimum.
Step number 34 out of a maximum of 177
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 24 25 26 27 28
29 30 31 32 33
34
DE= -5.73D-07 DEPred=-1.39D-07 R= 4.13D+00
Trust test= 4.13D+00 RLast= 4.18D-02 DXMaxT set to 1.94D+00
ITU= 0 1 1 0 1 1 1 1 1 1 1 1 1 1 1 1 -1 1 1
ITU= 1 1 1 1 1 1 1 1 1 0 1 0 1 0
Eigenvalues --- 0.00004 0.00060 0.00124 0.00234 0.00252
Eigenvalues --- 0.00328 0.00633 0.01007 0.01113 0.01313
Eigenvalues --- 0.01450 0.01649 0.01826 0.01956 0.02026
Eigenvalues --- 0.02168 0.02230 0.02321 0.02393 0.03021
Eigenvalues --- 0.03060 0.03136 0.03428 0.03577 0.03831
Eigenvalues --- 0.04413 0.04637 0.05213 0.05433 0.05592
Eigenvalues --- 0.05677 0.05934 0.06590 0.09296 0.09424
Eigenvalues --- 0.10422 0.11165 0.11472 0.11693 0.12942
Eigenvalues --- 0.13810 0.14159 0.14606 0.15904 0.15970
Eigenvalues --- 0.15997 0.16001 0.16002 0.16020 0.16031
Eigenvalues --- 0.16091 0.16955 0.19053 0.21233 0.22046
Eigenvalues --- 0.22838 0.23395 0.23926 0.24228 0.25035
Eigenvalues --- 0.27696 0.28579 0.30776 0.32052 0.33106
Eigenvalues --- 0.33346 0.34035 0.34199 0.34500 0.34838
Eigenvalues --- 0.35025 0.35685 0.35689 0.35857 0.36245
Eigenvalues --- 0.36436 0.36677 0.37200 0.37255 0.37600
Eigenvalues --- 0.38516 0.42169 0.42501 0.44883 0.45844
Eigenvalues --- 0.49499 0.54238 0.55195 0.56535 0.60401
Eigenvalue 1 is 3.86D-05 Eigenvector:
D52 D54 D53 D55 D25
1 0.50872 -0.49702 -0.49641 -0.48828 0.04005
D26 D45 D46 D47 D65
1 0.03547 -0.02920 -0.02795 -0.02530 -0.01706
En-DIIS/RFO-DIIS IScMMF= 0 using points: 34 33 32 31 30
RFO step: Lambda=-2.21950665D-08.
DidBck=F Rises=F RFO-DIIS coefs: 2.05039 -1.12205 -0.41259 0.84567 -0.36143
Iteration 1 RMS(Cart)= 0.00124965 RMS(Int)= 0.00000241
Iteration 2 RMS(Cart)= 0.00000399 RMS(Int)= 0.00000140
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000140
Variable Old X -DE/DX Delta X Delta X Delta X New X

			(Linear)	(Quad)	(Total)	
R1	2.56501	0.00000	-0.00001	0.00000	-0.00001	2.56500
R2	2.62011	0.00000	0.00003	-0.00001	0.00002	2.62013
R3	2.03418	0.00000	0.00000	0.00000	0.00000	2.03418
R4	2.62938	0.00000	0.00000	0.00000	0.00001	2.62939
R5	2.03076	0.00000	0.00000	0.00000	0.00000	2.03076
R6	2.54617	0.00001	0.00001	-0.00001	0.00000	2.54616
R7	2.68694	0.00000	0.00001	0.00000	0.00001	2.68695
R8	2.51709	0.00000	-0.00004	-0.00001	-0.00005	2.51704
R9	2.09962	0.00001	-0.00005	0.00004	-0.00001	2.09961
R10	2.79218	0.00001	0.00005	-0.00002	0.00002	2.79221
R11	2.90782	0.00001	0.00002	0.00002	0.00004	2.90786
R12	2.06206	0.00000	0.00000	0.00000	0.00000	2.06205
R13	2.06123	0.00000	0.00001	-0.00001	0.00000	2.06123
R14	2.07224	0.00001	0.00000	0.00000	-0.00001	2.07223
R15	2.07139	0.00000	0.00002	0.00000	0.00002	2.07141
R16	2.65412	-0.00004	-0.00010	-0.00001	-0.00011	2.65402
R17	4.15690	-0.00001	0.00004	-0.00025	-0.00021	4.15669
R18	8.46601	0.00000	-0.00124	0.00006	-0.00118	8.46483
R19	2.50679	0.00000	0.00000	0.00000	0.00000	2.50679
R20	2.04635	0.00000	0.00000	0.00000	0.00000	2.04635
R21	2.04299	0.00000	0.00000	0.00000	0.00000	2.04298
R22	2.04580	0.00000	0.00000	0.00000	0.00000	2.04580
R23	1.84640	0.00002	0.00002	0.00000	0.00001	1.84641
R24	3.41849	0.00000	0.00007	0.00006	0.00012	3.41861
R25	2.77426	0.00000	0.00003	-0.00003	0.00000	2.77426
R26	2.74088	0.00000	-0.00008	0.00002	-0.00006	2.74082
R27	2.05486	0.00000	0.00001	-0.00002	-0.00001	2.05485
R28	2.05336	0.00000	0.00000	-0.00001	-0.00001	2.05335
R29	2.73611	0.00001	-0.00004	0.00001	-0.00002	2.73609
R30	2.05777	0.00001	0.00001	-0.00001	0.00000	2.05777
R31	2.84185	0.00000	-0.00003	0.00000	-0.00003	2.84182
R32	2.06791	0.00000	0.00001	-0.00001	0.00000	2.06791
R33	2.06814	0.00000	0.00001	-0.00001	0.00000	2.06815
R34	2.06317	0.00000	0.00001	-0.00001	0.00000	2.06317
A1	1.87435	0.00000	-0.00002	-0.00001	-0.00002	1.87433
A2	2.27809	0.00000	0.00001	0.00000	0.00001	2.27810
A3	2.13070	0.00000	0.00001	0.00001	0.00002	2.13072
A4	1.86184	0.00000	0.00002	0.00000	0.00002	1.86186
A5	2.27712	0.00000	-0.00002	0.00000	-0.00002	2.27710
A6	2.14420	0.00000	0.00000	0.00001	0.00001	2.14421
A7	1.89723	0.00000	-0.00002	0.00000	-0.00002	1.89721
A8	2.24838	0.00000	0.00003	0.00001	0.00004	2.24841
A9	2.13757	0.00000	0.00000	-0.00001	-0.00001	2.13755

A10	1.88930	0.00000	0.00002	0.00000	0.00002	1.88932
A11	2.23470	0.00001	-0.00006	0.00000	-0.00006	2.23464
A12	2.15918	-0.00001	0.00003	0.00000	0.00004	2.15922
A13	1.90203	0.00000	0.00000	0.00001	0.00001	1.90204
A14	2.21189	0.00001	0.00003	0.00002	0.00006	2.21194
A15	2.16808	-0.00001	-0.00001	-0.00003	-0.00004	2.16804
A16	1.95075	0.00001	0.00003	0.00000	0.00003	1.95078
A17	1.86533	0.00000	-0.00005	-0.00001	-0.00007	1.86526
A18	1.88383	0.00000	0.00001	0.00002	0.00002	1.88385
A19	1.92518	0.00000	0.00005	0.00003	0.00009	1.92526
A20	1.92105	-0.00001	-0.00006	-0.00001	-0.00008	1.92097
A21	1.91645	0.00000	0.00003	-0.00003	0.00000	1.91645
A22	1.91307	-0.00001	-0.00003	-0.00001	-0.00003	1.91304
A23	1.90255	0.00000	0.00009	-0.00001	0.00008	1.90263
A24	1.91387	0.00001	0.00005	0.00007	0.00012	1.91400
A25	1.88705	0.00000	-0.00006	-0.00003	-0.00009	1.88696
A26	1.88678	0.00000	-0.00012	-0.00001	-0.00013	1.88665
A27	1.95999	0.00000	0.00006	-0.00002	0.00003	1.96002
A28	1.78869	-0.00001	-0.00011	-0.00022	-0.00033	1.78836
A29	2.83280	0.00003	0.00026	0.00035	0.00060	2.83340
A30	2.17706	0.00000	-0.00002	0.00000	-0.00002	2.17704
A31	1.95560	0.00000	-0.00001	-0.00001	-0.00002	1.95558
A32	2.15052	0.00000	0.00003	0.00001	0.00004	2.15056
A33	2.07968	0.00000	0.00002	0.00000	0.00002	2.07970
A34	2.15746	0.00000	-0.00003	0.00000	-0.00002	2.15744
A35	2.04604	0.00000	0.00000	0.00000	0.00001	2.04605
A36	1.91264	0.00001	0.00003	-0.00001	0.00001	1.91265
A37	3.05042	0.00002	-0.00008	0.00038	0.00031	3.05073
A38	2.07441	-0.00001	-0.00014	-0.00001	-0.00015	2.07426
A39	2.08776	0.00001	0.00010	-0.00004	0.00005	2.08781
A40	2.00204	-0.00001	-0.00017	0.00001	-0.00016	2.00188
A41	1.98447	0.00000	0.00005	0.00006	0.00011	1.98458
A42	2.04003	0.00000	0.00009	0.00000	0.00009	2.04012
A43	2.04576	-0.00001	-0.00001	-0.00005	-0.00006	2.04570
A44	2.13290	0.00002	0.00006	-0.00001	0.00005	2.13295
A45	1.94927	0.00000	-0.00008	0.00007	-0.00001	1.94926
A46	2.04629	0.00001	0.00009	0.00003	0.00011	2.04640
A47	2.02226	0.00000	-0.00003	0.00000	-0.00004	2.02222
A48	1.42812	0.00000	0.00098	0.00031	0.00128	1.42940
A49	0.99887	0.00002	0.00071	-0.00003	0.00069	0.99955
A50	2.37064	0.00002	0.00151	0.00041	0.00192	2.37256
A51	2.35069	0.00000	0.00029	-0.00005	0.00024	2.35093
A52	1.93141	0.00000	0.00005	-0.00003	0.00002	1.93143
A53	1.91243	0.00000	-0.00005	0.00000	-0.00005	1.91238

A54	1.93757	0.00000	0.00006	0.00000	0.00006	1.93763
A55	1.88378	0.00000	-0.00005	0.00001	-0.00004	1.88374
A56	1.91350	0.00000	-0.00001	0.00002	0.00001	1.91351
A57	1.88375	0.00000	-0.00001	-0.00001	-0.00001	1.88373
A58	3.77881	0.00000	0.00126	0.00026	0.00152	3.78033
A59	5.04628	0.00000	-0.00098	-0.00070	-0.00168	5.04460
D1	0.00452	-0.00001	-0.00004	0.00000	-0.00004	0.00448
D2	-3.13076	-0.00001	-0.00026	-0.00007	-0.00033	-3.13109
D3	3.13603	0.00000	0.00031	0.00007	0.00037	3.13640
D4	0.00075	0.00000	0.00008	0.00000	0.00008	0.00083
D5	-0.00696	0.00001	0.00008	0.00002	0.00010	-0.00686
D6	-3.09767	0.00000	-0.00043	0.00002	-0.00041	-3.09808
D7	-3.13950	0.00000	-0.00023	-0.00004	-0.00027	-3.13977
D8	0.05297	-0.00001	-0.00073	-0.00005	-0.00078	0.05219
D9	-0.00062	0.00000	-0.00002	-0.00002	-0.00004	-0.00065
D10	-3.13665	0.00000	-0.00003	-0.00004	-0.00007	-3.13673
D11	3.13526	0.00000	0.00018	0.00005	0.00023	3.13549
D12	-0.00078	0.00000	0.00017	0.00002	0.00019	-0.00059
D13	-0.00372	0.00000	0.00007	0.00003	0.00010	-0.00362
D14	3.13697	0.00001	0.00019	0.00005	0.00024	3.13721
D15	3.13275	0.00000	0.00008	0.00005	0.00014	3.13288
D16	-0.00975	0.00001	0.00021	0.00007	0.00028	-0.00948
D17	0.00030	0.00000	0.00006	0.00031	0.00037	0.00066
D18	-3.14146	0.00000	0.00009	0.00029	0.00038	-3.14108
D19	-3.13506	0.00000	0.00005	0.00028	0.00032	-3.13473
D20	0.00637	0.00000	0.00008	0.00026	0.00034	0.00671
D21	0.00657	-0.00001	-0.00010	-0.00003	-0.00013	0.00645
D22	3.09885	0.00000	0.00040	-0.00003	0.00037	3.09923
D23	-3.13416	-0.00001	-0.00021	-0.00005	-0.00026	-3.13442
D24	-0.04188	-0.00001	0.00028	-0.00004	0.00024	-0.04164
D25	-3.11420	-0.00001	0.00388	0.00073	0.00461	-3.10959
D26	0.02636	0.00000	0.00402	0.00075	0.00477	0.03113
D27	1.41052	0.00000	-0.00105	-0.00034	-0.00139	1.40913
D28	-2.76480	0.00000	-0.00100	-0.00031	-0.00131	-2.76610
D29	-0.70434	0.00000	-0.00099	-0.00034	-0.00133	-0.70567
D30	-1.67287	0.00000	-0.00163	-0.00035	-0.00198	-1.67485
D31	0.43499	0.00000	-0.00158	-0.00032	-0.00190	0.43309
D32	2.49545	0.00000	-0.00157	-0.00035	-0.00192	2.49353
D33	-0.93860	0.00000	-0.00002	-0.00015	-0.00017	-0.93877
D34	1.12368	-0.00001	-0.00006	-0.00019	-0.00025	1.12344
D35	-3.00729	0.00000	0.00011	-0.00018	-0.00007	-3.00736
D36	-3.01126	0.00000	-0.00001	-0.00015	-0.00016	-3.01142
D37	-0.94898	0.00000	-0.00005	-0.00019	-0.00024	-0.94922
D38	1.20324	0.00000	0.00012	-0.00018	-0.00006	1.20317

D39	1.15454	0.00000	-0.00004	-0.00013	-0.00017	1.15437
D40	-3.06636	0.00000	-0.00007	-0.00017	-0.00025	-3.06661
D41	-0.91415	0.00000	0.00009	-0.00016	-0.00007	-0.91422
D42	-1.64154	0.00000	0.00116	0.00031	0.00147	-1.64007
D43	2.55675	0.00000	0.00123	0.00028	0.00152	2.55827
D44	0.47646	0.00000	0.00135	0.00034	0.00169	0.47815
D45	0.44142	0.00000	-0.00482	-0.00099	-0.00581	0.43561
D46	-0.27475	0.00001	0.00054	0.00060	0.00114	-0.27361
D47	2.56309	0.00002	0.00041	0.00103	0.00143	2.56452
D48	-3.14158	0.00000	0.00001	0.00001	0.00002	-3.14156
D49	0.00046	0.00000	0.00002	0.00002	0.00004	0.00050
D50	0.00020	0.00000	-0.00002	0.00003	0.00001	0.00020
D51	-3.14095	0.00000	-0.00001	0.00003	0.00003	-3.14092
D52	-1.93252	0.00000	0.01073	-0.00291	0.00782	-1.92470
D53	2.44234	0.00000	-0.01095	0.00277	-0.00818	2.43416
D54	2.07307	-0.00001	-0.01189	0.00313	-0.00876	2.06432
D55	-2.60395	0.00000	-0.00997	0.00347	-0.00650	-2.61044
D56	-2.72894	0.00000	-0.00025	0.00014	-0.00011	-2.72905
D57	-0.02984	0.00000	-0.00022	-0.00002	-0.00024	-0.03007
D58	-0.02162	0.00000	-0.00012	0.00002	-0.00010	-0.02172
D59	2.67748	0.00000	-0.00008	-0.00014	-0.00022	2.67726
D60	-0.17079	0.00000	-0.00038	0.00036	-0.00002	-0.17081
D61	0.26804	0.00000	0.00061	-0.00005	0.00056	0.26860
D62	-2.58306	0.00000	-0.00038	0.00027	-0.00011	-2.58317
D63	-2.14423	0.00000	0.00061	-0.00014	0.00047	-2.14376
D64	2.14929	-0.00001	-0.00219	-0.00047	-0.00266	2.14664
D65	-0.24398	-0.00001	-0.00214	-0.00057	-0.00272	-0.24669
D66	2.48871	0.00001	0.00025	-0.00005	0.00020	2.48891
D67	-1.71922	0.00000	0.00019	-0.00005	0.00014	-1.71908
D68	0.35980	0.00000	0.00019	-0.00006	0.00013	0.35993
D69	1.27262	0.00000	0.00023	-0.00007	0.00016	1.27278
D70	-2.93531	0.00000	0.00016	-0.00007	0.00009	-2.93522
D71	-0.85629	0.00000	0.00016	-0.00008	0.00008	-0.85621
D72	-1.08985	0.00000	0.00029	-0.00021	0.00007	-1.08978
D73	0.98540	0.00000	0.00023	-0.00021	0.00001	0.98541
D74	3.06442	0.00000	0.00022	-0.00022	0.00000	3.06442

Item	Value	Threshold	Converged?
Maximum Force	0.000043	0.000450	YES
RMS Force	0.000007	0.000300	YES
Maximum Displacement	0.004363	0.001800	NO
RMS Displacement	0.001253	0.001200	NO

Predicted change in Energy=-7.504136D-08

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.377528	-1.908512	-0.259651
2	6	0	-2.509026	-1.168407	-0.139956
3	7	0	-2.111081	0.112342	0.230654
4	6	0	-0.767638	0.135275	0.330878
5	7	0	-0.307018	-1.080767	0.042459
6	6	0	1.126233	-1.436848	-0.004616
7	6	0	1.683704	-1.371854	-1.437382
8	1	0	-1.243345	-2.943548	-0.523124
9	1	0	-3.539008	-1.441386	-0.279423
10	1	0	1.650065	-0.727508	0.638143
11	1	0	1.234790	-2.446452	0.393709
12	1	0	1.065318	-1.987861	-2.101175
13	1	0	1.636797	-0.335771	-1.792156
14	35	0	1.653145	2.228819	1.028907
15	1	0	-0.115937	0.993272	0.602151
16	6	0	-2.915360	1.256551	0.486869
17	6	0	-4.239361	1.282558	0.409140
18	1	0	-2.319906	2.119672	0.757228
19	1	0	-4.761586	2.204545	0.623616
20	1	0	-4.840874	0.423593	0.140140
21	8	0	2.991233	-1.884051	-1.459438
22	1	0	3.631296	-1.152531	-1.360030
23	6	0	4.836615	1.611118	-1.122182
24	6	0	5.713034	0.752656	-0.315843
25	8	0	4.858576	0.176268	-1.332711
26	1	0	3.920245	1.991041	-0.676852
27	1	0	5.254374	2.180315	-1.948116
28	1	0	6.763347	0.706926	-0.599591
29	6	0	5.404956	0.412520	1.116251
30	1	0	5.686815	-0.621603	1.336754
31	1	0	5.978484	1.066906	1.780021
32	1	0	4.345107	0.558335	1.334082

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357339	0.000000			
3	N	2.205073	1.391413	0.000000		
4	C	2.213087	2.225692	1.347372	0.000000	

5	N	1.386515	2.211289	2.171076	1.331959	0.000000
6	C	2.560533	3.647669	3.596602	2.484125	1.477572
7	C	3.323581	4.393596	4.402905	3.377463	2.497525
8	H	1.076440	2.213570	3.264906	3.230289	2.160219
9	H	2.211468	1.074630	2.170996	3.246354	3.267937
10	H	3.371516	4.254159	3.875257	2.585362	2.076007
11	H	2.745991	3.991787	4.215314	3.267872	2.089413
12	H	3.060230	4.158584	4.465175	3.712454	2.702090
13	H	3.729375	4.539923	4.282424	3.241985	2.774751
14	Br	5.287993	5.498277	4.391592	3.275723	3.970979
15	H	3.279430	3.309147	2.212385	1.111063	2.156711
16	C	3.597199	2.537408	1.421873	2.427818	3.530439
17	C	4.338236	3.050048	2.435331	3.657218	4.602508
18	H	4.260092	3.413527	2.085728	2.555218	3.847781
19	H	5.399003	4.127211	3.399545	4.507681	5.565446
20	H	4.194438	2.837328	2.748970	4.087879	4.777917
21	O	4.530581	5.701406	5.733725	4.627313	3.712064
22	H	5.183692	6.260383	6.091394	4.885513	4.181201
23	C	7.193561	7.915110	7.235121	5.974709	5.921114
24	C	7.573708	8.445336	7.869272	6.542058	6.303241
25	O	6.662338	7.583691	7.143131	5.867154	5.491319
26	H	6.591431	7.183724	6.382004	5.141560	5.274766
27	H	7.971922	8.646026	7.954463	6.755785	6.747305
28	H	8.557448	9.471275	8.932990	7.609750	7.321075
29	C	7.299478	8.167527	7.573982	6.228531	6.000798
30	H	7.355922	8.345746	7.910077	6.576064	6.149151
31	H	8.192942	8.984474	8.291731	6.962623	6.865796
32	H	6.432252	7.220358	6.564970	5.227385	5.098746

		6	7	8	9	10
6	C	0.000000				
7	C	1.538771	0.000000			
8	H	2.855503	3.445824	0.000000		
9	H	4.673330	5.349992	2.754259	0.000000	
10	H	1.091192	2.173503	3.825075	5.317708	0.000000
11	H	1.090756	2.170065	2.688651	4.924673	1.785209
12	H	2.168614	1.096579	2.955251	4.981689	3.071527
13	H	2.160635	1.096144	4.087317	5.504516	2.461703
14	Br	3.844856	4.364443	6.127956	6.491578	2.982043
15	H	2.795824	3.604472	4.246863	4.292103	2.465997
16	C	4.881642	5.635835	4.632122	2.873153	4.980208
17	C	6.029591	6.748203	5.263573	2.895598	6.227210
18	H	5.010500	5.747691	5.332399	3.904099	4.886848
19	H	6.951318	7.653763	6.340023	3.950062	7.050277
20	H	6.252085	6.948548	4.971898	2.312799	6.611001

21	O	2.407223	1.404445	4.464401	6.650747	2.745208
22	H	2.862398	1.961429	5.260255	7.257024	2.845806
23	C	4.930110	4.351818	7.620352	8.954277	4.326894
24	C	5.092105	4.691151	7.880109	9.508703	4.428171
25	O	4.277424	3.533759	6.900878	8.616590	3.872417
26	H	4.473122	4.109694	7.143981	8.220703	3.778020
27	H	5.822594	5.062454	8.396721	9.655300	5.304264
28	H	6.060265	5.552117	8.799939	10.528830	5.453003
29	C	4.794160	4.853118	7.625658	9.240095	3.953158
30	H	4.823153	4.927840	7.541730	9.402121	4.098124
31	H	5.744393	5.894436	8.575724	10.055620	4.822761
32	H	4.016717	4.299966	6.851511	8.292258	3.066101

		11	12	13	14	15
11	H	0.000000				
12	H	2.542336	0.000000			
13	H	3.065060	1.775241	0.000000		
14	Br	4.736735	5.284254	3.812583	0.000000	
15	H	3.701299	4.194101	3.251328	2.199625	0.000000
16	C	5.562792	5.750650	5.334002	4.702163	2.814138
17	C	6.623601	6.718403	6.480272	6.000095	4.138063
18	H	5.798060	6.041691	5.308866	3.983824	2.479981
19	H	7.592177	7.678122	7.295784	6.427567	4.801010
20	H	6.724221	6.761783	6.802252	6.798605	4.781529
21	O	2.614487	2.032671	2.083835	4.989794	4.709951
22	H	3.239302	2.798448	2.198148	4.588424	4.743035
23	C	5.633378	5.304126	3.805006	3.891430	5.280419
24	C	5.549093	5.683230	4.469886	4.524391	5.905719
25	O	4.794894	4.434274	3.294409	4.479397	5.399719
26	H	5.296142	5.100094	3.445590	2.847086	4.349960
27	H	6.561111	5.911455	4.409294	4.672673	6.062439
28	H	6.441691	6.479519	5.365719	5.575153	6.989330
29	C	5.107453	5.911523	4.818484	4.169251	5.575108
30	H	4.903054	5.919818	5.125858	4.948755	6.067899
31	H	6.063678	6.966669	5.794669	4.541231	6.207638
32	H	4.425734	5.388981	4.231752	3.182814	4.541564

		16	17	18	19	20
16	C	0.000000				
17	C	1.326536	0.000000			
18	H	1.082884	2.122789	0.000000		
19	H	2.079890	1.081100	2.446805	0.000000	
20	H	2.126416	1.082589	3.100446	1.847113	0.000000
21	O	6.967017	8.111750	7.010820	9.008991	8.320203
22	H	7.216191	8.426557	7.113852	9.254473	8.747133
23	C	7.925142	9.210116	7.416643	9.773711	9.831453

24	C	8.680290	9.992826	8.218780	10.616413	10.568878
25	O	8.056795	9.329007	7.724976	10.024401	9.813755
26	H	6.972748	8.261991	6.404109	8.781286	8.937649
27	H	8.574791	9.823117	8.043151	10.340882	10.457577
28	H	9.754991	11.063837	9.292055	11.686025	11.631226
29	C	8.386665	9.709265	7.919391	10.335018	10.292227
30	H	8.845743	10.149644	8.482807	10.847339	10.646904
31	H	8.989364	10.311653	8.427200	10.861887	10.961824
32	H	7.343000	8.664474	6.869710	9.281520	9.264227

		21	22	23	24	25
21	O	0.000000				
22	H	0.977079	0.000000			
23	C	3.966784	3.024420	0.000000		
24	C	3.958312	3.008936	1.468077	0.000000	
25	O	2.783512	1.809052	1.450379	1.447876	0.000000
26	H	4.061014	3.229902	1.087380	2.208624	2.145697
27	H	4.677572	3.753410	1.086589	2.216505	2.133444
28	H	4.656323	3.720966	2.191566	1.088926	2.108843
29	C	4.211231	3.424503	2.601966	1.503828	2.520270
30	H	4.083947	3.432154	3.428447	2.149500	2.906651
31	H	5.303387	4.505010	3.165882	2.135851	3.425862
32	H	3.949934	3.270294	2.717198	2.152031	2.742519

		26	27	28	29	30
26	H	0.000000				
27	H	1.852522	0.000000			
28	H	3.120601	2.503277	0.000000		
29	C	2.812705	3.540920	2.208170	0.000000	
30	H	3.741829	4.339138	2.583281	1.094293	0.000000
31	H	3.335655	3.957653	2.531432	1.094416	1.769921
32	H	2.505396	3.772321	3.099848	1.091784	1.786741

		31	32
31	H	0.000000	
32	H	1.767888	0.000000

Stoichiometry C10H17BrN2O2
Framework group C1[X(C10H17BrN2O2)]
Deg. of freedom 90
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-2.711678	2.113406	-0.438522
2	6	0	-3.789603	1.349182	-0.128024
3	7	0	-3.322540	0.049238	0.039397
4	6	0	-1.991300	0.038381	-0.168187
5	7	0	-1.605065	1.278419	-0.463559
6	6	0	-0.202967	1.676406	-0.706345
7	6	0	0.455145	2.249857	0.560880
8	1	0	-2.638220	3.166438	-0.649359
9	1	0	-4.825203	1.615032	-0.019925
10	1	0	0.327433	0.781928	-1.036927
11	1	0	-0.198647	2.423511	-1.501056
12	1	0	-0.160817	3.065236	0.958666
13	1	0	0.511154	1.462679	1.321633
14	35	0	0.526846	-2.056555	-0.144835
15	1	0	-1.296895	-0.827201	-0.113129
16	6	0	-4.053841	-1.125599	0.366015
17	6	0	-5.363595	-1.167800	0.572080
18	1	0	-3.414940	-1.997625	0.429365
19	1	0	-5.828227	-2.112960	0.816146
20	1	0	-6.008304	-0.300347	0.509825
21	8	0	1.718668	2.773375	0.241655
22	1	0	2.403777	2.094873	0.399591
23	6	0	3.795113	-0.457265	1.234992
24	6	0	4.546595	0.009451	0.063369
25	8	0	3.723098	0.930199	0.818631
26	1	0	2.881568	-1.026241	1.079759
27	1	0	4.310538	-0.603535	2.180306
28	1	0	5.607492	0.212765	0.200923
29	6	0	4.115838	-0.305262	-1.342654
30	1	0	4.302944	0.546540	-2.003638
31	1	0	4.690078	-1.157077	-1.720022
32	1	0	3.057551	-0.571331	-1.377699

Rotational constants (GHZ): 0.6005774 0.2210490 0.1722658

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.

475 basis functions, 751 primitive gaussians, 492 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1307.2102452976 Hartrees.

NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 475 RedAO= T EigKep= 3.78D-06 NBF= 475
NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 0.000061 -0.000013 0.000029 Ang= 0.01 deg.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3225.52371282 A.U. after 8 cycles
NFock= 8 Conv=0.90D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000005726	-0.000003284	0.000025520
2	6	0.000001141	0.000006676	-0.000009374
3	7	-0.000006167	-0.000005649	0.000009959
4	6	-0.000024984	0.000026709	-0.000004063
5	7	0.000010391	-0.000022979	-0.000001278
6	6	-0.000004808	-0.000000092	-0.000002754
7	6	0.000027724	-0.000016553	0.000001721
8	1	-0.000000232	-0.000001782	0.000009604
9	1	-0.000001225	0.000000782	0.000002235
10	1	0.000004245	0.000006351	-0.000000531
11	1	-0.000001086	-0.000001958	0.000006260
12	1	-0.000008427	-0.000006367	0.000004750
13	1	-0.000005338	-0.000000411	0.000004844
14	35	-0.000012310	0.000005477	-0.000005075
15	1	0.000038900	0.000003794	-0.000002093
16	6	0.000002054	0.000001199	-0.000005710
17	6	-0.000001578	0.000002567	-0.000000826
18	1	0.000001271	0.000004576	-0.000007220
19	1	0.000000241	0.000004522	-0.000006124
20	1	-0.000000095	0.000000697	-0.000000055
21	8	-0.000022713	0.000001456	0.000022717
22	1	0.000018020	-0.000002588	-0.000027342
23	6	0.000018560	0.000009973	-0.000007213
24	6	-0.000005508	0.000001138	0.000001410

25	8	-0.000025255	-0.000007790	0.000014770
26	1	-0.000004610	-0.000003523	-0.000008690
27	1	-0.000003514	-0.000009121	-0.000007523
28	1	0.000006633	-0.000008170	-0.000007119
29	6	0.000004300	-0.000002693	0.000012553
30	1	0.000001154	0.000004518	-0.000002767
31	1	0.000001759	0.000005999	-0.000004751
32	1	-0.000002815	0.000006525	-0.000005836

Cartesian Forces: Max 0.000038900 RMS 0.000010567

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000020356 RMS 0.000005044
Search for a local minimum.
Step number 35 out of a maximum of 177
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 24 25 26 27 28
29 30 31 32 33
34 35
DE= -9.68D-08 DEPred=-7.50D-08 R= 1.29D+00
Trust test= 1.29D+00 RLast= 1.96D-02 DXMaxT set to 1.94D+00
ITU= 0 0 1 1 0 1 1 1 1 1 1 1 1 1 1 1 -1 1
ITU= 1 1 1 1 1 1 1 1 1 1 0 1 0 1 0

Eigenvalues ---	0.00004	0.00058	0.00126	0.00234	0.00235
Eigenvalues ---	0.00316	0.00631	0.00816	0.01120	0.01317
Eigenvalues ---	0.01499	0.01559	0.01826	0.01894	0.01980
Eigenvalues ---	0.02177	0.02240	0.02319	0.02389	0.02993
Eigenvalues ---	0.03060	0.03097	0.03403	0.03595	0.03795
Eigenvalues ---	0.04338	0.04636	0.05223	0.05407	0.05535
Eigenvalues ---	0.05669	0.05956	0.06635	0.08831	0.09390
Eigenvalues ---	0.10532	0.11036	0.11478	0.11775	0.12939
Eigenvalues ---	0.13802	0.14068	0.14203	0.15378	0.15977
Eigenvalues ---	0.16000	0.16001	0.16004	0.16015	0.16031
Eigenvalues ---	0.16051	0.17164	0.19162	0.21283	0.22051
Eigenvalues ---	0.22841	0.23402	0.23880	0.24247	0.25041
Eigenvalues ---	0.27673	0.28563	0.30737	0.32259	0.33106
Eigenvalues ---	0.33380	0.34037	0.34214	0.34481	0.34855
Eigenvalues ---	0.35068	0.35686	0.35690	0.35858	0.36147

Eigenvalues --- 0.36438 0.36672 0.37216 0.37259 0.37671
Eigenvalues --- 0.38501 0.42164 0.42623 0.44262 0.45712
Eigenvalues --- 0.49466 0.53984 0.55068 0.56875 0.60410
Eigenvalue 1 is 3.85D-05 Eigenvector:

	D52	D54	D53	D55	D25
1	0.50825	-0.49779	-0.49657	-0.48732	0.04038
	D26	D45	D46	D47	A48
1	0.03484	-0.02873	-0.02675	-0.02452	0.01853

En-DIIS/RFO-DIIS IScMMF= 0 using points: 35 34 33 32 31
RFO step: Lambda=-1.25327051D-08.
DidBck=F Rises=F RFO-DIIS coefs: 2.03997 -1.20611 -0.25134 0.67355 -0.25607
Iteration 1 RMS(Cart)= 0.00160779 RMS(Int)= 0.00000314
Iteration 2 RMS(Cart)= 0.00000717 RMS(Int)= 0.00000125
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000125

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56500	0.00000	-0.00001	0.00001	0.00000	2.56500
R2	2.62013	0.00000	0.00001	0.00000	0.00001	2.62015
R3	2.03418	0.00000	0.00000	0.00000	0.00000	2.03418
R4	2.62939	0.00000	0.00000	0.00000	0.00000	2.62939
R5	2.03076	0.00000	0.00000	0.00000	0.00000	2.03076
R6	2.54616	0.00001	0.00000	0.00000	0.00000	2.54617
R7	2.68695	0.00000	0.00000	0.00000	0.00001	2.68696
R8	2.51704	0.00002	0.00000	0.00002	0.00002	2.51706
R9	2.09961	0.00002	0.00006	0.00002	0.00008	2.09969
R10	2.79221	0.00000	0.00001	-0.00001	0.00000	2.79221
R11	2.90786	0.00000	0.00006	-0.00001	0.00005	2.90791
R12	2.06205	0.00000	0.00000	0.00000	0.00000	2.06206
R13	2.06123	0.00000	0.00000	0.00001	0.00001	2.06124
R14	2.07223	0.00001	0.00001	-0.00001	0.00000	2.07224
R15	2.07141	0.00000	0.00003	0.00001	0.00003	2.07144
R16	2.65402	-0.00002	-0.00013	0.00001	-0.00012	2.65390
R17	4.15669	-0.00001	-0.00043	-0.00018	-0.00061	4.15608
R18	8.46483	0.00000	-0.00055	-0.00036	-0.00091	8.46392
R19	2.50679	0.00000	0.00000	0.00000	0.00000	2.50679
R20	2.04635	0.00000	0.00000	0.00000	0.00000	2.04636
R21	2.04298	0.00000	0.00000	0.00000	0.00000	2.04298
R22	2.04580	0.00000	0.00000	0.00000	0.00000	2.04580
R23	1.84641	0.00001	0.00003	0.00001	0.00003	1.84645
R24	3.41861	0.00000	0.00002	-0.00017	-0.00015	3.41846
R25	2.77426	0.00000	0.00000	0.00002	0.00002	2.77428
R26	2.74082	0.00000	0.00001	0.00000	0.00000	2.74082
R27	2.05485	0.00000	0.00000	0.00001	0.00001	2.05486

R28	2.05335	0.00000	-0.00002	0.00001	-0.00001	2.05334
R29	2.73609	0.00001	0.00002	-0.00002	0.00000	2.73608
R30	2.05777	0.00001	0.00001	0.00001	0.00002	2.05779
R31	2.84182	0.00001	0.00000	0.00000	0.00000	2.84182
R32	2.06791	0.00000	0.00000	0.00000	0.00000	2.06791
R33	2.06815	0.00000	0.00000	0.00001	0.00001	2.06815
R34	2.06317	0.00000	0.00001	0.00000	0.00001	2.06318
A1	1.87433	0.00000	-0.00001	0.00001	-0.00001	1.87432
A2	2.27810	0.00000	0.00001	0.00000	0.00000	2.27810
A3	2.13072	0.00000	0.00001	0.00000	0.00001	2.13073
A4	1.86186	0.00000	0.00001	0.00001	0.00001	1.86187
A5	2.27710	0.00000	-0.00002	0.00000	-0.00002	2.27708
A6	2.14421	0.00000	0.00002	-0.00001	0.00001	2.14422
A7	1.89721	0.00000	0.00001	-0.00001	0.00000	1.89721
A8	2.24841	0.00000	0.00001	0.00000	0.00002	2.24843
A9	2.13755	0.00000	-0.00002	0.00001	-0.00002	2.13753
A10	1.88932	0.00000	-0.00002	0.00001	-0.00001	1.88932
A11	2.23464	0.00001	0.00000	-0.00002	-0.00002	2.23462
A12	2.15922	-0.00001	0.00002	0.00001	0.00003	2.15924
A13	1.90204	0.00000	0.00001	-0.00001	0.00000	1.90204
A14	2.21194	0.00001	0.00005	-0.00001	0.00004	2.21199
A15	2.16804	-0.00001	-0.00005	0.00002	-0.00003	2.16801
A16	1.95078	0.00000	0.00004	0.00000	0.00004	1.95082
A17	1.86526	0.00000	-0.00003	0.00001	-0.00002	1.86524
A18	1.88385	0.00000	0.00000	0.00002	0.00002	1.88387
A19	1.92526	-0.00001	-0.00001	-0.00002	-0.00002	1.92524
A20	1.92097	0.00000	-0.00002	0.00000	-0.00002	1.92095
A21	1.91645	0.00000	0.00001	-0.00001	0.00000	1.91645
A22	1.91304	0.00000	-0.00002	-0.00002	-0.00004	1.91300
A23	1.90263	-0.00001	-0.00001	0.00000	-0.00001	1.90262
A24	1.91400	0.00000	0.00008	0.00001	0.00009	1.91408
A25	1.88696	0.00000	-0.00008	0.00001	-0.00007	1.88689
A26	1.88665	0.00001	-0.00002	-0.00003	-0.00005	1.88660
A27	1.96002	0.00000	0.00006	0.00002	0.00008	1.96010
A28	1.78836	-0.00001	-0.00022	-0.00012	-0.00034	1.78802
A29	2.83340	0.00002	0.00053	0.00018	0.00071	2.83412
A30	2.17704	0.00000	-0.00001	0.00000	-0.00001	2.17703
A31	1.95558	0.00000	-0.00001	0.00000	-0.00001	1.95557
A32	2.15056	0.00000	0.00003	0.00000	0.00002	2.15059
A33	2.07970	0.00000	0.00001	0.00000	0.00001	2.07971
A34	2.15744	0.00000	-0.00002	0.00000	-0.00002	2.15742
A35	2.04605	0.00000	0.00001	0.00000	0.00001	2.04605
A36	1.91265	0.00001	0.00006	0.00004	0.00010	1.91275
A37	3.05073	0.00002	0.00048	0.00021	0.00069	3.05142

A38	2.07426	0.00000	-0.00006	0.00001	-0.00005	2.07421
A39	2.08781	0.00000	0.00005	0.00001	0.00006	2.08788
A40	2.00188	0.00000	-0.00014	0.00002	-0.00012	2.00176
A41	1.98458	0.00000	0.00008	-0.00007	0.00002	1.98460
A42	2.04012	0.00000	0.00003	0.00001	0.00004	2.04015
A43	2.04570	-0.00001	-0.00006	0.00006	0.00000	2.04570
A44	2.13295	0.00001	0.00006	-0.00001	0.00005	2.13300
A45	1.94926	0.00000	0.00000	-0.00008	-0.00008	1.94918
A46	2.04640	0.00000	0.00009	-0.00002	0.00007	2.04647
A47	2.02222	0.00000	-0.00004	0.00001	-0.00003	2.02219
A48	1.42940	0.00001	0.00064	0.00028	0.00092	1.43031
A49	0.99955	0.00000	0.00024	0.00006	0.00031	0.99987
A50	2.37256	0.00001	0.00096	0.00020	0.00116	2.37372
A51	2.35093	0.00000	-0.00001	0.00026	0.00025	2.35119
A52	1.93143	0.00000	-0.00001	0.00001	0.00000	1.93143
A53	1.91238	0.00000	-0.00005	0.00000	-0.00004	1.91233
A54	1.93763	-0.00001	0.00002	-0.00003	-0.00001	1.93763
A55	1.88374	0.00000	0.00000	0.00000	0.00000	1.88374
A56	1.91351	0.00001	0.00002	0.00002	0.00004	1.91355
A57	1.88373	0.00000	0.00000	0.00000	0.00001	1.88374
A58	3.78033	0.00001	0.00063	0.00054	0.00117	3.78150
A59	5.04460	0.00000	-0.00103	0.00001	-0.00102	5.04358
D1	0.00448	-0.00001	-0.00011	-0.00001	-0.00012	0.00436
D2	-3.13109	0.00000	-0.00029	0.00002	-0.00026	-3.13135
D3	3.13640	0.00000	0.00027	-0.00005	0.00022	3.13662
D4	0.00083	0.00000	0.00009	-0.00002	0.00007	0.00090
D5	-0.00686	0.00001	0.00008	0.00001	0.00009	-0.00676
D6	-3.09808	0.00001	-0.00020	0.00011	-0.00009	-3.09817
D7	-3.13977	0.00000	-0.00026	0.00005	-0.00021	-3.13998
D8	0.05219	0.00000	-0.00054	0.00015	-0.00039	0.05179
D9	-0.00065	0.00001	0.00010	0.00000	0.00010	-0.00055
D10	-3.13673	0.00000	0.00001	0.00001	0.00002	-3.13670
D11	3.13549	0.00000	0.00026	-0.00003	0.00024	3.13572
D12	-0.00059	0.00000	0.00017	-0.00002	0.00016	-0.00043
D13	-0.00362	0.00000	-0.00005	0.00000	-0.00005	-0.00366
D14	3.13721	0.00000	0.00037	-0.00005	0.00032	3.13753
D15	3.13288	0.00000	0.00003	-0.00001	0.00003	3.13291
D16	-0.00948	0.00000	0.00045	-0.00006	0.00039	-0.00908
D17	0.00066	0.00000	0.00049	0.00018	0.00067	0.00133
D18	-3.14108	0.00000	0.00049	0.00016	0.00064	-3.14044
D19	-3.13473	0.00000	0.00039	0.00019	0.00058	-3.13415
D20	0.00671	0.00000	0.00039	0.00017	0.00055	0.00726
D21	0.00645	0.00000	-0.00002	-0.00001	-0.00003	0.00642
D22	3.09923	0.00000	0.00026	-0.00010	0.00015	3.09938

D23	-3.13442	-0.00001	-0.00041	0.00004	-0.00037	-3.13479
D24	-0.04164	-0.00001	-0.00014	-0.00006	-0.00019	-0.04183
D25	-3.10959	-0.00001	0.00180	-0.00020	0.00160	-3.10799
D26	0.03113	0.00000	0.00227	-0.00025	0.00202	0.03315
D27	1.40913	0.00000	-0.00030	0.00001	-0.00029	1.40885
D28	-2.76610	0.00000	-0.00030	0.00000	-0.00030	-2.76641
D29	-0.70567	0.00000	-0.00030	0.00000	-0.00030	-0.70597
D30	-1.67485	0.00000	-0.00062	0.00013	-0.00049	-1.67535
D31	0.43309	0.00000	-0.00062	0.00011	-0.00051	0.43258
D32	2.49353	0.00000	-0.00062	0.00011	-0.00051	2.49302
D33	-0.93877	0.00000	-0.00016	0.00000	-0.00015	-0.93893
D34	1.12344	0.00000	-0.00028	0.00001	-0.00026	1.12317
D35	-3.00736	0.00000	-0.00016	0.00004	-0.00012	-3.00748
D36	-3.01142	0.00000	-0.00015	0.00001	-0.00014	-3.01157
D37	-0.94922	0.00000	-0.00027	0.00001	-0.00025	-0.94947
D38	1.20317	0.00000	-0.00015	0.00005	-0.00011	1.20307
D39	1.15437	0.00000	-0.00014	0.00003	-0.00011	1.15426
D40	-3.06661	0.00000	-0.00026	0.00004	-0.00022	-3.06683
D41	-0.91422	0.00000	-0.00015	0.00007	-0.00007	-0.91429
D42	-1.64007	0.00000	0.00092	0.00049	0.00141	-1.63865
D43	2.55827	0.00000	0.00092	0.00052	0.00144	2.55971
D44	0.47815	-0.00001	0.00100	0.00051	0.00151	0.47966
D45	0.43561	0.00000	-0.00298	-0.00011	-0.00310	0.43251
D46	-0.27361	0.00001	0.00146	0.00076	0.00222	-0.27139
D47	2.56452	0.00001	0.00187	0.00042	0.00228	2.56681
D48	-3.14156	0.00000	0.00004	-0.00001	0.00003	-3.14153
D49	0.00050	0.00000	0.00004	0.00001	0.00005	0.00055
D50	0.00020	0.00000	0.00004	0.00002	0.00006	0.00027
D51	-3.14092	0.00000	0.00005	0.00003	0.00008	-3.14084
D52	-1.92470	0.00000	-0.00259	-0.00127	-0.00386	-1.92856
D53	2.43416	0.00000	0.00198	0.00072	0.00269	2.43685
D54	2.06432	0.00000	0.00203	0.00020	0.00223	2.06655
D55	-2.61044	0.00000	0.00300	0.00071	0.00371	-2.60673
D56	-2.72905	0.00000	-0.00011	-0.00011	-0.00022	-2.72927
D57	-0.03007	0.00000	-0.00023	0.00004	-0.00019	-0.03026
D58	-0.02172	0.00000	-0.00005	-0.00003	-0.00008	-0.02181
D59	2.67726	0.00000	-0.00017	0.00012	-0.00005	2.67720
D60	-0.17081	-0.00001	0.00015	-0.00023	-0.00008	-0.17089
D61	0.26860	0.00000	0.00005	0.00039	0.00045	0.26904
D62	-2.58317	0.00000	0.00016	-0.00019	-0.00003	-2.58319
D63	-2.14376	0.00000	0.00007	0.00043	0.00050	-2.14326
D64	2.14664	-0.00001	-0.00127	-0.00042	-0.00169	2.14495
D65	-0.24669	-0.00001	-0.00132	-0.00031	-0.00162	-0.24832
D66	2.48891	0.00000	0.00008	-0.00014	-0.00006	2.48885

D67	-1.71908	0.00000	0.00005	-0.00013	-0.00009	-1.71917
D68	0.35993	0.00000	0.00004	-0.00015	-0.00011	0.35982
D69	1.27278	0.00000	0.00001	-0.00012	-0.00011	1.27267
D70	-2.93522	0.00000	-0.00001	-0.00012	-0.00013	-2.93535
D71	-0.85621	0.00000	-0.00003	-0.00013	-0.00016	-0.85637
D72	-1.08978	0.00000	-0.00005	0.00003	-0.00003	-1.08980
D73	0.98541	0.00000	-0.00008	0.00003	-0.00005	0.98536
D74	3.06442	0.00000	-0.00009	0.00002	-0.00007	3.06435

Item	Value	Threshold	Converged?
Maximum Force	0.000020	0.000450	YES
RMS Force	0.000005	0.000300	YES
Maximum Displacement	0.007028	0.001800	NO
RMS Displacement	0.001615	0.001200	NO

Predicted change in Energy=-3.639421D-08

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.376911	-1.908535	-0.259205
2	6	0	-2.508464	-1.168572	-0.139164
3	7	0	-2.110546	0.112362	0.230830
4	6	0	-0.767044	0.135590	0.330232
5	7	0	-0.306365	-1.080473	0.041942
6	6	0	1.126931	-1.436297	-0.005689
7	6	0	1.683629	-1.372304	-1.438830
8	1	0	-1.242686	-2.943589	-0.522591
9	1	0	-3.538462	-1.441747	-0.278133
10	1	0	1.650974	-0.726336	0.636214
11	1	0	1.235952	-2.445568	0.393361
12	1	0	1.065078	-1.989087	-2.101749
13	1	0	1.636068	-0.336532	-1.794476
14	35	0	1.652539	2.231071	1.026072
15	1	0	-0.115359	0.993771	0.601140
16	6	0	-2.914870	1.256526	0.487122
17	6	0	-4.238963	1.282097	0.410795
18	1	0	-2.319356	2.119987	0.756268
19	1	0	-4.761230	2.204085	0.625161
20	1	0	-4.840504	0.422750	0.143077
21	8	0	2.991253	-1.884071	-1.461281
22	1	0	3.631189	-1.152460	-1.361552
23	6	0	4.837603	1.611250	-1.122003

24	6	0	5.712338	0.752008	-0.314648
25	8	0	4.858304	0.176343	-1.332280
26	1	0	3.921130	1.992063	-0.677637
27	1	0	5.256706	2.179902	-1.947625
28	1	0	6.762877	0.705083	-0.597398
29	6	0	5.402583	0.412441	1.117219
30	1	0	5.683096	-0.621959	1.338142
31	1	0	5.976274	1.066303	1.781370
32	1	0	4.342702	0.559513	1.334074

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357339	0.000000			
3	N	2.205080	1.391411	0.000000		
4	C	2.213102	2.225693	1.347374	0.000000	
5	N	1.386522	2.211289	2.171083	1.331971	0.000000
6	C	2.560567	3.647682	3.596601	2.484112	1.477571
7	C	3.323546	4.393663	4.403153	3.377739	2.497584
8	H	1.076441	2.213571	3.264913	3.230307	2.160230
9	H	2.211459	1.074632	2.171000	3.246360	3.267937
10	H	3.371566	4.254139	3.875149	2.585218	2.075993
11	H	2.746143	3.991861	4.215266	3.267776	2.089431
12	H	3.060191	4.158748	4.465602	3.712877	2.702193
13	H	3.729114	4.539767	4.282579	3.242257	2.774694
14	Br	5.288274	5.498117	4.391144	3.275610	3.971416
15	H	3.279495	3.309188	2.212416	1.111108	2.156775
16	C	3.597212	2.537419	1.421877	2.427811	3.530446
17	C	4.338245	3.050059	2.435329	3.657210	4.602512
18	H	4.260091	3.413528	2.085724	2.555192	3.847770
19	H	5.399015	4.127222	3.399549	4.507680	5.565455
20	H	4.194425	2.837318	2.748948	4.087855	4.777899
21	O	4.530612	5.701475	5.733876	4.627456	3.712107
22	H	5.183424	6.260178	6.091221	4.885250	4.180827
23	C	7.193990	7.915686	7.235578	5.974833	5.921195
24	C	7.572253	8.443992	7.867922	6.540508	6.301582
25	O	6.661539	7.582980	7.142287	5.866016	5.490162
26	H	6.592343	7.184653	6.382766	5.142108	5.275414
27	H	7.973139	8.647581	7.955928	6.756731	6.748050
28	H	8.555788	9.469863	8.931680	7.608188	7.319231
29	C	7.296781	8.164727	7.571185	6.225777	5.998092
30	H	7.351904	8.341634	7.906087	6.572220	6.145243
31	H	8.190417	8.981864	8.289199	6.960199	6.863368
32	H	6.429912	7.217699	6.562126	5.224645	5.096370

		6	7	8	9	10
6	C	0.000000				
7	C	1.538798	0.000000			
8	H	2.855556	3.445540	0.000000		
9	H	4.673344	5.349978	2.754247	0.000000	
10	H	1.091194	2.173510	3.825220	5.317714	0.000000
11	H	1.090759	2.170076	2.688985	4.924794	1.785211
12	H	2.168610	1.096580	2.954758	4.981741	3.071523
13	H	2.160662	1.096161	4.086766	5.504230	2.461793
14	Br	3.845827	4.365893	6.128442	6.491304	2.982994
15	H	2.795846	3.605016	4.246934	4.292145	2.465752
16	C	4.881630	5.636154	4.632136	2.873179	4.980050
17	C	6.029588	6.748633	5.263583	2.895625	6.227035
18	H	5.010451	5.747907	5.332401	3.904120	4.886664
19	H	6.951316	7.654203	6.340034	3.950087	7.050096
20	H	6.252077	6.949026	4.971886	2.312807	6.610814
21	O	2.407270	1.404383	4.464299	6.650765	2.745211
22	H	2.861859	1.961452	5.259911	7.256816	2.844979
23	C	4.929786	4.353106	7.620746	8.954964	4.325534
24	C	5.090196	4.691161	7.878645	9.507429	4.425418
25	O	4.275932	3.533868	6.900120	8.615980	3.869982
26	H	4.473557	4.111544	7.144907	8.221689	3.777501
27	H	5.822632	5.063983	8.397796	9.657045	5.303183
28	H	6.058012	5.551784	8.798150	10.527506	5.449983
29	C	4.791655	4.852765	7.623091	9.237278	3.950032
30	H	4.819509	4.926492	7.537821	9.397953	4.094094
31	H	5.742187	5.894344	8.573264	10.052963	4.820079
32	H	4.014898	4.300184	6.849488	8.289571	3.063628

		11	12	13	14	15
11	H	0.000000				
12	H	2.542272	0.000000			
13	H	3.065086	1.775213	0.000000		
14	Br	4.737597	5.285652	3.814230	0.000000	
15	H	3.701117	4.194816	3.252103	2.199304	0.000000
16	C	5.562699	5.751195	5.334281	4.701216	2.814126
17	C	6.623480	6.719105	6.480676	5.999075	4.138052
18	H	5.797948	6.042114	5.309064	3.982597	2.479925
19	H	7.592049	7.678841	7.296218	6.426344	4.800996
20	H	6.724077	6.762551	6.802691	6.797743	4.781515
21	O	2.614586	2.032579	2.083848	4.991340	4.710265
22	H	3.238674	2.798707	2.198561	4.589563	4.742899
23	C	5.632583	5.306060	3.807349	3.891407	5.280372
24	C	5.546513	5.683692	4.471106	4.524062	5.904165
25	O	4.793087	4.435057	3.295371	4.478913	5.398483

26	H	5.296205	5.102419	3.448361	2.847149	4.350298
27	H	6.560613	5.913879	4.411906	4.672849	6.063183
28	H	6.438563	6.479701	5.366761	5.574930	6.987843
29	C	5.104214	5.911264	4.819291	4.168760	5.572429
30	H	4.898494	5.918444	5.125739	4.947985	6.064308
31	H	6.060566	6.966625	5.795861	4.541129	6.205336
32	H	4.423499	5.389161	4.232799	3.182130	4.538730

		16	17	18	19	20
16	C	0.000000				
17	C	1.326537	0.000000			
18	H	1.082886	2.122805	0.000000		
19	H	2.079897	1.081100	2.446838	0.000000	
20	H	2.126409	1.082591	3.100453	1.847118	0.000000
21	O	6.967203	8.112047	7.010889	9.009288	8.320566
22	H	7.216072	8.426599	7.113582	9.254519	8.747273
23	C	7.925652	9.210964	7.416790	9.774541	9.832534
24	C	8.679061	9.991779	8.217441	10.615433	10.567895
25	O	8.056007	9.328518	7.723896	10.023909	9.813474
26	H	6.973419	8.262920	6.404382	8.782119	8.938823
27	H	8.576437	9.825269	8.044336	10.343059	10.460032
28	H	9.753925	11.062995	9.290926	11.685320	11.630411
29	C	8.383886	9.706428	7.916713	10.332242	10.289310
30	H	8.841830	10.145573	8.479155	10.843377	10.642638
31	H	8.986863	10.309030	8.424877	10.859345	10.959053
32	H	7.339993	8.661382	6.866728	9.278403	9.261126

		21	22	23	24	25
21	O	0.000000				
22	H	0.977097	0.000000			
23	C	3.967541	3.025047	0.000000		
24	C	3.958280	3.009018	1.468087	0.000000	
25	O	2.783491	1.808973	1.450379	1.447874	0.000000
26	H	4.062411	3.231073	1.087384	2.208602	2.145621
27	H	4.678106	3.753721	1.086583	2.216550	2.133452
28	H	4.655658	3.720465	2.191580	1.088935	2.108794
29	C	4.211548	3.425063	2.602011	1.503828	2.520323
30	H	4.083591	3.432215	3.428468	2.149501	2.906668
31	H	5.303757	4.505584	3.165930	2.135822	3.425887
32	H	3.951142	3.271620	2.717240	2.152032	2.742645

		26	27	28	29	30
26	H	0.000000				
27	H	1.852543	0.000000			
28	H	3.120622	2.503348	0.000000		
29	C	2.812725	3.540970	2.208155	0.000000	
30	H	3.741791	4.339181	2.583270	1.094293	0.000000

31	H	3.335771	3.957687	2.531356	1.094419	1.769924
32	H	2.505375	3.772348	3.099842	1.091790	1.786770

		31	32
31	H	0.000000	
32	H	1.767899	0.000000

Stoichiometry C10H17BrN2O2
Framework group C1[X(C10H17BrN2O2)]
Deg. of freedom 90
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.711066	2.113818	-0.438377
2	6	0	-3.789079	1.349467	-0.128499
3	7	0	-3.322032	0.049507	0.038821
4	6	0	-1.990683	0.038773	-0.168085
5	7	0	-1.604375	1.278911	-0.462995
6	6	0	-0.202185	1.676957	-0.705154
7	6	0	0.455306	2.250750	0.562270
8	1	0	-2.637547	3.166936	-0.648767
9	1	0	-4.824717	1.615279	-0.020654
10	1	0	0.328440	0.782433	-1.035259
11	1	0	-0.197495	2.423882	-1.500036
12	1	0	-0.160844	3.066278	0.959462
13	1	0	0.510761	1.463801	1.323325
14	35	0	0.526460	-2.057173	-0.143252
15	1	0	-1.296293	-0.826885	-0.113160
16	6	0	-4.053406	-1.125456	0.364842
17	6	0	-5.363355	-1.167901	0.569619
18	1	0	-3.414372	-1.997336	0.428887
19	1	0	-5.828039	-2.113119	0.813360
20	1	0	-6.008172	-0.300584	0.506586
21	8	0	1.718968	2.774150	0.243678
22	1	0	2.403922	2.095307	0.400931
23	6	0	3.796211	-0.458073	1.233210
24	6	0	4.545758	0.009419	0.060644
25	8	0	3.722938	0.929505	0.817446
26	1	0	2.882648	-1.027320	1.079056
27	1	0	4.313028	-0.604449	2.177740
28	1	0	5.606749	0.213270	0.196738

29	6	0	4.113189	-0.305025	-1.344883
30	1	0	4.298862	0.547129	-2.005818
31	1	0	4.687429	-1.156356	-1.723350
32	1	0	3.055013	-0.571743	-1.378513

Rotational constants (GHZ): 0.6003620 0.2211187 0.1722799

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.

475 basis functions, 751 primitive gaussians, 492 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1307.2206229554 Hartrees.

NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 475 RedAO= T EigKep= 3.78D-06 NBF= 475

NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000033 -0.000035 0.000039 Ang= -0.01 deg.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3225.52371261 A.U. after 8 cycles

NFock= 8 Conv=0.85D-08 -V/T= 2.0018

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000000799	0.000002449	0.000004609
2	6	-0.000001685	0.000002477	-0.000005961
3	7	0.000001951	-0.000001931	-0.000000457
4	6	-0.000020978	0.000015075	0.000018762
5	7	0.000007422	-0.000015744	0.000008841
6	6	-0.000003047	0.000002096	-0.000008306
7	6	-0.000011846	0.000000177	0.000001576
8	1	-0.000001254	-0.000002863	0.000014590

9	1	-0.000001028	0.000000780	0.000005677
10	1	0.000002606	0.000002024	0.000001145
11	1	-0.000000589	0.000000576	0.000007591
12	1	-0.000003078	-0.000006138	0.000005932
13	1	0.000000638	-0.000004382	0.000007765
14	35	-0.000008564	0.000006677	-0.000001413
15	1	0.000028816	0.000003110	-0.000021802
16	6	0.000001537	0.000001174	-0.000003650
17	6	0.000000305	0.000000969	-0.000001623
18	1	0.000000450	0.000004270	-0.000006723
19	1	0.000000608	0.000004287	-0.000005910
20	1	-0.000000715	0.000001859	-0.000000269
21	8	0.000014559	-0.000005337	0.000019539
22	1	-0.000001839	-0.000006978	-0.000022151
23	6	0.000000042	-0.000003369	0.000001302
24	6	0.000011252	-0.000002906	-0.000014659
25	8	-0.000019131	-0.000007140	0.000018293
26	1	0.000000349	0.000002300	-0.000009833
27	1	0.000000044	-0.000008050	-0.000007307
28	1	0.000003428	-0.000001309	-0.000002813
29	6	-0.000001638	0.000002198	0.000008876
30	1	0.000000794	0.000004435	-0.000002812
31	1	-0.000000061	0.000003819	-0.000003620
32	1	-0.000000148	0.000005394	-0.000005187

Cartesian Forces: Max 0.000028816 RMS 0.000008224

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000018157 RMS 0.000003496
Search for a local minimum.
Step number 36 out of a maximum of 177
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 24 25 26 27 28
29 30 31 32 33
34 35 36
DE= 2.13D-07 DEPred=-3.64D-08 R=-5.84D+00
Trust test=-5.84D+00 RLast= 9.52D-03 DXMaxT set to 9.71D-01
ITU= -1 0 0 1 1 0 1 1 1 1 1 1 1 1 1 1 1 1 -1

ITU= 1 1 1 1 1 1 1 1 1 1 1 0 1 0 1 0

Eigenvalues ---	0.00004	0.00053	0.00127	0.00208	0.00235
Eigenvalues ---	0.00310	0.00559	0.00705	0.01119	0.01310
Eigenvalues ---	0.01394	0.01577	0.01823	0.01903	0.01994
Eigenvalues ---	0.02150	0.02231	0.02319	0.02395	0.02899
Eigenvalues ---	0.03049	0.03073	0.03302	0.03481	0.03726
Eigenvalues ---	0.04066	0.04632	0.05162	0.05381	0.05460
Eigenvalues ---	0.05670	0.05921	0.06479	0.09129	0.09396
Eigenvalues ---	0.10427	0.11036	0.11498	0.11692	0.13017
Eigenvalues ---	0.13828	0.14140	0.14304	0.15231	0.15976
Eigenvalues ---	0.15999	0.16001	0.16005	0.16016	0.16039
Eigenvalues ---	0.16050	0.17171	0.19247	0.21311	0.22056
Eigenvalues ---	0.22852	0.23399	0.23866	0.24250	0.25034
Eigenvalues ---	0.27777	0.28499	0.30765	0.32063	0.33105
Eigenvalues ---	0.33219	0.34046	0.34197	0.34466	0.34843
Eigenvalues ---	0.35046	0.35686	0.35690	0.35859	0.36205
Eigenvalues ---	0.36437	0.36670	0.37211	0.37238	0.37606
Eigenvalues ---	0.38291	0.42167	0.42561	0.45258	0.45614
Eigenvalues ---	0.49328	0.54101	0.55180	0.56041	0.60394

Eigenvalue 1 is 3.58D-05 Eigenvector:

	D52	D53	D54	D55	D25
1	0.51036	-0.49569	-0.49555	-0.48986	0.03359
	D46	D47	D26	D45	A48
1	-0.03335	-0.03112	0.02630	-0.01704	0.01455

En-DIIS/RFO-DIIS IScMMF= 0 using points: 36 35 34 33 32

RFO step: Lambda=-7.22988457D-09.

DidBck=F Rises=F RFO-DIIS coefs: 1.99929 -1.05181 -0.28624 0.49883 -0.16006

Iteration 1 RMS(Cart)= 0.00159794 RMS(Int)= 0.00000374

Iteration 2 RMS(Cart)= 0.00001205 RMS(Int)= 0.00000073

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000073

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56500	0.00000	0.00000	0.00000	0.00000	2.56500
R2	2.62015	0.00000	0.00000	0.00000	0.00001	2.62015
R3	2.03418	0.00000	0.00000	0.00000	0.00000	2.03418
R4	2.62939	0.00000	-0.00001	0.00001	0.00000	2.62939
R5	2.03076	0.00000	0.00000	0.00000	0.00000	2.03076
R6	2.54617	0.00000	0.00000	-0.00001	-0.00001	2.54616
R7	2.68696	0.00000	0.00001	0.00000	0.00000	2.68696
R8	2.51706	0.00001	0.00004	-0.00002	0.00002	2.51708
R9	2.09969	0.00001	0.00010	0.00000	0.00010	2.09979
R10	2.79221	-0.00001	-0.00001	-0.00002	-0.00003	2.79218
R11	2.90791	-0.00001	0.00005	-0.00002	0.00003	2.90794

R12	2.06206	0.00000	0.00001	-0.00001	0.00000	2.06205
R13	2.06124	0.00000	0.00001	-0.00001	0.00000	2.06124
R14	2.07224	0.00000	0.00000	-0.00001	0.00000	2.07223
R15	2.07144	0.00000	0.00003	-0.00001	0.00002	2.07146
R16	2.65390	0.00001	-0.00008	0.00003	-0.00006	2.65384
R17	4.15608	-0.00001	-0.00062	-0.00009	-0.00070	4.15538
R18	8.46392	0.00000	-0.00045	-0.00044	-0.00089	8.46303
R19	2.50679	0.00000	0.00000	0.00000	0.00000	2.50679
R20	2.04636	0.00000	0.00000	0.00000	0.00000	2.04636
R21	2.04298	0.00000	0.00000	0.00000	0.00000	2.04298
R22	2.04580	0.00000	0.00000	0.00000	0.00000	2.04580
R23	1.84645	0.00000	0.00003	-0.00001	0.00002	1.84646
R24	3.41846	0.00000	-0.00016	0.00003	-0.00013	3.41834
R25	2.77428	0.00000	0.00001	0.00000	0.00001	2.77429
R26	2.74082	0.00000	0.00002	-0.00003	0.00000	2.74082
R27	2.05486	0.00000	0.00001	-0.00001	0.00000	2.05486
R28	2.05334	0.00000	0.00000	0.00000	-0.00001	2.05334
R29	2.73608	0.00000	0.00001	0.00000	0.00000	2.73609
R30	2.05779	0.00000	0.00002	0.00000	0.00001	2.05780
R31	2.84182	0.00000	0.00000	0.00001	0.00002	2.84184
R32	2.06791	0.00000	0.00000	0.00000	-0.00001	2.06791
R33	2.06815	0.00000	0.00000	0.00000	0.00000	2.06815
R34	2.06318	0.00000	0.00001	0.00000	0.00001	2.06319
A1	1.87432	0.00000	0.00000	-0.00001	-0.00001	1.87431
A2	2.27810	0.00000	0.00000	0.00000	0.00000	2.27810
A3	2.13073	0.00000	0.00000	0.00001	0.00001	2.13074
A4	1.86187	0.00000	0.00001	-0.00001	0.00000	1.86187
A5	2.27708	0.00000	-0.00001	0.00001	0.00000	2.27708
A6	2.14422	0.00000	0.00000	0.00000	0.00001	2.14423
A7	1.89721	0.00000	0.00000	0.00002	0.00002	1.89723
A8	2.24843	0.00000	0.00001	0.00000	0.00001	2.24844
A9	2.13753	0.00000	-0.00001	-0.00002	-0.00003	2.13751
A10	1.88932	0.00000	-0.00001	-0.00001	-0.00002	1.88930
A11	2.23462	0.00001	-0.00001	0.00001	0.00000	2.23462
A12	2.15924	-0.00001	0.00002	0.00000	0.00002	2.15927
A13	1.90204	0.00000	-0.00001	0.00002	0.00001	1.90205
A14	2.21199	0.00000	0.00002	0.00001	0.00003	2.21202
A15	2.16801	0.00000	-0.00001	-0.00003	-0.00004	2.16796
A16	1.95082	-0.00001	0.00003	-0.00002	0.00001	1.95083
A17	1.86524	0.00000	-0.00001	0.00003	0.00002	1.86526
A18	1.88387	0.00000	0.00003	-0.00001	0.00002	1.88389
A19	1.92524	0.00000	-0.00004	0.00002	-0.00002	1.92522
A20	1.92095	0.00000	0.00000	0.00000	0.00001	1.92096
A21	1.91645	0.00000	-0.00001	-0.00002	-0.00003	1.91641

A22	1.91300	0.00000	-0.00003	0.00000	-0.00002	1.91298
A23	1.90262	0.00000	-0.00004	0.00001	-0.00003	1.90259
A24	1.91408	0.00000	0.00008	-0.00001	0.00007	1.91416
A25	1.88689	0.00000	-0.00005	0.00003	-0.00002	1.88688
A26	1.88660	0.00000	-0.00003	-0.00001	-0.00005	1.88655
A27	1.96010	0.00000	0.00006	-0.00003	0.00003	1.96013
A28	1.78802	-0.00001	-0.00033	-0.00012	-0.00045	1.78758
A29	2.83412	0.00002	0.00060	0.00024	0.00084	2.83496
A30	2.17703	0.00000	0.00000	-0.00001	-0.00001	2.17702
A31	1.95557	0.00000	-0.00001	0.00000	-0.00001	1.95556
A32	2.15059	0.00000	0.00001	0.00001	0.00002	2.15061
A33	2.07971	0.00000	0.00000	-0.00001	0.00000	2.07971
A34	2.15742	0.00000	-0.00001	0.00001	0.00000	2.15742
A35	2.04605	0.00000	0.00000	0.00000	0.00000	2.04606
A36	1.91275	0.00000	0.00007	-0.00004	0.00004	1.91279
A37	3.05142	0.00001	0.00070	0.00010	0.00079	3.05221
A38	2.07421	0.00001	-0.00001	0.00003	0.00002	2.07423
A39	2.08788	0.00000	0.00003	-0.00003	0.00000	2.08787
A40	2.00176	0.00000	-0.00004	-0.00002	-0.00007	2.00170
A41	1.98460	0.00000	-0.00001	0.00002	0.00001	1.98461
A42	2.04015	0.00000	0.00001	0.00000	0.00001	2.04017
A43	2.04570	0.00000	0.00001	-0.00003	-0.00002	2.04568
A44	2.13300	0.00000	0.00003	-0.00001	0.00001	2.13301
A45	1.94918	0.00000	-0.00008	0.00009	0.00002	1.94920
A46	2.04647	0.00000	0.00004	-0.00003	0.00001	2.04648
A47	2.02219	0.00000	-0.00002	0.00001	-0.00001	2.02218
A48	1.43031	0.00001	0.00067	0.00013	0.00081	1.43112
A49	0.99987	0.00000	0.00010	0.00011	0.00020	1.00007
A50	2.37372	0.00000	0.00071	0.00032	0.00103	2.37475
A51	2.35119	0.00000	0.00027	-0.00006	0.00021	2.35140
A52	1.93143	-0.00001	-0.00001	-0.00002	-0.00003	1.93140
A53	1.91233	0.00000	-0.00002	0.00002	0.00000	1.91233
A54	1.93763	0.00000	-0.00003	0.00001	-0.00002	1.93760
A55	1.88374	0.00000	0.00001	-0.00001	0.00001	1.88375
A56	1.91355	0.00000	0.00004	0.00000	0.00004	1.91359
A57	1.88374	0.00000	0.00001	0.00000	0.00001	1.88375
A58	3.78150	0.00001	0.00095	0.00007	0.00102	3.78252
A59	5.04358	-0.00001	-0.00071	-0.00047	-0.00118	5.04240
D1	0.00436	0.00000	-0.00008	0.00002	-0.00006	0.00430
D2	-3.13135	0.00000	-0.00017	0.00005	-0.00012	-3.13147
D3	3.13662	0.00000	0.00012	-0.00006	0.00006	3.13668
D4	0.00090	0.00000	0.00003	-0.00003	0.00001	0.00091
D5	-0.00676	0.00000	0.00008	-0.00003	0.00004	-0.00672
D6	-3.09817	0.00001	0.00006	0.00009	0.00015	-3.09802

D7	-3.13998	0.00000	-0.00010	0.00003	-0.00007	-3.14005
D8	0.05179	0.00001	-0.00011	0.00015	0.00004	0.05183
D9	-0.00055	0.00000	0.00006	0.00001	0.00007	-0.00048
D10	-3.13670	0.00000	0.00000	0.00003	0.00003	-3.13667
D11	3.13572	0.00000	0.00014	-0.00002	0.00011	3.13584
D12	-0.00043	0.00000	0.00008	0.00000	0.00008	-0.00035
D13	-0.00366	0.00000	-0.00001	-0.00003	-0.00004	-0.00370
D14	3.13753	0.00000	0.00021	-0.00010	0.00011	3.13764
D15	3.13291	0.00000	0.00004	-0.00005	-0.00001	3.13290
D16	-0.00908	0.00000	0.00026	-0.00012	0.00014	-0.00895
D17	0.00133	0.00000	0.00062	0.00010	0.00072	0.00205
D18	-3.14044	0.00000	0.00057	0.00012	0.00069	-3.13975
D19	-3.13415	0.00000	0.00055	0.00013	0.00068	-3.13347
D20	0.00726	0.00000	0.00051	0.00014	0.00065	0.00791
D21	0.00642	0.00000	-0.00004	0.00004	0.00000	0.00642
D22	3.09938	0.00000	-0.00003	-0.00008	-0.00010	3.09928
D23	-3.13479	0.00000	-0.00025	0.00011	-0.00014	-3.13493
D24	-0.04183	0.00000	-0.00024	-0.00001	-0.00025	-0.04208
D25	-3.10799	0.00000	0.00066	-0.00041	0.00025	-3.10774
D26	0.03315	0.00000	0.00092	-0.00050	0.00042	0.03357
D27	1.40885	0.00000	-0.00017	0.00027	0.00010	1.40895
D28	-2.76641	0.00000	-0.00021	0.00030	0.00009	-2.76632
D29	-0.70597	0.00000	-0.00022	0.00029	0.00007	-0.70590
D30	-1.67535	0.00001	-0.00019	0.00041	0.00022	-1.67512
D31	0.43258	0.00000	-0.00022	0.00044	0.00022	0.43280
D32	2.49302	0.00000	-0.00023	0.00042	0.00020	2.49321
D33	-0.93893	0.00000	-0.00016	0.00001	-0.00015	-0.93908
D34	1.12317	0.00000	-0.00025	0.00006	-0.00020	1.12298
D35	-3.00748	0.00000	-0.00015	0.00003	-0.00012	-3.00760
D36	-3.01157	0.00000	-0.00014	-0.00002	-0.00016	-3.01173
D37	-0.94947	0.00000	-0.00024	0.00002	-0.00021	-0.94968
D38	1.20307	0.00000	-0.00013	-0.00001	-0.00014	1.20293
D39	1.15426	0.00000	-0.00010	-0.00002	-0.00011	1.15414
D40	-3.06683	0.00000	-0.00019	0.00003	-0.00016	-3.06699
D41	-0.91429	0.00000	-0.00009	0.00000	-0.00009	-0.91438
D42	-1.63865	0.00000	0.00113	-0.00002	0.00111	-1.63755
D43	2.55971	0.00000	0.00113	-0.00001	0.00112	2.56083
D44	0.47966	-0.00001	0.00118	-0.00003	0.00115	0.48081
D45	0.43251	0.00000	-0.00175	0.00038	-0.00138	0.43114
D46	-0.27139	0.00001	0.00194	0.00033	0.00228	-0.26912
D47	2.56681	0.00001	0.00194	0.00061	0.00255	2.56936
D48	-3.14153	0.00000	0.00001	0.00004	0.00005	-3.14147
D49	0.00055	0.00000	0.00004	0.00001	0.00005	0.00061
D50	0.00027	0.00000	0.00006	0.00002	0.00008	0.00035

D51	-3.14084	0.00000	0.00009	-0.00001	0.00008	-3.14076
D52	-1.92856	0.00000	-0.00635	-0.00029	-0.00664	-1.93520
D53	2.43685	0.00000	0.00532	-0.00001	0.00531	2.44216
D54	2.06655	0.00000	0.00500	0.00019	0.00519	2.07173
D55	-2.60673	0.00000	0.00603	0.00047	0.00650	-2.60024
D56	-2.72927	0.00000	-0.00015	0.00008	-0.00007	-2.72934
D57	-0.03026	0.00000	-0.00010	0.00000	-0.00010	-0.03036
D58	-0.02181	0.00000	-0.00007	0.00009	0.00001	-0.02179
D59	2.67720	0.00000	-0.00002	0.00000	-0.00002	2.67718
D60	-0.17089	0.00000	0.00003	0.00015	0.00017	-0.17072
D61	0.26904	0.00000	0.00043	-0.00011	0.00032	0.26936
D62	-2.58319	0.00000	0.00007	0.00015	0.00022	-2.58297
D63	-2.14326	0.00000	0.00047	-0.00010	0.00037	-2.14289
D64	2.14495	0.00000	-0.00107	-0.00037	-0.00144	2.14351
D65	-0.24832	0.00000	-0.00100	-0.00046	-0.00146	-0.24978
D66	2.48885	0.00000	-0.00014	-0.00002	-0.00016	2.48870
D67	-1.71917	0.00000	-0.00014	-0.00003	-0.00017	-1.71934
D68	0.35982	0.00000	-0.00016	-0.00001	-0.00018	0.35964
D69	1.27267	0.00000	-0.00018	0.00001	-0.00016	1.27251
D70	-2.93535	0.00000	-0.00018	0.00000	-0.00017	-2.93553
D71	-0.85637	0.00000	-0.00020	0.00002	-0.00018	-0.85655
D72	-1.08980	0.00000	-0.00008	-0.00011	-0.00019	-1.08999
D73	0.98536	0.00000	-0.00009	-0.00012	-0.00021	0.98516
D74	3.06435	0.00000	-0.00011	-0.00010	-0.00021	3.06414

Item	Value	Threshold	Converged?
Maximum Force	0.000018	0.000450	YES
RMS Force	0.000003	0.000300	YES
Maximum Displacement	0.006720	0.001800	NO
RMS Displacement	0.001610	0.001200	NO

Predicted change in Energy=-4.057922D-08

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.376322	-1.908773	-0.258238
2	6	0	-2.507926	-1.168912	-0.138059
3	7	0	-2.110009	0.112318	0.230908
4	6	0	-0.766458	0.135865	0.329498
5	7	0	-0.305742	-1.080321	0.041728
6	6	0	1.127589	-1.435840	-0.006635
7	6	0	1.683395	-1.372410	-1.440163

8	1	0	-1.242076	-2.943962	-0.521087
9	1	0	-3.537953	-1.442332	-0.276345
10	1	0	1.651891	-0.725458	0.634589
11	1	0	1.237113	-2.444884	0.392852
12	1	0	1.064651	-1.989775	-2.102355
13	1	0	1.635184	-0.336838	-1.796329
14	35	0	1.651750	2.233513	1.022977
15	1	0	-0.114754	0.994355	0.599593
16	6	0	-2.914368	1.256518	0.486944
17	6	0	-4.238554	1.281623	0.412108
18	1	0	-2.318783	2.120414	0.754542
19	1	0	-4.760841	2.203693	0.626076
20	1	0	-4.840153	0.421811	0.146011
21	8	0	2.991157	-1.883717	-1.463246
22	1	0	3.630912	-1.151965	-1.363304
23	6	0	4.838602	1.611607	-1.121551
24	6	0	5.711752	0.751372	-0.313527
25	8	0	4.858021	0.176706	-1.331979
26	1	0	3.922077	1.993242	-0.677993
27	1	0	5.259014	2.179934	-1.946725
28	1	0	6.762498	0.703442	-0.595361
29	6	0	5.400412	0.411942	1.118040
30	1	0	5.679540	-0.622820	1.339002
31	1	0	5.974328	1.065021	1.782766
32	1	0	4.340520	0.560245	1.334021

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357338	0.000000			
3	N	2.205079	1.391411	0.000000		
4	C	2.213123	2.225706	1.347370	0.000000	
5	N	1.386526	2.211286	2.171073	1.331983	0.000000
6	C	2.560575	3.647670	3.596563	2.484080	1.477556
7	C	3.323628	4.393639	4.403046	3.377628	2.497596
8	H	1.076442	2.213570	3.264912	3.230331	2.160240
9	H	2.211457	1.074633	2.171005	3.246373	3.267937
10	H	3.371565	4.254141	3.875142	2.585221	2.075991
11	H	2.746157	3.991903	4.215298	3.267809	2.089431
12	H	3.060339	4.158796	4.465577	3.712844	2.702254
13	H	3.729058	4.539557	4.282278	3.241986	2.774602
14	Br	5.288598	5.497946	4.390635	3.275480	3.971917
15	H	3.279571	3.309249	2.212456	1.111159	2.156843
16	C	3.597214	2.537427	1.421879	2.427791	3.530434

17	C	4.338244	3.050062	2.435325	3.657190	4.602496
18	H	4.260083	3.413529	2.085720	2.555154	3.847746
19	H	5.399015	4.127226	3.399546	4.507657	5.565440
20	H	4.194421	2.837319	2.748941	4.087838	4.777882
21	O	4.530733	5.701490	5.733778	4.627344	3.712134
22	H	5.183274	6.259940	6.090822	4.884767	4.180490
23	C	7.194697	7.916440	7.236035	5.974952	5.921484
24	C	7.571013	8.442831	7.866686	6.539078	6.300123
25	O	6.661019	7.582434	7.141443	5.864890	5.489229
26	H	6.593554	7.185798	6.383576	5.142689	5.276291
27	H	7.974723	8.649359	7.957363	6.757642	6.749054
28	H	8.554397	9.468664	8.930483	7.606752	7.317630
29	C	7.294106	8.162028	7.568567	6.223206	5.995456
30	H	7.347792	8.337537	7.902239	6.568530	6.141321
31	H	8.187869	8.979346	8.286882	6.957982	6.860976
32	H	6.427568	7.215139	6.559484	5.222106	5.094039

		6	7	8	9	10
6	C	0.000000				
7	C	1.538813	0.000000			
8	H	2.855592	3.445701	0.000000		
9	H	4.673336	5.349938	2.754241	0.000000	
10	H	1.091192	2.173507	3.825230	5.317724	0.000000
11	H	1.090760	2.170095	2.689004	4.924855	1.785190
12	H	2.168605	1.096578	2.954973	4.981763	3.071516
13	H	2.160663	1.096170	4.086803	5.503982	2.461842
14	Br	3.846946	4.367006	6.128998	6.491001	2.984352
15	H	2.795850	3.604930	4.247013	4.292203	2.465769
16	C	4.881580	5.635993	4.632140	2.873197	4.980035
17	C	6.029548	6.748650	5.263583	2.895641	6.226975
18	H	5.010371	5.747520	5.332395	3.904134	4.886679
19	H	6.951269	7.654152	6.340035	3.950103	7.050045
20	H	6.252049	6.949234	4.971882	2.312820	6.610716
21	O	2.407321	1.404353	4.464531	6.650777	2.745197
22	H	2.861427	1.961460	5.259904	7.256612	2.844294
23	C	4.929663	4.354446	7.621575	8.955869	4.324468
24	C	5.088480	4.691207	7.877455	9.506354	4.422943
25	O	4.274688	3.534079	6.899804	8.615569	3.867888
26	H	4.474202	4.113419	7.146263	8.222928	3.777294
27	H	5.822924	5.065650	8.399460	9.659069	5.302436
28	H	6.056015	5.551588	8.796719	10.526414	5.447278
29	C	4.789175	4.852270	7.620464	9.234555	3.947000
30	H	4.815806	4.924918	7.533684	9.393781	4.090072
31	H	5.739959	5.894102	8.570657	10.050385	4.817425
32	H	4.013058	4.300182	6.847355	8.286974	3.061203

		11	12	13	14	15
11	H	0.000000				
12	H	2.542229	0.000000			
13	H	3.065100	1.775208	0.000000		
14	Br	4.738817	5.286639	3.815163	0.000000	
15	H	3.701170	4.194825	3.251892	2.198932	0.000000
16	C	5.562735	5.751128	5.333905	4.700136	2.814117
17	C	6.623455	6.719267	6.480541	5.997911	4.138043
18	H	5.798032	6.041783	5.308379	3.981204	2.479872
19	H	7.592043	7.678923	7.295991	6.424932	4.800971
20	H	6.723989	6.762958	6.802810	6.796774	4.781520
21	O	2.614705	2.032519	2.083852	4.992685	4.710126
22	H	3.238210	2.798896	2.198835	4.590521	4.742328
23	C	5.631985	5.307979	3.809678	3.891245	5.280063
24	C	5.544134	5.684131	4.472283	4.524003	5.902627
25	O	4.791529	4.435851	3.296365	4.478442	5.397037
26	H	5.296481	5.104716	3.451062	2.847001	4.350403
27	H	6.560355	5.916366	4.414624	4.672724	6.063557
28	H	6.435713	6.479962	5.367853	5.574933	6.986354
29	C	5.101020	5.910838	4.819871	4.168887	5.570013
30	H	4.893902	5.916816	5.125319	4.947889	6.061009
31	H	6.057433	6.966410	5.796835	4.541732	6.203371
32	H	4.421282	5.389119	4.233520	3.182147	4.536221

		16	17	18	19	20
16	C	0.000000				
17	C	1.326537	0.000000			
18	H	1.082888	2.122817	0.000000		
19	H	2.079895	1.081101	2.446852	0.000000	
20	H	2.126410	1.082592	3.100462	1.847121	0.000000
21	O	6.967032	8.112031	7.010500	9.009199	8.320732
22	H	7.215601	8.426324	7.112849	9.254167	8.747214
23	C	7.926025	9.211718	7.416655	9.775176	9.833647
24	C	8.677895	9.990811	8.216115	10.614486	10.567047
25	O	8.055091	9.327934	7.722570	10.023231	9.813210
26	H	6.974010	8.263814	6.404426	8.782822	8.940081
27	H	8.577856	9.827251	8.045085	10.344920	10.462491
28	H	9.752897	11.062207	9.289764	11.684605	11.629722
29	C	8.381357	9.703832	7.914353	10.329737	10.286598
30	H	8.838165	10.141727	8.475854	10.839695	10.638534
31	H	8.984694	10.306725	8.422992	10.857180	10.956536
32	H	7.337284	8.658570	6.864128	9.275607	9.258255

		21	22	23	24	25
21	O	0.000000				
22	H	0.977106	0.000000			

23	C	3.968261	3.025606	0.000000		
24	C	3.958180	3.009090	1.468093	0.000000	
25	O	2.783479	1.808907	1.450378	1.447876	0.000000
26	H	4.063748	3.232145	1.087385	2.208623	2.145575
27	H	4.678695	3.754018	1.086579	2.216551	2.133455
28	H	4.655065	3.720094	2.191578	1.088942	2.108812
29	C	4.211603	3.425493	2.602036	1.503838	2.520340
30	H	4.082874	3.432103	3.428434	2.149487	2.906592
31	H	5.303863	4.506038	3.166020	2.135828	3.425913
32	H	3.952017	3.272732	2.717219	2.152027	2.742711

		26	27	28	29	30
26	H	0.000000				
27	H	1.852548	0.000000			
28	H	3.120641	2.503333	0.000000		
29	C	2.812777	3.540984	2.208165	0.000000	
30	H	3.741755	4.339156	2.583318	1.094290	0.000000
31	H	3.335965	3.957752	2.531292	1.094419	1.769925
32	H	2.505349	3.772309	3.099838	1.091793	1.786797

		31	32
31	H	0.000000	
32	H	1.767908	0.000000

Stoichiometry C10H17BrN2O2
Framework group C1[X(C10H17BrN2O2)]
Deg. of freedom 90
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.710548	2.114242	-0.438495
2	6	0	-3.788608	1.349742	-0.129150
3	7	0	-3.321483	0.049822	0.038265
4	6	0	-1.990033	0.039250	-0.167975
5	7	0	-1.603739	1.279469	-0.462616
6	6	0	-0.201464	1.677677	-0.703916
7	6	0	0.455321	2.251221	0.564007
8	1	0	-2.637053	3.167395	-0.648717
9	1	0	-4.824317	1.615440	-0.021693
10	1	0	0.329425	0.783282	-1.033941
11	1	0	-0.196378	2.424774	-1.498633
12	1	0	-0.161036	3.066705	0.960961

13	1	0	0.510235	1.464125	1.324962
14	35	0	0.526011	-2.057797	-0.141762
15	1	0	-1.295563	-0.826400	-0.112880
16	6	0	-4.052858	-1.125267	0.363835
17	6	0	-5.363011	-1.168031	0.567235
18	1	0	-3.413631	-1.996944	0.428765
19	1	0	-5.827674	-2.113308	0.810790
20	1	0	-6.008016	-0.300922	0.503234
21	8	0	1.719168	2.774661	0.246344
22	1	0	2.403940	2.095466	0.402920
23	6	0	3.797379	-0.459287	1.231085
24	6	0	4.545076	0.009538	0.057862
25	8	0	3.722824	0.928586	0.816542
26	1	0	2.883844	-1.028803	1.077750
27	1	0	4.315573	-0.606170	2.174777
28	1	0	5.606159	0.213794	0.192677
29	6	0	4.110752	-0.303990	-1.347339
30	1	0	4.294950	0.548868	-2.007774
31	1	0	4.685040	-1.154605	-1.727340
32	1	0	3.052707	-0.571396	-1.379696

Rotational constants (GHZ): 0.6001623 0.2211833 0.1722952

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.

475 basis functions, 751 primitive gaussians, 492 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1307.2303066825 Hartrees.

NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 475 RedAO= T EigKep= 3.78D-06 NBF= 475

NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000087 -0.000034 0.000035 Ang= -0.01 deg.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3225.52371228 A.U. after 8 cycles

NFock= 8 Conv=0.82D-08 -V/T= 2.0018

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000003721	0.000003546	-0.000004026
2	6	-0.000001075	0.000000779	0.000000163
3	7	0.000002024	0.000004377	-0.000005233
4	6	-0.000014264	0.000003410	0.000024032
5	7	0.000004824	-0.000007526	0.000010968
6	6	0.000001175	0.000000632	-0.000007262
7	6	-0.000028214	0.000008115	0.000000601
8	1	-0.000000984	-0.000002388	0.000015090
9	1	-0.000000488	0.000001112	0.000007047
10	1	0.000000457	0.000000159	0.000002075
11	1	0.000000067	0.000001441	0.000007532
12	1	-0.000000508	-0.000005382	0.000006731
13	1	0.000002915	-0.000006404	0.000007447
14	35	-0.000003850	0.000007750	0.000001205
15	1	0.000016123	-0.000000121	-0.000029528
16	6	0.000000002	0.000002097	-0.000002311
17	6	0.000000849	0.000001597	-0.000003290
18	1	0.000000122	0.000003680	-0.000005640
19	1	0.000000453	0.000003645	-0.000005287
20	1	-0.000000601	0.000002430	-0.000000326
21	8	0.000030666	-0.000006420	0.000015437
22	1	-0.000010984	-0.000012068	-0.000013291
23	6	-0.000010746	-0.000010191	0.000003375
24	6	0.000011802	0.000000259	-0.000019273
25	8	-0.000004470	-0.000003314	0.000020358
26	1	0.000002755	0.000004417	-0.000008114
27	1	0.000000840	-0.000007348	-0.000009216
28	1	-0.000000100	-0.000003455	-0.000001533
29	6	-0.000002915	0.000005593	-0.000000006
30	1	-0.000000257	0.000002997	0.000000237
31	1	-0.000000104	0.000003201	-0.000003234
32	1	0.000000764	0.000003381	-0.000004727

Cartesian Forces: Max 0.000030666 RMS 0.000008575

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000019220 RMS 0.000003384
Search for a local minimum.
Step number 37 out of a maximum of 177
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 24 25 26 27 28
29 30 31 32 33
34 35 36 37
DE= 3.26D-07 DEPred=-4.06D-08 R=-8.03D+00
Trust test=-8.03D+00 RLast= 1.32D-02 DXMaxT set to 4.86D-01
ITU= -1 -1 0 0 1 1 0 1 1 1 1 1 1 1 1 1 1 1 1
ITU= -1 1 1 1 1 1 1 1 1 1 1 1 0 1 0 1 0
Eigenvalues --- 0.00003 0.00055 0.00117 0.00190 0.00235
Eigenvalues --- 0.00313 0.00430 0.00696 0.01121 0.01241
Eigenvalues --- 0.01316 0.01560 0.01824 0.01961 0.02014
Eigenvalues --- 0.02121 0.02237 0.02322 0.02397 0.02623
Eigenvalues --- 0.03043 0.03067 0.03226 0.03477 0.03710
Eigenvalues --- 0.04092 0.04625 0.05168 0.05391 0.05450
Eigenvalues --- 0.05670 0.05889 0.06487 0.09328 0.09434
Eigenvalues --- 0.10318 0.11088 0.11496 0.11632 0.12997
Eigenvalues --- 0.13825 0.14132 0.14397 0.15162 0.15973
Eigenvalues --- 0.15998 0.16001 0.16004 0.16018 0.16035
Eigenvalues --- 0.16060 0.17013 0.19060 0.21303 0.22051
Eigenvalues --- 0.22847 0.23398 0.23861 0.24273 0.25033
Eigenvalues --- 0.27749 0.28410 0.30896 0.31944 0.33107
Eigenvalues --- 0.33228 0.34052 0.34195 0.34472 0.34837
Eigenvalues --- 0.35029 0.35685 0.35690 0.35857 0.36251
Eigenvalues --- 0.36435 0.36674 0.37203 0.37245 0.37610
Eigenvalues --- 0.38533 0.42178 0.42516 0.45346 0.45852
Eigenvalues --- 0.49380 0.54399 0.55453 0.55767 0.60391
Eigenvalue 1 is 3.49D-05 Eigenvector:

	D52	D54	D53	D55	D25
1	0.50791	-0.49863	-0.49468	-0.48826	0.04247
	D26	D47	D45	D46	D28
1	0.03632	-0.03010	-0.03000	-0.02985	-0.01778

En-DIIS/RFO-DIIS IScMMF= 0 using points: 37 36 35 34 33
RFO step: Lambda=-5.29641283D-09.
DidBck=F Rises=F RFO-DIIS coefs: 2.12806 -1.34009 -0.24000 0.64223 -0.19019

Iteration 1 RMS(Cart)= 0.00126201 RMS(Int)= 0.00000244
Iteration 2 RMS(Cart)= 0.00000731 RMS(Int)= 0.00000051
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000051

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56500	0.00000	0.00000	0.00001	0.00001	2.56500
R2	2.62015	0.00000	0.00000	0.00000	0.00000	2.62015
R3	2.03418	0.00000	0.00000	0.00000	0.00000	2.03418
R4	2.62939	0.00000	0.00000	0.00000	0.00000	2.62939
R5	2.03076	0.00000	0.00000	0.00000	0.00000	2.03076
R6	2.54616	0.00000	-0.00001	0.00000	-0.00001	2.54615
R7	2.68696	0.00000	0.00000	0.00001	0.00001	2.68697
R8	2.51708	0.00000	0.00002	0.00001	0.00003	2.51711
R9	2.09979	0.00000	0.00008	0.00000	0.00008	2.09986
R10	2.79218	0.00000	-0.00004	0.00001	-0.00002	2.79215
R11	2.90794	-0.00001	0.00000	0.00000	0.00000	2.90794
R12	2.06205	0.00000	0.00000	0.00000	-0.00001	2.06205
R13	2.06124	0.00000	0.00000	0.00000	0.00000	2.06124
R14	2.07223	0.00000	-0.00001	0.00000	-0.00001	2.07222
R15	2.07146	0.00000	0.00000	0.00000	0.00000	2.07146
R16	2.65384	0.00002	0.00001	0.00002	0.00003	2.65387
R17	4.15538	0.00000	-0.00051	-0.00003	-0.00054	4.15484
R18	8.46303	0.00000	-0.00062	0.00013	-0.00049	8.46254
R19	2.50679	0.00000	0.00000	0.00000	0.00000	2.50679
R20	2.04636	0.00000	0.00000	0.00000	0.00000	2.04637
R21	2.04298	0.00000	0.00000	0.00000	0.00000	2.04299
R22	2.04580	0.00000	0.00000	0.00000	0.00000	2.04580
R23	1.84646	-0.00001	0.00000	-0.00001	-0.00001	1.84646
R24	3.41834	0.00000	-0.00014	0.00003	-0.00011	3.41822
R25	2.77429	0.00000	0.00001	0.00000	0.00001	2.77431
R26	2.74082	0.00000	0.00000	0.00000	0.00000	2.74082
R27	2.05486	0.00000	0.00000	0.00000	0.00000	2.05486
R28	2.05334	0.00000	0.00000	0.00000	0.00000	2.05334
R29	2.73609	-0.00001	0.00000	-0.00003	-0.00002	2.73606
R30	2.05780	0.00000	0.00001	0.00000	0.00000	2.05780
R31	2.84184	0.00000	0.00003	-0.00001	0.00001	2.84186
R32	2.06791	0.00000	0.00000	0.00000	0.00000	2.06791
R33	2.06815	0.00000	0.00000	0.00000	0.00000	2.06815
R34	2.06319	0.00000	0.00000	0.00000	0.00000	2.06319
A1	1.87431	0.00000	0.00000	0.00000	0.00000	1.87431
A2	2.27810	0.00000	-0.00001	0.00001	0.00000	2.27810
A3	2.13074	0.00000	0.00001	-0.00001	0.00000	2.13074
A4	1.86187	0.00000	-0.00001	0.00001	0.00000	1.86187
A5	2.27708	0.00000	0.00001	0.00000	0.00000	2.27708

A6	2.14423	0.00000	0.00000	-0.00001	-0.00001	2.14422
A7	1.89723	0.00000	0.00003	-0.00002	0.00000	1.89723
A8	2.24844	0.00000	0.00000	0.00001	0.00001	2.24845
A9	2.13751	0.00000	-0.00002	0.00001	-0.00001	2.13749
A10	1.88930	0.00000	-0.00003	0.00002	-0.00001	1.88929
A11	2.23462	0.00000	0.00001	-0.00003	-0.00002	2.23460
A12	2.15927	0.00000	0.00002	0.00001	0.00002	2.15929
A13	1.90205	0.00000	0.00001	-0.00001	0.00000	1.90205
A14	2.21202	0.00000	0.00000	0.00000	0.00001	2.21202
A15	2.16796	0.00000	-0.00003	0.00001	-0.00002	2.16794
A16	1.95083	-0.00001	-0.00001	0.00002	0.00001	1.95084
A17	1.86526	0.00000	0.00004	-0.00001	0.00003	1.86529
A18	1.88389	0.00000	0.00001	0.00000	0.00001	1.88390
A19	1.92522	0.00000	-0.00003	0.00001	-0.00002	1.92520
A20	1.92096	0.00000	0.00003	-0.00002	0.00001	1.92097
A21	1.91641	0.00000	-0.00004	0.00000	-0.00004	1.91637
A22	1.91298	0.00000	0.00000	-0.00001	-0.00001	1.91297
A23	1.90259	0.00000	-0.00003	0.00000	-0.00003	1.90257
A24	1.91416	0.00000	0.00002	0.00000	0.00003	1.91418
A25	1.88688	0.00000	0.00003	0.00001	0.00003	1.88691
A26	1.88655	0.00000	-0.00002	0.00000	-0.00002	1.88654
A27	1.96013	0.00000	0.00000	-0.00001	0.00000	1.96013
A28	1.78758	-0.00001	-0.00034	-0.00018	-0.00051	1.78706
A29	2.83496	0.00002	0.00058	0.00017	0.00076	2.83572
A30	2.17702	0.00000	0.00000	0.00000	0.00000	2.17702
A31	1.95556	0.00000	0.00000	0.00000	-0.00001	1.95555
A32	2.15061	0.00000	0.00000	0.00000	0.00001	2.15061
A33	2.07971	0.00000	-0.00001	0.00000	-0.00001	2.07970
A34	2.15742	0.00000	0.00001	0.00000	0.00001	2.15743
A35	2.04606	0.00000	0.00000	0.00000	0.00000	2.04605
A36	1.91279	0.00000	0.00000	-0.00002	-0.00001	1.91278
A37	3.05221	0.00000	0.00057	0.00008	0.00065	3.05286
A38	2.07423	0.00001	0.00008	-0.00003	0.00005	2.07428
A39	2.08787	0.00000	-0.00003	0.00000	-0.00003	2.08784
A40	2.00170	0.00000	-0.00001	0.00004	0.00003	2.00172
A41	1.98461	0.00000	-0.00003	-0.00001	-0.00004	1.98456
A42	2.04017	0.00000	-0.00001	0.00001	0.00000	2.04016
A43	2.04568	0.00000	0.00000	0.00004	0.00004	2.04572
A44	2.13301	0.00000	-0.00001	-0.00002	-0.00003	2.13298
A45	1.94920	0.00000	0.00004	-0.00004	0.00000	1.94921
A46	2.04648	0.00000	-0.00005	0.00000	-0.00005	2.04643
A47	2.02218	0.00000	0.00001	0.00000	0.00001	2.02219
A48	1.43112	0.00000	0.00043	0.00013	0.00057	1.43169
A49	1.00007	0.00000	0.00002	0.00004	0.00006	1.00013

A50	2.37475	0.00000	0.00047	0.00011	0.00058	2.37533
A51	2.35140	0.00000	0.00019	0.00012	0.00032	2.35172
A52	1.93140	0.00000	-0.00003	0.00001	-0.00003	1.93137
A53	1.91233	0.00000	0.00002	0.00001	0.00003	1.91236
A54	1.93760	0.00000	-0.00004	-0.00002	-0.00005	1.93755
A55	1.88375	0.00000	0.00001	0.00000	0.00001	1.88375
A56	1.91359	0.00000	0.00003	0.00000	0.00003	1.91362
A57	1.88375	0.00000	0.00001	0.00001	0.00002	1.88377
A58	3.78252	0.00001	0.00063	0.00026	0.00089	3.78341
A59	5.04240	0.00000	-0.00066	-0.00003	-0.00069	5.04171
D1	0.00430	0.00000	-0.00003	0.00002	-0.00001	0.00429
D2	-3.13147	0.00000	0.00004	0.00001	0.00005	-3.13142
D3	3.13668	0.00000	-0.00011	0.00000	-0.00011	3.13657
D4	0.00091	0.00000	-0.00004	-0.00001	-0.00005	0.00086
D5	-0.00672	0.00000	-0.00002	0.00001	0.00000	-0.00673
D6	-3.09802	0.00000	0.00029	0.00000	0.00030	-3.09773
D7	-3.14005	0.00000	0.00006	0.00003	0.00009	-3.13997
D8	0.05183	0.00000	0.00037	0.00002	0.00038	0.05222
D9	-0.00048	0.00000	0.00006	-0.00005	0.00002	-0.00046
D10	-3.13667	0.00000	0.00005	0.00003	0.00008	-3.13659
D11	3.13584	0.00000	0.00000	-0.00004	-0.00003	3.13580
D12	-0.00035	0.00000	-0.00001	0.00004	0.00003	-0.00032
D13	-0.00370	0.00000	-0.00008	0.00006	-0.00002	-0.00372
D14	3.13764	0.00000	-0.00010	0.00003	-0.00006	3.13757
D15	3.13290	0.00000	-0.00006	-0.00002	-0.00008	3.13282
D16	-0.00895	0.00000	-0.00008	-0.00004	-0.00012	-0.00907
D17	0.00205	0.00000	0.00049	-0.00001	0.00049	0.00254
D18	-3.13975	0.00000	0.00048	-0.00005	0.00043	-3.13932
D19	-3.13347	0.00000	0.00048	0.00008	0.00056	-3.13291
D20	0.00791	0.00000	0.00046	0.00004	0.00051	0.00842
D21	0.00642	0.00000	0.00006	-0.00004	0.00001	0.00644
D22	3.09928	0.00000	-0.00024	-0.00003	-0.00027	3.09900
D23	-3.13493	0.00000	0.00008	-0.00002	0.00006	-3.13488
D24	-0.04208	0.00000	-0.00022	-0.00001	-0.00023	-0.04231
D25	-3.10774	0.00000	-0.00097	-0.00065	-0.00162	-3.10936
D26	0.03357	0.00000	-0.00100	-0.00068	-0.00167	0.03189
D27	1.40895	0.00000	0.00033	0.00029	0.00063	1.40957
D28	-2.76632	0.00000	0.00031	0.00031	0.00062	-2.76569
D29	-0.70590	0.00000	0.00029	0.00030	0.00060	-0.70530
D30	-1.67512	0.00001	0.00068	0.00028	0.00097	-1.67416
D31	0.43280	0.00000	0.00066	0.00030	0.00096	0.43376
D32	2.49321	0.00000	0.00064	0.00029	0.00094	2.49415
D33	-0.93908	0.00000	-0.00007	0.00004	-0.00003	-0.93910
D34	1.12298	0.00000	-0.00006	0.00005	-0.00001	1.12296

D35	-3.00760	0.00000	-0.00006	0.00004	-0.00002	-3.00762
D36	-3.01173	0.00000	-0.00009	0.00003	-0.00005	-3.01178
D37	-0.94968	0.00000	-0.00008	0.00004	-0.00004	-0.94971
D38	1.20293	0.00000	-0.00008	0.00004	-0.00004	1.20289
D39	1.15414	0.00000	-0.00004	0.00004	0.00000	1.15415
D40	-3.06699	0.00000	-0.00003	0.00005	0.00002	-3.06697
D41	-0.91438	0.00000	-0.00003	0.00004	0.00001	-0.91437
D42	-1.63755	0.00000	0.00058	-0.00005	0.00052	-1.63703
D43	2.56083	0.00000	0.00058	-0.00005	0.00053	2.56136
D44	0.48081	-0.00001	0.00055	-0.00005	0.00050	0.48131
D45	0.43114	0.00000	0.00045	0.00065	0.00110	0.43224
D46	-0.26912	0.00000	0.00155	0.00006	0.00162	-0.26750
D47	2.56936	0.00000	0.00168	-0.00008	0.00160	2.57096
D48	-3.14147	0.00000	0.00005	-0.00005	0.00000	-3.14148
D49	0.00061	0.00000	0.00003	-0.00001	0.00002	0.00063
D50	0.00035	0.00000	0.00007	-0.00001	0.00006	0.00040
D51	-3.14076	0.00000	0.00005	0.00004	0.00008	-3.14067
D52	-1.93520	0.00000	-0.00643	0.00110	-0.00534	-1.94053
D53	2.44216	0.00000	0.00540	-0.00122	0.00418	2.44634
D54	2.07173	0.00000	0.00537	-0.00145	0.00391	2.07565
D55	-2.60024	0.00000	0.00607	-0.00119	0.00487	-2.59536
D56	-2.72934	0.00000	0.00000	-0.00001	-0.00001	-2.72935
D57	-0.03036	0.00000	0.00001	0.00005	0.00005	-0.03031
D58	-0.02179	0.00000	0.00008	-0.00005	0.00003	-0.02176
D59	2.67718	0.00000	0.00008	0.00001	0.00009	2.67728
D60	-0.17072	0.00000	0.00015	-0.00003	0.00011	-0.17060
D61	0.26936	0.00000	0.00021	0.00024	0.00046	0.26982
D62	-2.58297	0.00000	0.00022	-0.00008	0.00014	-2.58283
D63	-2.14289	0.00000	0.00029	0.00019	0.00048	-2.14241
D64	2.14351	0.00000	-0.00065	-0.00024	-0.00089	2.14262
D65	-0.24978	0.00000	-0.00067	-0.00019	-0.00086	-0.25064
D66	2.48870	0.00000	-0.00019	-0.00005	-0.00024	2.48846
D67	-1.71934	0.00000	-0.00018	-0.00004	-0.00023	-1.71957
D68	0.35964	0.00000	-0.00018	-0.00004	-0.00022	0.35943
D69	1.27251	0.00000	-0.00016	-0.00005	-0.00020	1.27230
D70	-2.93553	0.00000	-0.00015	-0.00004	-0.00020	-2.93572
D71	-0.85655	0.00000	-0.00015	-0.00004	-0.00018	-0.85673
D72	-1.08999	0.00000	-0.00019	0.00002	-0.00017	-1.09016
D73	0.98516	0.00000	-0.00018	0.00002	-0.00016	0.98500
D74	3.06414	0.00000	-0.00018	0.00003	-0.00015	3.06400

Item	Value	Threshold	Converged?
Maximum Force	0.000019	0.000450	YES
RMS Force	0.000003	0.000300	YES
Maximum Displacement	0.005034	0.001800	NO

RMS Displacement 0.001269 0.001200 NO
Predicted change in Energy=-1.846804D-08
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.375937	-1.909159	-0.257127
2	6	0	-2.507539	-1.169286	-0.136969
3	7	0	-2.109544	0.112244	0.230872
4	6	0	-0.765952	0.135973	0.328804
5	7	0	-0.305277	-1.080409	0.041723
6	6	0	1.128060	-1.435750	-0.007376
7	6	0	1.683166	-1.372128	-1.441169
8	1	0	-1.241745	-2.944555	-0.519190
9	1	0	-3.537615	-1.442885	-0.274530
10	1	0	1.652616	-0.725377	0.633642
11	1	0	1.237917	-2.444805	0.391992
12	1	0	1.064187	-1.989531	-2.103097
13	1	0	1.634638	-0.336524	-1.797197
14	35	0	1.651146	2.235278	1.020791
15	1	0	-0.114180	0.994772	0.597919
16	6	0	-2.913864	1.256560	0.486529
17	6	0	-4.238125	1.281364	0.412903
18	1	0	-2.318177	2.120807	0.752771
19	1	0	-4.760365	2.203558	0.626453
20	1	0	-4.839833	0.421186	0.148238
21	8	0	2.991001	-1.883257	-1.464964
22	1	0	3.630683	-1.151475	-1.364803
23	6	0	4.839246	1.611869	-1.121148
24	6	0	5.711324	0.750973	-0.312657
25	8	0	4.857892	0.176979	-1.331721
26	1	0	3.922672	1.994070	-0.678183
27	1	0	5.260579	2.179980	-1.946002
28	1	0	6.762228	0.702359	-0.593789
29	6	0	5.398763	0.411550	1.118653
30	1	0	5.676876	-0.623493	1.339582
31	1	0	5.972781	1.064012	1.783895
32	1	0	4.338844	0.560714	1.333913

Distance matrix (angstroms):

	1	2	3	4	5

1	C	0.000000				
2	C	1.357341	0.000000			
3	N	2.205084	1.391412	0.000000		
4	C	2.213133	2.225706	1.347365	0.000000	
5	N	1.386524	2.211287	2.171078	1.331999	0.000000
6	C	2.560565	3.647654	3.596545	2.484072	1.477543
7	C	3.323924	4.393643	4.402697	3.377181	2.497594
8	H	1.076443	2.213573	3.264918	3.230344	2.160239
9	H	2.211463	1.074633	2.171001	3.246370	3.267938
10	H	3.371489	4.254149	3.875266	2.585406	2.075996
11	H	2.745998	3.991890	4.215443	3.268011	2.089428
12	H	3.060763	4.158809	4.465137	3.712320	2.702256
13	H	3.729418	4.539546	4.281747	3.241291	2.774574
14	Br	5.288918	5.497828	4.390220	3.275407	3.972398
15	H	3.279626	3.309286	2.212478	1.111200	2.156907
16	C	3.597224	2.537435	1.421882	2.427781	3.530440
17	C	4.338259	3.050077	2.435329	3.657181	4.602504
18	H	4.260087	3.413533	2.085721	2.555136	3.847746
19	H	5.399029	4.127241	3.399548	4.507642	5.565444
20	H	4.194449	2.837347	2.748954	4.087842	4.777900
21	O	4.530970	5.701515	5.733537	4.627050	3.712159
22	H	5.183365	6.259845	6.090433	4.884283	4.180328
23	C	7.195323	7.916987	7.236195	5.974854	5.921718
24	C	7.570248	8.442036	7.865709	6.537951	6.299129
25	O	6.660882	7.582179	7.140802	5.864013	5.488687
26	H	6.594524	7.186609	6.383987	5.142932	5.276954
27	H	7.976008	8.650656	7.958206	6.758091	6.749811
28	H	8.553543	9.467857	8.929538	7.605621	7.316540
29	C	7.292120	8.159978	7.566533	6.221215	5.993479
30	H	7.344698	8.334431	7.899297	6.565706	6.138352
31	H	8.185913	8.977370	8.285030	6.956226	6.859134
32	H	6.425761	7.213138	6.557403	5.220114	5.092239

		6	7	8	9	10
6	C	0.000000				
7	C	1.538815	0.000000			
8	H	2.855595	3.446401	0.000000		
9	H	4.673323	5.350011	2.754249	0.000000	
10	H	1.091189	2.173491	3.825061	5.317715	0.000000
11	H	1.090759	2.170106	2.688629	4.924815	1.785162
12	H	2.168594	1.096573	2.956037	4.981873	3.071495
13	H	2.160643	1.096169	4.087628	5.504067	2.461810
14	Br	3.848011	4.367568	6.129520	6.490761	2.985860
15	H	2.795886	3.604240	4.247073	4.292231	2.466122
16	C	4.881560	5.635487	4.632151	2.873201	4.980207

17	C	6.029534	6.748355	5.263599	2.895654	6.227083
18	H	5.010337	5.746714	5.332399	3.904136	4.886937
19	H	6.951249	7.653737	6.340051	3.950119	7.050180
20	H	6.252054	6.949224	4.971912	2.312848	6.610757
21	O	2.407358	1.404368	4.465085	6.650857	2.745198
22	H	2.861213	1.961464	5.260299	7.256591	2.843957
23	C	4.929642	4.355168	7.622454	8.956567	4.323959
24	C	5.087363	4.691178	7.876849	9.505648	4.421335
25	O	4.273924	3.534203	6.899982	8.615460	3.866613
26	H	4.474763	4.114465	7.147482	8.223836	3.777491
27	H	5.823185	5.066578	8.401004	9.660600	5.302176
28	H	6.054687	5.551433	8.795972	10.525719	5.445471
29	C	4.787417	4.851789	7.618550	9.232483	3.944801
30	H	4.813085	4.923693	7.530583	9.390613	4.086980
31	H	5.738361	5.893778	8.568675	10.048347	4.815478
32	H	4.011740	4.299951	6.845719	8.284933	3.059449

		11	12	13	14	15
11	H	0.000000				
12	H	2.542229	0.000000			
13	H	3.065091	1.775225	0.000000		
14	Br	4.740181	5.286985	3.815166	0.000000	
15	H	3.701521	4.194055	3.250737	2.198647	0.000000
16	C	5.562942	5.750492	5.333122	4.699217	2.814103
17	C	6.623579	6.718893	6.480081	5.996915	4.138029
18	H	5.798343	6.040799	5.307124	3.980008	2.479827
19	H	7.592209	7.678401	7.295352	6.423704	4.800939
20	H	6.724013	6.762952	6.802765	6.795960	4.781528
21	O	2.614752	2.032516	2.083862	4.993647	4.709637
22	H	3.237957	2.798985	2.198933	4.591265	4.741587
23	C	5.631676	5.308990	3.810878	3.891083	5.279434
24	C	5.542644	5.684358	4.472793	4.523968	5.901278
25	O	4.790528	4.436326	3.296926	4.478184	5.395720
26	H	5.296867	5.105918	3.452385	2.846845	4.350081
27	H	6.560234	5.917703	4.416151	4.672572	6.063356
28	H	6.433850	6.480120	5.368393	5.574932	6.985031
29	C	5.098965	5.910450	4.819796	4.168956	5.568110
30	H	4.890753	5.915658	5.124590	4.947797	6.058479
31	H	6.055422	6.966142	5.797000	4.542106	6.201808
32	H	4.419967	5.388893	4.233393	3.182127	4.534260

		16	17	18	19	20
16	C	0.000000				
17	C	1.326538	0.000000			
18	H	1.082890	2.122822	0.000000		
19	H	2.079892	1.081102	2.446852	0.000000	

20	H	2.126416	1.082592	3.100471	1.847121	0.000000
21	O	6.966650	8.111811	7.009869	9.008871	8.320747
22	H	7.215065	8.425976	7.112024	9.253704	8.747125
23	C	7.926007	9.212014	7.416152	9.775313	9.834309
24	C	8.676876	9.989959	8.214893	10.613585	10.566366
25	O	8.054298	9.327427	7.721370	10.022591	9.813041
26	H	6.974145	8.264201	6.404053	8.783000	8.940829
27	H	8.578545	9.828394	8.045150	10.345888	10.464106
28	H	9.751973	11.061484	9.288648	11.683866	11.629164
29	C	8.379343	9.701766	7.912433	10.327702	10.284485
30	H	8.835333	10.138760	8.473276	10.836825	10.635404
31	H	8.982911	10.304827	8.421403	10.855352	10.954507
32	H	7.335124	8.656327	6.862037	9.273351	9.255993

		21	22	23	24	25
21	O	0.000000				
22	H	0.977103	0.000000			
23	C	3.968642	3.025898	0.000000		
24	C	3.958173	3.009217	1.468100	0.000000	
25	O	2.783452	1.808846	1.450379	1.447863	0.000000
26	H	4.064566	3.232825	1.087384	2.208659	2.145593
27	H	4.678918	3.754057	1.086580	2.216539	2.133427
28	H	4.654729	3.719910	2.191614	1.088944	2.108806
29	C	4.211714	3.425888	2.602025	1.503845	2.520297
30	H	4.082451	3.432109	3.428361	2.149474	2.906433
31	H	5.304007	4.506452	3.166121	2.135857	3.425912
32	H	3.952643	3.273553	2.717104	2.151997	2.742675

		26	27	28	29	30
26	H	0.000000				
27	H	1.852545	0.000000			
28	H	3.120692	2.503356	0.000000		
29	C	2.812799	3.540981	2.208182	0.000000	
30	H	3.741690	4.339104	2.583369	1.094290	0.000000
31	H	3.336134	3.957871	2.531285	1.094418	1.769928
32	H	2.505243	3.772196	3.099821	1.091794	1.786815

		31	32
31	H	0.000000	
32	H	1.767921	0.000000

Stoichiometry C10H17BrN2O2

Framework group C1[X(C10H17BrN2O2)]

Deg. of freedom 90

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.710301	2.114523	-0.438953
2	6	0	-3.788323	1.349861	-0.129869
3	7	0	-3.321004	0.050062	0.037951
4	6	0	-1.989477	0.039714	-0.167772
5	7	0	-1.603316	1.279969	-0.462506
6	6	0	-0.200996	1.678453	-0.703010
7	6	0	0.455264	2.251244	0.565527
8	1	0	-2.636951	3.167638	-0.649424
9	1	0	-4.824133	1.615357	-0.022885
10	1	0	0.330122	0.784335	-1.033404
11	1	0	-0.195656	2.426040	-1.497265
12	1	0	-0.161304	3.066434	0.962743
13	1	0	0.509936	1.463650	1.325983
14	35	0	0.525692	-2.058259	-0.140782
15	1	0	-1.294842	-0.825827	-0.112197
16	6	0	-4.052272	-1.125139	0.363372
17	6	0	-5.362583	-1.168251	0.565680
18	1	0	-3.412817	-1.996587	0.429138
19	1	0	-5.827136	-2.113588	0.809217
20	1	0	-6.007830	-0.301389	0.500767
21	8	0	1.719213	2.774992	0.248712
22	1	0	2.403915	2.095591	0.404680
23	6	0	3.798160	-0.460163	1.229461
24	6	0	4.544580	0.009632	0.055806
25	8	0	3.722804	0.927949	0.815861
26	1	0	2.884642	-1.029860	1.076705
27	1	0	4.317333	-0.607444	2.172554
28	1	0	5.605736	0.214143	0.189677
29	6	0	4.108908	-0.303105	-1.349163
30	1	0	4.292008	0.550327	-2.009162
31	1	0	4.683173	-1.153179	-1.730404
32	1	0	3.050948	-0.570966	-1.380529

Rotational constants (GHZ): 0.6000074 0.2212335 0.1723102

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.

475 basis functions, 751 primitive gaussians, 492 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1307.2399090046 Hartrees.

NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 475 RedAO= T EigKep= 3.78D-06 NBF= 475

NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000081 -0.000027 0.000019 Ang= -0.01 deg.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3225.52371204 A.U. after 8 cycles

NFock= 8 Conv=0.55D-08 -V/T= 2.0018

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000000310	0.000002011	-0.000000591
2	6	-0.000001207	-0.000002073	0.000006222
3	7	0.000004130	0.000002714	-0.000004954
4	6	-0.000001541	0.000001269	0.000012036
5	7	-0.000002843	0.000003320	0.000006553
6	6	0.000004326	0.000002330	0.000001701
7	6	-0.000018443	0.000005387	0.000000369
8	1	-0.000000829	-0.000000979	0.000010949
9	1	-0.000000398	0.000000475	0.000005985
10	1	-0.000000417	-0.000000763	0.000002705
11	1	-0.000001063	0.000002233	0.000006930
12	1	0.000000362	-0.000004947	0.000006113
13	1	0.000002532	-0.000006837	0.000004084
14	35	-0.000001326	0.000007840	0.000000892
15	1	0.000006505	-0.000005637	-0.000023470
16	6	-0.000000437	0.000003261	-0.000000593
17	6	0.000001640	0.000001726	-0.000003865
18	1	0.000000612	0.000002861	-0.000005190
19	1	0.000000646	0.000003224	-0.000005854
20	1	-0.000000141	0.000002299	-0.000000864

21	8	0.000017005	-0.000004300	0.000011113
22	1	-0.000009289	-0.000012471	-0.000004000
23	6	-0.000002707	-0.000011215	-0.000006458
24	6	0.000008644	-0.000002232	-0.000015058
25	8	-0.000005176	0.000000260	0.000017681
26	1	0.000001894	0.000000266	-0.000005252
27	1	0.000000299	-0.000004999	-0.000007851
28	1	-0.000001205	-0.000000140	-0.000000932
29	6	-0.000001802	0.000006481	-0.000005815
30	1	-0.000000818	0.000003099	0.000002413
31	1	-0.000000446	0.000003527	-0.000003505
32	1	0.000001184	0.000002010	-0.000001494

Cartesian Forces: Max 0.000023470 RMS 0.000006142

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000014469 RMS 0.000002703
Search for a local minimum.
Step number 38 out of a maximum of 177
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 24 25 26 27 28
29 30 31 32 33
34 35 36 37 38
DE= 2.43D-07 DEPred=-1.85D-08 R=-1.32D+01
Trust test=-1.32D+01 RLast= 1.04D-02 DXMaxT set to 2.43D-01
ITU= -1 -1 -1 0 0 1 1 0 1 1 1 1 1 1 1 1 1 1 1
ITU= 1 -1 1 1 1 1 1 1 1 1 1 1 1 0 1 0 1 0

Eigenvalues ---	0.00004	0.00052	0.00097	0.00196	0.00235
Eigenvalues ---	0.00318	0.00337	0.00695	0.01079	0.01184
Eigenvalues ---	0.01328	0.01555	0.01826	0.01920	0.01993
Eigenvalues ---	0.02125	0.02248	0.02281	0.02329	0.02416
Eigenvalues ---	0.03027	0.03065	0.03142	0.03502	0.03704
Eigenvalues ---	0.04144	0.04622	0.05198	0.05407	0.05425
Eigenvalues ---	0.05670	0.05878	0.06514	0.09153	0.09348
Eigenvalues ---	0.10350	0.11079	0.11465	0.11586	0.12921
Eigenvalues ---	0.13806	0.14126	0.14160	0.15167	0.15983
Eigenvalues ---	0.15996	0.16001	0.16001	0.16012	0.16042
Eigenvalues ---	0.16060	0.16969	0.18782	0.21081	0.22048
Eigenvalues ---	0.22837	0.23407	0.23869	0.24298	0.25050

Eigenvalues --- 0.27661 0.28378 0.30769 0.32071 0.33105
Eigenvalues --- 0.33277 0.34035 0.34203 0.34474 0.34842
Eigenvalues --- 0.35038 0.35683 0.35689 0.35856 0.36188
Eigenvalues --- 0.36436 0.36673 0.37198 0.37249 0.37606
Eigenvalues --- 0.38375 0.42174 0.42536 0.44591 0.45694
Eigenvalues --- 0.49401 0.54022 0.55069 0.56343 0.60404
Eigenvalue 1 is 3.78D-05 Eigenvector:

	D52	D53	D54	D55	D25
1	0.50817	-0.49686	-0.49580	-0.48892	0.04423
	D26	D45	D46	D47	D64
1	0.03950	-0.03361	-0.02667	-0.02255	-0.01671

En-DIIS/RFO-DIIS IScMMF= 0 using points: 38 37 36 35 34
RFO step: Lambda=-3.37506151D-09.
DidBck=F Rises=F RFO-DIIS coefs: 1.86661 -0.84071 -0.38641 0.48164 -0.12113
Iteration 1 RMS(Cart)= 0.00070170 RMS(Int)= 0.00000057
Iteration 2 RMS(Cart)= 0.00000094 RMS(Int)= 0.00000032

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56500	0.00000	0.00000	0.00000	0.00000	2.56500
R2	2.62015	0.00000	0.00000	0.00001	0.00000	2.62015
R3	2.03418	0.00000	0.00000	0.00000	0.00000	2.03418
R4	2.62939	0.00000	0.00000	0.00000	0.00000	2.62939
R5	2.03076	0.00000	0.00000	0.00000	0.00000	2.03076
R6	2.54615	0.00000	-0.00001	0.00000	-0.00001	2.54614
R7	2.68697	0.00000	0.00000	0.00000	0.00000	2.68697
R8	2.51711	-0.00001	0.00001	-0.00001	0.00000	2.51712
R9	2.09986	-0.00001	0.00004	0.00000	0.00004	2.09990
R10	2.79215	0.00000	-0.00002	0.00000	-0.00002	2.79213
R11	2.90794	-0.00001	-0.00001	-0.00001	-0.00002	2.90792
R12	2.06205	0.00000	-0.00001	0.00000	-0.00001	2.06204
R13	2.06124	0.00000	0.00000	0.00000	0.00000	2.06123
R14	2.07222	0.00000	-0.00001	0.00000	-0.00001	2.07221
R15	2.07146	0.00000	-0.00001	0.00000	-0.00001	2.07145
R16	2.65387	0.00001	0.00005	-0.00001	0.00004	2.65391
R17	4.15484	0.00000	-0.00029	-0.00008	-0.00037	4.15447
R18	8.46254	0.00000	-0.00026	-0.00009	-0.00035	8.46220
R19	2.50679	0.00000	0.00000	0.00000	0.00000	2.50679
R20	2.04637	0.00000	0.00000	0.00000	0.00000	2.04637
R21	2.04299	0.00000	0.00000	0.00000	0.00000	2.04299
R22	2.04580	0.00000	0.00000	0.00000	0.00000	2.04580
R23	1.84646	-0.00001	-0.00002	0.00000	-0.00002	1.84644
R24	3.41822	0.00000	-0.00003	0.00001	-0.00002	3.41820
R25	2.77431	0.00000	0.00000	0.00001	0.00001	2.77432

R26	2.74082	0.00000	-0.00001	-0.00001	-0.00002	2.74080
R27	2.05486	0.00000	0.00000	0.00000	0.00000	2.05486
R28	2.05334	0.00000	0.00000	0.00000	0.00000	2.05334
R29	2.73606	0.00000	-0.00002	-0.00001	-0.00003	2.73604
R30	2.05780	0.00000	0.00000	0.00000	0.00000	2.05780
R31	2.84186	0.00000	0.00001	0.00000	0.00001	2.84187
R32	2.06791	0.00000	0.00000	0.00000	0.00000	2.06791
R33	2.06815	0.00000	0.00000	0.00000	0.00000	2.06815
R34	2.06319	0.00000	0.00000	0.00000	0.00000	2.06319
A1	1.87431	0.00000	0.00000	0.00000	0.00000	1.87431
A2	2.27810	0.00000	0.00000	0.00000	0.00000	2.27810
A3	2.13074	0.00000	0.00000	0.00000	0.00000	2.13074
A4	1.86187	0.00000	0.00000	-0.00001	-0.00001	1.86186
A5	2.27708	0.00000	0.00001	0.00000	0.00001	2.27709
A6	2.14422	0.00000	-0.00001	0.00001	0.00000	2.14422
A7	1.89723	0.00000	0.00000	0.00001	0.00001	1.89725
A8	2.24845	0.00000	0.00001	0.00000	0.00001	2.24845
A9	2.13749	0.00000	-0.00001	-0.00001	-0.00002	2.13747
A10	1.88929	0.00000	0.00000	-0.00001	-0.00001	1.88928
A11	2.23460	0.00000	-0.00002	0.00000	-0.00001	2.23459
A12	2.15929	0.00000	0.00002	0.00001	0.00002	2.15932
A13	1.90205	0.00000	0.00000	0.00001	0.00001	1.90205
A14	2.21202	0.00000	0.00000	0.00001	0.00001	2.21203
A15	2.16794	0.00000	-0.00001	-0.00002	-0.00003	2.16792
A16	1.95084	0.00000	0.00000	0.00000	-0.00001	1.95083
A17	1.86529	0.00000	0.00002	0.00002	0.00004	1.86532
A18	1.88390	0.00000	0.00001	-0.00001	0.00000	1.88390
A19	1.92520	0.00000	0.00000	0.00000	0.00000	1.92520
A20	1.92097	0.00000	0.00001	0.00000	0.00001	1.92098
A21	1.91637	0.00000	-0.00003	0.00000	-0.00003	1.91634
A22	1.91297	0.00000	0.00000	-0.00001	-0.00001	1.91296
A23	1.90257	0.00000	-0.00001	0.00000	-0.00001	1.90256
A24	1.91418	-0.00001	0.00001	-0.00001	0.00000	1.91418
A25	1.88691	0.00000	0.00004	0.00000	0.00004	1.88695
A26	1.88654	0.00000	-0.00001	0.00001	0.00000	1.88654
A27	1.96013	0.00000	-0.00003	0.00001	-0.00002	1.96011
A28	1.78706	-0.00001	-0.00037	-0.00017	-0.00054	1.78653
A29	2.83572	0.00001	0.00049	0.00012	0.00061	2.83633
A30	2.17702	0.00000	0.00000	-0.00001	0.00000	2.17702
A31	1.95555	0.00000	0.00000	0.00000	-0.00001	1.95555
A32	2.15061	0.00000	0.00000	0.00001	0.00001	2.15062
A33	2.07970	0.00000	-0.00001	0.00000	-0.00001	2.07969
A34	2.15743	0.00000	0.00001	0.00000	0.00001	2.15744
A35	2.04605	0.00000	0.00000	0.00000	0.00000	2.04605

A36	1.91278	-0.00001	-0.00004	0.00000	-0.00004	1.91274
A37	3.05286	-0.00001	0.00037	0.00007	0.00044	3.05330
A38	2.07428	0.00000	0.00004	0.00000	0.00004	2.07432
A39	2.08784	0.00000	-0.00004	0.00001	-0.00003	2.08781
A40	2.00172	0.00000	0.00005	-0.00003	0.00002	2.00174
A41	1.98456	0.00000	-0.00003	0.00001	-0.00002	1.98454
A42	2.04016	0.00000	-0.00001	0.00000	0.00000	2.04016
A43	2.04572	0.00000	0.00003	-0.00001	0.00002	2.04574
A44	2.13298	0.00000	-0.00004	0.00000	-0.00004	2.13294
A45	1.94921	0.00000	0.00003	0.00001	0.00005	1.94925
A46	2.04643	0.00000	-0.00006	0.00000	-0.00005	2.04638
A47	2.02219	0.00000	0.00002	0.00000	0.00002	2.02221
A48	1.43169	0.00000	0.00034	0.00016	0.00050	1.43219
A49	1.00013	0.00000	0.00003	-0.00001	0.00002	1.00015
A50	2.37533	0.00000	0.00034	0.00005	0.00040	2.37573
A51	2.35172	0.00001	0.00022	0.00029	0.00050	2.35222
A52	1.93137	0.00000	-0.00002	0.00001	-0.00001	1.93136
A53	1.91236	0.00000	0.00004	0.00000	0.00003	1.91239
A54	1.93755	0.00000	-0.00004	0.00001	-0.00003	1.93752
A55	1.88375	0.00000	0.00000	0.00000	0.00000	1.88375
A56	1.91362	0.00000	0.00001	-0.00001	0.00000	1.91362
A57	1.88377	0.00000	0.00001	0.00000	0.00001	1.88378
A58	3.78341	0.00001	0.00056	0.00045	0.00101	3.78442
A59	5.04171	0.00000	-0.00047	-0.00003	-0.00050	5.04120
D1	0.00429	0.00000	0.00003	-0.00001	0.00002	0.00431
D2	-3.13142	0.00000	0.00009	-0.00001	0.00009	-3.13134
D3	3.13657	0.00000	-0.00013	0.00001	-0.00012	3.13645
D4	0.00086	0.00000	-0.00006	0.00001	-0.00005	0.00081
D5	-0.00673	0.00000	-0.00002	-0.00001	-0.00004	-0.00676
D6	-3.09773	0.00000	0.00024	-0.00003	0.00021	-3.09752
D7	-3.13997	0.00000	0.00012	-0.00003	0.00009	-3.13988
D8	0.05222	0.00000	0.00038	-0.00005	0.00033	0.05255
D9	-0.00046	0.00000	-0.00002	0.00003	0.00000	-0.00046
D10	-3.13659	0.00000	0.00006	0.00005	0.00010	-3.13649
D11	3.13580	0.00000	-0.00008	0.00003	-0.00006	3.13575
D12	-0.00032	0.00000	0.00000	0.00004	0.00004	-0.00028
D13	-0.00372	0.00000	0.00001	-0.00004	-0.00003	-0.00375
D14	3.13757	0.00000	-0.00014	0.00007	-0.00006	3.13751
D15	3.13282	0.00000	-0.00006	-0.00005	-0.00012	3.13270
D16	-0.00907	0.00000	-0.00021	0.00006	-0.00015	-0.00922
D17	0.00254	0.00000	0.00025	-0.00006	0.00018	0.00272
D18	-3.13932	0.00000	0.00021	-0.00004	0.00017	-3.13915
D19	-3.13291	0.00000	0.00033	-0.00004	0.00029	-3.13262
D20	0.00842	0.00000	0.00030	-0.00002	0.00027	0.00869

D21	0.00644	0.00000	0.00001	0.00003	0.00004	0.00648
D22	3.09900	0.00000	-0.00025	0.00005	-0.00020	3.09881
D23	-3.13488	0.00000	0.00015	-0.00007	0.00007	-3.13480
D24	-0.04231	0.00000	-0.00011	-0.00005	-0.00016	-0.04247
D25	-3.10936	0.00000	-0.00142	-0.00080	-0.00222	-3.11158
D26	0.03189	0.00000	-0.00159	-0.00067	-0.00226	0.02963
D27	1.40957	0.00000	0.00048	0.00016	0.00064	1.41022
D28	-2.76569	0.00000	0.00049	0.00017	0.00066	-2.76503
D29	-0.70530	0.00000	0.00047	0.00017	0.00064	-0.70467
D30	-1.67416	0.00000	0.00078	0.00014	0.00092	-1.67324
D31	0.43376	0.00000	0.00079	0.00015	0.00094	0.43470
D32	2.49415	0.00000	0.00077	0.00015	0.00092	2.49507
D33	-0.93910	0.00000	0.00001	0.00005	0.00005	-0.93905
D34	1.12296	0.00000	0.00005	0.00004	0.00009	1.12305
D35	-3.00762	0.00000	0.00002	0.00004	0.00006	-3.00756
D36	-3.01178	0.00000	-0.00002	0.00003	0.00001	-3.01177
D37	-0.94971	0.00000	0.00003	0.00002	0.00005	-0.94967
D38	1.20289	0.00000	-0.00001	0.00003	0.00002	1.20291
D39	1.15415	0.00000	0.00002	0.00003	0.00005	1.15419
D40	-3.06697	0.00000	0.00006	0.00002	0.00008	-3.06689
D41	-0.91437	0.00000	0.00003	0.00003	0.00005	-0.91432
D42	-1.63703	0.00000	0.00015	0.00006	0.00021	-1.63682
D43	2.56136	0.00000	0.00015	0.00007	0.00022	2.56157
D44	0.48131	0.00000	0.00012	0.00006	0.00018	0.48149
D45	0.43224	0.00000	0.00133	0.00073	0.00206	0.43430
D46	-0.26750	0.00000	0.00080	-0.00008	0.00072	-0.26678
D47	2.57096	0.00000	0.00081	-0.00034	0.00047	2.57143
D48	-3.14148	0.00000	-0.00001	0.00003	0.00002	-3.14146
D49	0.00063	0.00000	0.00001	0.00000	0.00001	0.00064
D50	0.00040	0.00000	0.00003	0.00001	0.00004	0.00044
D51	-3.14067	0.00000	0.00005	-0.00002	0.00003	-3.14064
D52	-1.94053	0.00000	-0.00246	0.00177	-0.00069	-1.94122
D53	2.44634	0.00000	0.00180	-0.00181	-0.00002	2.44633
D54	2.07565	0.00000	0.00166	-0.00216	-0.00050	2.07515
D55	-2.59536	0.00000	0.00227	-0.00178	0.00049	-2.59488
D56	-2.72935	0.00000	0.00006	-0.00001	0.00005	-2.72930
D57	-0.03031	0.00000	0.00008	-0.00003	0.00005	-0.03026
D58	-0.02176	0.00000	0.00004	0.00002	0.00006	-0.02170
D59	2.67728	0.00000	0.00007	0.00000	0.00007	2.67735
D60	-0.17060	0.00000	0.00013	-0.00001	0.00012	-0.17048
D61	0.26982	0.00000	0.00031	0.00042	0.00073	0.27054
D62	-2.58283	0.00000	0.00012	0.00001	0.00013	-2.58270
D63	-2.14241	0.00000	0.00030	0.00043	0.00074	-2.14168
D64	2.14262	0.00000	-0.00053	-0.00007	-0.00060	2.14202

D65	-0.25064	0.00000	-0.00053	-0.00010	-0.00062	-0.25127
D66	2.48846	0.00000	-0.00016	0.00006	-0.00010	2.48836
D67	-1.71957	0.00000	-0.00015	0.00006	-0.00009	-1.71966
D68	0.35943	0.00000	-0.00014	0.00006	-0.00008	0.35935
D69	1.27230	0.00000	-0.00012	0.00006	-0.00006	1.27224
D70	-2.93572	0.00000	-0.00011	0.00006	-0.00005	-2.93578
D71	-0.85673	0.00000	-0.00010	0.00006	-0.00003	-0.85676
D72	-1.09016	0.00000	-0.00013	0.00004	-0.00010	-1.09025
D73	0.98500	0.00000	-0.00012	0.00003	-0.00009	0.98491
D74	3.06400	0.00000	-0.00011	0.00004	-0.00007	3.06393

Item	Value	Threshold	Converged?
Maximum Force	0.000014	0.000450	YES
RMS Force	0.000003	0.000300	YES
Maximum Displacement	0.002413	0.001800	NO
RMS Displacement	0.000702	0.001200	YES

Predicted change in Energy=-1.731604D-08

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.375827	-1.909489	-0.256433
2	6	0	-2.507367	-1.169513	-0.136314
3	7	0	-2.109205	0.112189	0.230754
4	6	0	-0.765589	0.135926	0.328268
5	7	0	-0.305050	-1.080631	0.041699
6	6	0	1.128263	-1.435960	-0.007869
7	6	0	1.682989	-1.371921	-1.441782
8	1	0	-1.241756	-2.945048	-0.517914
9	1	0	-3.537500	-1.443149	-0.273374
10	1	0	1.653015	-0.725808	0.633225
11	1	0	1.238213	-2.445128	0.391180
12	1	0	1.063801	-1.989086	-2.103728
13	1	0	1.634450	-0.336198	-1.797450
14	35	0	1.650753	2.236135	1.019971
15	1	0	-0.113707	0.994880	0.596701
16	6	0	-2.913399	1.256647	0.486178
17	6	0	-4.237698	1.281388	0.413254
18	1	0	-2.317572	2.121049	0.751611
19	1	0	-4.759829	2.203709	0.626530
20	1	0	-4.839546	0.421051	0.149426
21	8	0	2.990808	-1.883126	-1.466080

22	1	0	3.630515	-1.151414	-1.365668
23	6	0	4.839295	1.611970	-1.120831
24	6	0	5.711026	0.750879	-0.312166
25	8	0	4.857632	0.177077	-1.331348
26	1	0	3.922732	1.994431	-0.678069
27	1	0	5.260934	2.179930	-1.945634
28	1	0	6.761978	0.702019	-0.593078
29	6	0	5.398056	0.411549	1.119083
30	1	0	5.675791	-0.623589	1.340048
31	1	0	5.972127	1.063807	1.784476
32	1	0	4.338133	0.561041	1.334087

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357341	0.000000			
3	N	2.205080	1.391414	0.000000		
4	C	2.213140	2.225713	1.347359	0.000000	
5	N	1.386525	2.211286	2.171068	1.332002	0.000000
6	C	2.560563	3.647642	3.596513	2.484046	1.477532
7	C	3.324213	4.393665	4.402351	3.376716	2.497572
8	H	1.076443	2.213575	3.264915	3.230350	2.160240
9	H	2.211468	1.074634	2.171002	3.246374	3.267939
10	H	3.371421	4.254156	3.875374	2.585581	2.076011
11	H	2.745818	3.991843	4.215545	3.268183	2.089414
12	H	3.061146	4.158804	4.464653	3.711731	2.702203
13	H	3.729846	4.539651	4.281311	3.240643	2.774583
14	Br	5.289196	5.497763	4.389908	3.275369	3.972797
15	H	3.279656	3.309307	2.212481	1.111219	2.156939
16	C	3.597224	2.537442	1.421884	2.427764	3.530427
17	C	4.338259	3.050081	2.435327	3.657165	4.602490
18	H	4.260079	3.413536	2.085720	2.555110	3.847723
19	H	5.399027	4.127245	3.399545	4.507621	5.565427
20	H	4.194459	2.837358	2.748958	4.087836	4.777897
21	O	4.531164	5.701530	5.733294	4.626746	3.712153
22	H	5.183487	6.259810	6.090126	4.883891	4.180235
23	C	7.195527	7.917030	7.235868	5.974389	5.921644
24	C	7.569951	8.441612	7.865031	6.537191	6.298637
25	O	6.660721	7.581861	7.140111	5.863159	5.488203
26	H	6.594930	7.186808	6.383812	5.142675	5.277141
27	H	7.976425	8.650948	7.958089	6.757778	6.749884
28	H	8.553197	9.467418	8.928857	7.604840	7.315987
29	C	7.291417	8.159135	7.565561	6.220279	5.992727
30	H	7.343542	8.333172	7.897979	6.564445	6.137187

31	H	8.185245	8.976579	8.284176	6.955453	6.858487
32	H	6.425154	7.212334	6.556445	5.219231	5.091611

		6	7	8	9	10
6	C	0.000000				
7	C	1.538807	0.000000			
8	H	2.855606	3.447085	0.000000		
9	H	4.673317	5.350118	2.754259	0.000000	
10	H	1.091184	2.173480	3.824899	5.317702	0.000000
11	H	1.090757	2.170104	2.688237	4.924737	1.785135
12	H	2.168577	1.096567	2.957070	4.981989	3.071475
13	H	2.160625	1.096165	4.088506	5.504291	2.461772
14	Br	3.848861	4.367990	6.129956	6.490597	2.987086
15	H	2.795885	3.603509	4.247104	4.292246	2.466456
16	C	4.881521	5.634996	4.632153	2.873208	4.980350
17	C	6.029500	6.748018	5.263603	2.895659	6.227177
18	H	5.010279	5.745981	5.332393	3.904142	4.887144
19	H	6.951207	7.653297	6.340055	3.950126	7.050297
20	H	6.252037	6.949112	4.971927	2.312861	6.610801
21	O	2.407366	1.404390	4.465568	6.650935	2.745206
22	H	2.861092	1.961446	5.260687	7.256628	2.843803
23	C	4.929535	4.355328	7.622933	8.956709	4.323690
24	C	5.086903	4.691204	7.876763	9.505288	4.420613
25	O	4.273368	3.534112	6.900136	8.615259	3.865788
26	H	4.475020	4.114855	7.148150	8.224099	3.777672
27	H	5.823106	5.066676	8.401712	9.661035	5.301972
28	H	6.054103	5.551365	8.795823	10.525360	5.444631
29	C	4.786903	4.851857	7.617979	9.231631	3.943979
30	H	4.812155	4.923520	7.529519	9.389332	4.085679
31	H	5.737975	5.893914	8.568082	10.047517	4.814855
32	H	4.011499	4.300184	6.845270	8.284099	3.058928

		11	12	13	14	15
11	H	0.000000				
12	H	2.542236	0.000000			
13	H	3.065076	1.775243	0.000000		
14	Br	4.741285	5.287201	3.815105	0.000000	
15	H	3.701835	4.193196	3.249582	2.198452	0.000000
16	C	5.563097	5.749827	5.332452	4.698490	2.814073
17	C	6.623671	6.718414	6.479655	5.996124	4.138000
18	H	5.798576	6.039855	5.306058	3.979054	2.479773
19	H	7.592337	7.677793	7.294767	6.422726	4.800896
20	H	6.724030	6.762763	6.802674	6.795319	4.781515
21	O	2.614737	2.032531	2.083867	4.994448	4.709140
22	H	3.237795	2.799008	2.198928	4.591973	4.740957
23	C	5.631520	5.309242	3.811063	3.890940	5.278537

24	C	5.542131	5.684524	4.472838	4.523980	5.900263
25	O	4.789912	4.436439	3.296908	4.478001	5.394478
26	H	5.297134	5.106310	3.452692	2.846691	4.349366
27	H	6.560042	5.917907	4.416361	4.672406	6.062556
28	H	6.433139	6.480226	5.368421	5.574949	6.984009
29	C	5.098504	5.910611	4.819753	4.169079	5.567108
30	H	4.889832	5.915626	5.124346	4.947868	6.057252
31	H	6.055068	6.966345	5.797038	4.542367	6.201044
32	H	4.419912	5.389153	4.233375	3.182235	4.533303

		16	17	18	19	20
16	C	0.000000				
17	C	1.326537	0.000000			
18	H	1.082891	2.122828	0.000000		
19	H	2.079887	1.081103	2.446855	0.000000	
20	H	2.126421	1.082592	3.100479	1.847120	0.000000
21	O	6.966287	8.111557	7.009313	9.008531	8.320669
22	H	7.214631	8.425667	7.111373	9.253301	8.747004
23	C	7.925465	9.211651	7.415251	9.774795	9.834216
24	C	8.676051	9.989234	8.213853	10.612760	10.565814
25	O	8.053434	9.326745	7.720188	10.021781	9.812618
26	H	6.973699	8.263900	6.403235	8.782519	8.940793
27	H	8.578222	9.828314	8.044399	10.345642	10.464351
28	H	9.751170	11.060798	9.287629	11.683088	11.628654
29	C	8.378248	9.700649	7.911280	10.326523	10.283424
30	H	8.833944	10.137315	8.471904	10.835354	10.633963
31	H	8.981945	10.303792	8.420433	10.854267	10.953483
32	H	7.333998	8.655155	6.860854	9.272104	9.254880

		21	22	23	24	25
21	O	0.000000				
22	H	0.977092	0.000000			
23	C	3.968854	3.026118	0.000000		
24	C	3.958420	3.009504	1.468105	0.000000	
25	O	2.783455	1.808835	1.450370	1.447848	0.000000
26	H	4.065083	3.233346	1.087383	2.208689	2.145598
27	H	4.678875	3.753996	1.086581	2.216526	2.133406
28	H	4.654764	3.719969	2.191630	1.088943	2.108824
29	C	4.212296	3.426520	2.602007	1.503851	2.520247
30	H	4.082882	3.432587	3.428320	2.149468	2.906339
31	H	5.304601	4.507079	3.166165	2.135885	3.425894
32	H	3.953501	3.274432	2.717028	2.151982	2.742600

		26	27	28	29	30
26	H	0.000000				
27	H	1.852543	0.000000			
28	H	3.120716	2.503349	0.000000		

29	C	2.812802	3.540969	2.208200	0.000000	
30	H	3.741663	4.339070	2.583412	1.094290	0.000000
31	H	3.336197	3.957934	2.531307	1.094416	1.769925
32	H	2.505183	3.772126	3.099817	1.091794	1.786816

		31	32
31	H	0.000000	
32	H	1.767926	0.000000

Stoichiometry C10H17BrN2O2

Framework group C1[X(C10H17BrN2O2)]

Deg. of freedom 90

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.710288	2.114647	-0.439449
2	6	0	-3.788208	1.349821	-0.130412
3	7	0	-3.320620	0.050176	0.037868
4	6	0	-1.989047	0.040072	-0.167530
5	7	0	-1.603110	1.280335	-0.462537
6	6	0	-0.200799	1.679089	-0.702580
7	6	0	0.455157	2.251286	0.566373
8	1	0	-2.637144	3.167704	-0.650282
9	1	0	-4.824115	1.615089	-0.023796
10	1	0	0.330501	0.785230	-1.033363
11	1	0	-0.195400	2.427086	-1.496446
12	1	0	-0.161603	3.066161	0.963921
13	1	0	0.509850	1.463271	1.326386
14	35	0	0.525507	-2.058574	-0.140372
15	1	0	-1.294223	-0.825310	-0.111494
16	6	0	-4.051697	-1.125136	0.363325
17	6	0	-5.362091	-1.168563	0.565018
18	1	0	-3.412012	-1.996374	0.429666
19	1	0	-5.826476	-2.113956	0.808661
20	1	0	-6.007569	-0.301919	0.499503
21	8	0	1.719095	2.775412	0.250044
22	1	0	2.403821	2.095952	0.405584
23	6	0	3.798293	-0.460475	1.228700
24	6	0	4.544288	0.009676	0.054910
25	8	0	3.722578	0.927690	0.815374
26	1	0	2.884828	-1.030309	1.076149

27	1	0	4.317795	-0.607816	2.171603
28	1	0	5.605457	0.214313	0.188477
29	6	0	4.108174	-0.302847	-1.349975
30	1	0	4.290842	0.550783	-2.009838
31	1	0	4.682471	-1.152705	-1.731646
32	1	0	3.050256	-0.570916	-1.380990

Rotational constants (GHZ): 0.5998721 0.2212703 0.1723208

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.

475 basis functions, 751 primitive gaussians, 492 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1307.2430481336 Hartrees.

NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 475 RedAO= T EigKep= 3.78D-06 NBF= 475

NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000036 -0.000010 0.000001 Ang= 0.00 deg.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3225.52371196 A.U. after 8 cycles

NFock= 8 Conv=0.46D-08 -V/T= 2.0018

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

1	6	-0.000000551	-0.000001126	0.000006535
2	6	0.000000671	-0.000000984	0.000010745
3	7	0.000000531	0.000003701	-0.000001949
4	6	0.000001258	-0.000000595	-0.000000582
5	7	-0.000003897	0.000005752	-0.000000082
6	6	0.000003021	0.000000928	0.000007911

7	6	-0.000002762	-0.000001169	0.000001176
8	1	-0.000000225	0.000000049	0.000007150
9	1	0.000000165	0.000000375	0.000005056
10	1	-0.000001158	0.000000201	0.000003455
11	1	-0.000000960	0.000001905	0.000006513
12	1	0.000000534	-0.000004856	0.000004749
13	1	0.000001119	-0.000005967	0.000000790
14	35	-0.000000312	0.000007405	-0.000000188
15	1	0.000002448	-0.000005452	-0.000012399
16	6	-0.000000627	0.000004203	-0.000002664
17	6	0.000000793	0.000003236	-0.000005113
18	1	0.000000657	0.000002448	-0.000004308
19	1	0.000000443	0.000002769	-0.000005263
20	1	0.000000340	0.000002122	-0.000000806
21	8	0.000001524	-0.000003085	0.000006506
22	1	-0.000004775	-0.000009617	0.000002731
23	6	0.000002804	-0.000008297	-0.000012641
24	6	0.000000883	0.000000286	-0.000006206
25	8	-0.000001942	-0.000001763	0.000010268
26	1	0.000001394	-0.000001950	-0.000003049
27	1	-0.000000425	-0.000003531	-0.000007264
28	1	-0.000001690	-0.000001689	-0.000002078
29	6	0.000000649	0.000004896	-0.000007677
30	1	-0.000000859	0.000003157	0.000003190
31	1	0.000000075	0.000004757	-0.000003923
32	1	0.000000874	0.000001889	-0.000000583

Cartesian Forces: Max 0.000012641 RMS 0.000004219

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000011627 RMS 0.000002053
Search for a local minimum.
Step number 39 out of a maximum of 177
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 24 25 26 27 28
29 30 31 32 33
34 35 36 37 38
39

DE= 7.77D-08 DEPred=-1.73D-08 R=-4.49D+00

Trust test=-4.49D+00 RLast= 5.05D-03 DXMaxT set to 1.21D-01

ITU= -1 -1 -1 -1 0 0 1 1 0 1 1 1 1 1 1 1 1 1 1

ITU= 1 1 -1 1 1 1 1 1 1 1 1 1 1 1 0 1 0 1 0

Eigenvalues ---	0.00004	0.00046	0.00081	0.00204	0.00234
Eigenvalues ---	0.00259	0.00347	0.00683	0.01025	0.01203
Eigenvalues ---	0.01365	0.01613	0.01709	0.01852	0.02044
Eigenvalues ---	0.02085	0.02197	0.02256	0.02325	0.02406
Eigenvalues ---	0.02997	0.03063	0.03101	0.03517	0.03719
Eigenvalues ---	0.04128	0.04623	0.05190	0.05392	0.05421
Eigenvalues ---	0.05670	0.05893	0.06487	0.08770	0.09356
Eigenvalues ---	0.10416	0.11032	0.11465	0.11584	0.12865
Eigenvalues ---	0.13828	0.14080	0.14263	0.15134	0.15969
Eigenvalues ---	0.15990	0.16001	0.16003	0.16010	0.16028
Eigenvalues ---	0.16050	0.17172	0.18455	0.20519	0.22048
Eigenvalues ---	0.22875	0.23409	0.23858	0.24336	0.25047
Eigenvalues ---	0.27837	0.28380	0.30707	0.32044	0.33105
Eigenvalues ---	0.33246	0.34030	0.34199	0.34470	0.34847
Eigenvalues ---	0.35044	0.35684	0.35689	0.35856	0.36087
Eigenvalues ---	0.36436	0.36670	0.37184	0.37240	0.37513
Eigenvalues ---	0.38075	0.42173	0.42559	0.44780	0.45619
Eigenvalues ---	0.49380	0.53712	0.54972	0.56080	0.60397

Eigenvalue 1 is 3.96D-05 Eigenvector:

	D52	D53	D54	D55	D25
1	-0.50594	0.49855	0.49825	0.49016	-0.03062
	D26	D46	D47	D45	D65
1	-0.02475	0.02433	0.02098	0.01875	0.01648

En-DIIS/RFO-DIIS IScMMF= 0 using points: 39 38 37 36 35

RFO step: Lambda=-2.17041196D-09.

DidBck=F Rises=F RFO-DIIS coefs: 2.66175 -2.12471 -0.19465 1.06864 -0.41104

Iteration 1 RMS(Cart)= 0.00062612 RMS(Int)= 0.00000093

Iteration 2 RMS(Cart)= 0.00000204 RMS(Int)= 0.00000039

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000039

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56500	0.00000	0.00000	0.00000	0.00000	2.56501
R2	2.62015	0.00000	0.00000	0.00000	0.00000	2.62015
R3	2.03418	0.00000	0.00000	0.00000	0.00000	2.03418
R4	2.62939	0.00000	0.00000	0.00000	0.00000	2.62939
R5	2.03076	0.00000	0.00000	0.00000	0.00000	2.03076
R6	2.54614	0.00000	-0.00001	0.00000	-0.00001	2.54613
R7	2.68697	0.00000	0.00000	0.00001	0.00001	2.68698
R8	2.51712	-0.00001	-0.00001	0.00001	-0.00001	2.51711

R9	2.09990	0.00000	-0.00001	0.00002	0.00001	2.09991
R10	2.79213	0.00000	0.00000	0.00000	0.00000	2.79213
R11	2.90792	0.00000	-0.00003	0.00002	-0.00001	2.90792
R12	2.06204	0.00000	-0.00001	0.00000	-0.00001	2.06203
R13	2.06123	0.00000	0.00000	0.00000	-0.00001	2.06123
R14	2.07221	0.00000	-0.00001	0.00000	-0.00001	2.07221
R15	2.07145	0.00000	-0.00001	0.00000	-0.00001	2.07144
R16	2.65391	0.00000	0.00004	-0.00001	0.00004	2.65395
R17	4.15447	0.00000	-0.00015	-0.00006	-0.00021	4.15426
R18	8.46220	0.00000	-0.00014	0.00032	0.00018	8.46237
R19	2.50679	0.00000	0.00000	0.00000	0.00000	2.50679
R20	2.04637	0.00000	0.00000	0.00000	0.00000	2.04637
R21	2.04299	0.00000	0.00000	0.00000	0.00000	2.04299
R22	2.04580	0.00000	0.00000	0.00000	0.00000	2.04580
R23	1.84644	0.00000	-0.00003	0.00000	-0.00003	1.84641
R24	3.41820	0.00000	0.00004	0.00000	0.00003	3.41824
R25	2.77432	0.00000	0.00001	-0.00001	0.00000	2.77432
R26	2.74080	0.00000	-0.00003	0.00001	-0.00002	2.74079
R27	2.05486	0.00000	0.00000	0.00000	0.00000	2.05485
R28	2.05334	0.00000	0.00000	0.00000	0.00000	2.05334
R29	2.73604	0.00000	-0.00004	0.00001	-0.00003	2.73600
R30	2.05780	0.00000	0.00000	0.00000	0.00000	2.05780
R31	2.84187	0.00000	0.00000	0.00000	0.00000	2.84186
R32	2.06791	0.00000	0.00001	0.00000	0.00000	2.06791
R33	2.06815	0.00000	0.00000	0.00000	0.00000	2.06814
R34	2.06319	0.00000	0.00000	0.00000	0.00000	2.06319
A1	1.87431	0.00000	0.00000	-0.00001	-0.00001	1.87430
A2	2.27810	0.00000	0.00000	0.00001	0.00001	2.27811
A3	2.13074	0.00000	0.00000	0.00000	0.00000	2.13073
A4	1.86186	0.00000	-0.00001	0.00001	0.00000	1.86187
A5	2.27709	0.00000	0.00001	-0.00001	0.00000	2.27709
A6	2.14422	0.00000	0.00000	0.00000	-0.00001	2.14421
A7	1.89725	0.00000	0.00001	-0.00001	0.00000	1.89724
A8	2.24845	0.00000	0.00001	0.00001	0.00002	2.24847
A9	2.13747	0.00000	-0.00001	0.00000	-0.00001	2.13746
A10	1.88928	0.00000	0.00000	0.00001	0.00001	1.88929
A11	2.23459	0.00000	-0.00002	-0.00002	-0.00004	2.23454
A12	2.15932	0.00000	0.00002	0.00001	0.00004	2.15935
A13	1.90205	0.00000	0.00000	0.00000	0.00000	1.90206
A14	2.21203	0.00000	0.00001	0.00001	0.00002	2.21205
A15	2.16792	0.00000	-0.00002	0.00000	-0.00003	2.16789
A16	1.95083	0.00000	-0.00001	0.00001	0.00000	1.95084
A17	1.86532	0.00000	0.00003	-0.00001	0.00002	1.86535
A18	1.88390	0.00000	-0.00002	0.00000	-0.00001	1.88388

A19	1.92520	0.00000	0.00001	0.00001	0.00003	1.92522
A20	1.92098	0.00000	0.00000	-0.00001	-0.00001	1.92097
A21	1.91634	0.00000	-0.00002	-0.00001	-0.00003	1.91631
A22	1.91296	0.00000	-0.00001	0.00001	0.00000	1.91296
A23	1.90256	0.00000	0.00001	0.00001	0.00001	1.90257
A24	1.91418	0.00000	-0.00003	0.00001	-0.00002	1.91416
A25	1.88695	0.00000	0.00003	-0.00001	0.00003	1.88698
A26	1.88654	0.00000	0.00002	0.00000	0.00002	1.88656
A27	1.96011	0.00000	-0.00002	-0.00002	-0.00004	1.96008
A28	1.78653	-0.00001	-0.00050	-0.00024	-0.00075	1.78578
A29	2.83633	0.00001	0.00041	0.00019	0.00059	2.83693
A30	2.17702	0.00000	-0.00001	0.00000	0.00000	2.17701
A31	1.95555	0.00000	-0.00001	0.00000	-0.00001	1.95554
A32	2.15062	0.00000	0.00001	0.00000	0.00001	2.15063
A33	2.07969	0.00000	0.00000	0.00000	0.00000	2.07969
A34	2.15744	0.00000	0.00000	0.00000	0.00000	2.15744
A35	2.04605	0.00000	0.00000	0.00000	0.00000	2.04605
A36	1.91274	-0.00001	-0.00005	-0.00004	-0.00010	1.91264
A37	3.05330	-0.00001	0.00020	0.00007	0.00027	3.05357
A38	2.07432	0.00000	0.00001	-0.00002	-0.00001	2.07431
A39	2.08781	0.00000	-0.00001	0.00000	-0.00001	2.08780
A40	2.00174	0.00000	0.00001	0.00001	0.00003	2.00177
A41	1.98454	0.00000	-0.00002	0.00002	0.00000	1.98454
A42	2.04016	0.00000	0.00000	0.00000	0.00001	2.04017
A43	2.04574	0.00000	0.00002	-0.00001	0.00002	2.04575
A44	2.13294	0.00000	-0.00004	0.00000	-0.00003	2.13291
A45	1.94925	0.00000	0.00003	0.00000	0.00003	1.94929
A46	2.04638	0.00000	-0.00005	0.00001	-0.00003	2.04634
A47	2.02221	0.00000	0.00002	0.00000	0.00001	2.02223
A48	1.43219	0.00000	0.00042	0.00009	0.00051	1.43271
A49	1.00015	0.00000	0.00000	-0.00001	0.00000	1.00014
A50	2.37573	0.00000	0.00019	0.00011	0.00029	2.37602
A51	2.35222	0.00000	0.00066	-0.00001	0.00065	2.35287
A52	1.93136	0.00000	0.00001	0.00000	0.00000	1.93136
A53	1.91239	0.00000	0.00003	0.00000	0.00002	1.91242
A54	1.93752	0.00000	-0.00001	0.00000	-0.00001	1.93752
A55	1.88375	0.00000	-0.00001	0.00000	-0.00001	1.88374
A56	1.91362	0.00000	-0.00002	0.00000	-0.00002	1.91361
A57	1.88378	0.00000	0.00001	0.00000	0.00001	1.88379
A58	3.78442	0.00000	0.00107	0.00009	0.00116	3.78558
A59	5.04120	0.00000	-0.00015	-0.00014	-0.00029	5.04091
D1	0.00431	0.00000	0.00003	0.00001	0.00004	0.00435
D2	-3.13134	0.00000	0.00009	-0.00002	0.00007	-3.13127
D3	3.13645	0.00000	-0.00010	0.00005	-0.00005	3.13641

D4	0.00081	0.00000	-0.00004	0.00002	-0.00002	0.00079
D5	-0.00676	0.00000	-0.00005	0.00002	-0.00003	-0.00679
D6	-3.09752	0.00000	0.00007	-0.00005	0.00002	-3.09749
D7	-3.13988	0.00000	0.00007	-0.00002	0.00005	-3.13983
D8	0.05255	0.00000	0.00019	-0.00009	0.00010	0.05265
D9	-0.00046	0.00000	0.00000	-0.00004	-0.00004	-0.00050
D10	-3.13649	0.00000	0.00012	-0.00002	0.00010	-3.13639
D11	3.13575	0.00000	-0.00006	-0.00001	-0.00006	3.13568
D12	-0.00028	0.00000	0.00006	0.00001	0.00008	-0.00020
D13	-0.00375	0.00000	-0.00003	0.00005	0.00002	-0.00373
D14	3.13751	0.00000	-0.00002	0.00014	0.00012	3.13763
D15	3.13270	0.00000	-0.00014	0.00003	-0.00011	3.13260
D16	-0.00922	0.00000	-0.00013	0.00012	-0.00001	-0.00923
D17	0.00272	0.00000	-0.00012	-0.00008	-0.00020	0.00252
D18	-3.13915	0.00000	-0.00012	-0.00012	-0.00023	-3.13939
D19	-3.13262	0.00000	0.00001	-0.00006	-0.00004	-3.13267
D20	0.00869	0.00000	0.00002	-0.00010	-0.00008	0.00861
D21	0.00648	0.00000	0.00005	-0.00005	0.00000	0.00648
D22	3.09881	0.00000	-0.00007	0.00003	-0.00004	3.09876
D23	-3.13480	0.00000	0.00004	-0.00013	-0.00009	-3.13490
D24	-0.04247	0.00000	-0.00008	-0.00006	-0.00014	-0.04261
D25	-3.11158	0.00000	-0.00244	-0.00056	-0.00300	-3.11458
D26	0.02963	0.00000	-0.00243	-0.00046	-0.00289	0.02675
D27	1.41022	0.00000	0.00060	0.00022	0.00081	1.41103
D28	-2.76503	0.00000	0.00063	0.00023	0.00086	-2.76417
D29	-0.70467	0.00000	0.00062	0.00021	0.00083	-0.70383
D30	-1.67324	0.00000	0.00074	0.00013	0.00087	-1.67237
D31	0.43470	0.00000	0.00077	0.00015	0.00092	0.43562
D32	2.49507	0.00000	0.00076	0.00013	0.00088	2.49595
D33	-0.93905	0.00000	0.00013	-0.00010	0.00003	-0.93902
D34	1.12305	0.00000	0.00017	-0.00010	0.00007	1.12313
D35	-3.00756	0.00000	0.00014	-0.00012	0.00002	-3.00754
D36	-3.01177	0.00000	0.00009	-0.00011	-0.00002	-3.01179
D37	-0.94967	0.00000	0.00013	-0.00010	0.00003	-0.94964
D38	1.20291	0.00000	0.00010	-0.00012	-0.00003	1.20288
D39	1.15419	0.00000	0.00011	-0.00010	0.00001	1.15420
D40	-3.06689	0.00000	0.00015	-0.00009	0.00005	-3.06683
D41	-0.91432	0.00000	0.00011	-0.00011	0.00000	-0.91432
D42	-1.63682	0.00000	-0.00005	-0.00022	-0.00027	-1.63709
D43	2.56157	0.00000	-0.00003	-0.00024	-0.00027	2.56130
D44	0.48149	0.00000	-0.00007	-0.00023	-0.00030	0.48119
D45	0.43430	0.00000	0.00255	0.00068	0.00322	0.43752
D46	-0.26678	0.00000	-0.00013	-0.00031	-0.00043	-0.26721
D47	2.57143	0.00000	-0.00070	-0.00024	-0.00093	2.57050

D48	-3.14146	0.00000	0.00001	-0.00006	-0.00004	-3.14150
D49	0.00064	0.00000	-0.00001	-0.00002	-0.00002	0.00062
D50	0.00044	0.00000	0.00001	-0.00002	-0.00001	0.00044
D51	-3.14064	0.00000	-0.00001	0.00003	0.00002	-3.14063
D52	-1.94122	0.00000	0.00411	0.00088	0.00499	-1.93623
D53	2.44633	0.00000	-0.00435	-0.00066	-0.00501	2.44131
D54	2.07515	0.00000	-0.00513	-0.00062	-0.00575	2.06940
D55	-2.59488	0.00000	-0.00420	-0.00053	-0.00472	-2.59960
D56	-2.72930	0.00000	0.00004	0.00003	0.00007	-2.72924
D57	-0.03026	0.00000	0.00005	0.00001	0.00006	-0.03020
D58	-0.02170	0.00000	0.00005	-0.00002	0.00003	-0.02167
D59	2.67735	0.00000	0.00007	-0.00004	0.00003	2.67737
D60	-0.17048	0.00000	0.00000	0.00007	0.00006	-0.17042
D61	0.27054	0.00000	0.00097	0.00002	0.00099	0.27154
D62	-2.58270	0.00000	-0.00001	0.00003	0.00002	-2.58268
D63	-2.14168	0.00000	0.00097	-0.00002	0.00095	-2.14072
D64	2.14202	0.00000	-0.00033	-0.00014	-0.00046	2.14155
D65	-0.25127	0.00000	-0.00034	-0.00014	-0.00049	-0.25175
D66	2.48836	0.00000	0.00002	0.00006	0.00008	2.48844
D67	-1.71966	0.00000	0.00003	0.00006	0.00009	-1.71957
D68	0.35935	0.00000	0.00004	0.00006	0.00011	0.35946
D69	1.27224	0.00000	0.00006	0.00005	0.00011	1.27235
D70	-2.93578	0.00000	0.00006	0.00005	0.00012	-2.93566
D71	-0.85676	0.00000	0.00008	0.00005	0.00013	-0.85663
D72	-1.09025	0.00000	0.00003	0.00004	0.00008	-1.09018
D73	0.98491	0.00000	0.00004	0.00004	0.00008	0.98500
D74	3.06393	0.00000	0.00006	0.00004	0.00010	3.06403

Item	Value	Threshold	Converged?
Maximum Force	0.000012	0.000450	YES
RMS Force	0.000002	0.000300	YES
Maximum Displacement	0.002347	0.001800	NO
RMS Displacement	0.000628	0.001200	YES

Predicted change in Energy=-6.413508D-09

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.376068	-1.909799	-0.256212
2	6	0	-2.507435	-1.169551	-0.136119
3	7	0	-2.108951	0.112172	0.230533
4	6	0	-0.765323	0.135640	0.327875

5	7	0	-0.305080	-1.081088	0.041573
6	6	0	1.128159	-1.436688	-0.008119
7	6	0	1.682978	-1.371965	-1.441961
8	1	0	-1.242247	-2.945467	-0.517390
9	1	0	-3.537649	-1.443013	-0.272918
10	1	0	1.653038	-0.727050	0.633433
11	1	0	1.237860	-2.446108	0.390355
12	1	0	1.063682	-1.988603	-2.104293
13	1	0	1.634753	-0.336030	-1.797036
14	35	0	1.650507	2.235984	1.021083
15	1	0	-0.113261	0.994533	0.596091
16	6	0	-2.912857	1.256856	0.485879
17	6	0	-4.237157	1.281890	0.413072
18	1	0	-2.316797	2.121141	0.751173
19	1	0	-4.759058	2.204349	0.626313
20	1	0	-4.839227	0.421662	0.149396
21	8	0	2.990699	-1.883469	-1.466442
22	1	0	3.630492	-1.151883	-1.365816
23	6	0	4.838567	1.611984	-1.120641
24	6	0	5.710755	0.751214	-0.312124
25	8	0	4.857127	0.177062	-1.330888
26	1	0	3.922100	1.994362	-0.677611
27	1	0	5.259815	2.179876	-1.945693
28	1	0	6.761625	0.702528	-0.593362
29	6	0	5.398294	0.412083	1.119281
30	1	0	5.676385	-0.622933	1.340379
31	1	0	5.972356	1.064631	1.784396
32	1	0	4.338385	0.561297	1.334549

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357343	0.000000			
3	N	2.205086	1.391416	0.000000		
4	C	2.213140	2.225706	1.347354	0.000000	
5	N	1.386525	2.211281	2.171066	1.331999	0.000000
6	C	2.560573	3.647641	3.596498	2.484025	1.477530
7	C	3.324609	4.393831	4.402115	3.376295	2.497570
8	H	1.076443	2.213581	3.264923	3.230348	2.160238
9	H	2.211470	1.074633	2.171000	3.246365	3.267934
10	H	3.371327	4.254122	3.875459	2.585744	2.076022
11	H	2.745596	3.991742	4.215624	3.268343	2.089400
12	H	3.061698	4.159018	4.464333	3.711215	2.702191
13	H	3.730405	4.539947	4.281032	3.240075	2.774625

14	Br	5.289532	5.497751	4.389655	3.275395	3.973251
15	H	3.279671	3.309299	2.212458	1.111225	2.156962
16	C	3.597238	2.537459	1.421889	2.427754	3.530423
17	C	4.338277	3.050101	2.435328	3.657154	4.602489
18	H	4.260078	3.413544	2.085718	2.555086	3.847702
19	H	5.399045	4.127264	3.399546	4.507609	5.565423
20	H	4.194485	2.837382	2.748959	4.087831	4.777905
21	O	4.531446	5.701658	5.733126	4.626454	3.712153
22	H	5.183753	6.259921	6.089939	4.883594	4.180249
23	C	7.195267	7.916436	7.234854	5.973388	5.921189
24	C	7.570150	8.441502	7.864518	6.536674	6.298627
25	O	6.660528	7.581399	7.139222	5.862180	5.487712
26	H	6.594743	7.186270	6.382863	5.141769	5.276805
27	H	7.975884	8.650051	7.956762	6.756501	6.749161
28	H	8.553360	9.467271	8.928294	7.604274	7.315924
29	C	7.292125	8.159543	7.565616	6.220363	5.993287
30	H	7.344536	8.333891	7.898328	6.564769	6.137974
31	H	8.186003	8.977015	8.284273	6.955630	6.859136
32	H	6.425870	7.212763	6.556577	5.219426	5.092247

		6	7	8	9	10
6	C	0.000000				
7	C	1.538803	0.000000			
8	H	2.855625	3.447851	0.000000		
9	H	4.673320	5.350388	2.754270	0.000000	
10	H	1.091180	2.173493	3.824715	5.317641	0.000000
11	H	1.090754	2.170091	2.687805	4.924593	1.785111
12	H	2.168575	1.096564	2.958236	4.982354	3.071482
13	H	2.160627	1.096159	4.089472	5.504733	2.461790
14	Br	3.849756	4.368630	6.130445	6.490486	2.988285
15	H	2.795894	3.602838	4.247122	4.292229	2.466790
16	C	4.881498	5.634621	4.632170	2.873226	4.980467
17	C	6.029484	6.747746	5.263629	2.895685	6.227262
18	H	5.010228	5.745417	5.332393	3.904155	4.887294
19	H	6.951185	7.652947	6.340080	3.950152	7.050399
20	H	6.252038	6.949005	4.971964	2.312892	6.610850
21	O	2.407358	1.404411	4.466136	6.651152	2.745199
22	H	2.861141	1.961389	5.261212	7.256819	2.843906
23	C	4.929425	4.354876	7.623029	8.956150	4.323823
24	C	5.087192	4.691206	7.877298	9.505216	4.420905
25	O	4.273068	3.533702	6.900314	8.614883	3.865509
26	H	4.475090	4.114615	7.148291	8.223574	3.778036
27	H	5.822741	5.065875	8.401548	9.660169	5.301976
28	H	6.054312	5.551243	8.796340	10.525258	5.444848
29	C	4.787801	4.852459	7.618964	9.232045	3.944694

30	H	4.813211	4.924405	7.530799	9.390084	4.086310
31	H	5.738985	5.894501	8.569107	10.047935	4.815739
32	H	4.012512	4.300895	6.846205	8.284510	3.059818

		11	12	13	14	15
11	H	0.000000				
12	H	2.542227	0.000000			
13	H	3.065066	1.775254	0.000000		
14	Br	4.742370	5.287672	3.815403	0.000000	
15	H	3.702143	4.192418	3.248539	2.198339	0.000000
16	C	5.563229	5.749336	5.331954	4.697810	2.814018
17	C	6.623767	6.718046	6.479318	5.995377	4.137944
18	H	5.798753	6.039149	5.305262	3.978133	2.479691
19	H	7.592460	7.677328	7.294310	6.421788	4.800833
20	H	6.724073	6.762606	6.802581	6.794722	4.781472
21	O	2.614709	2.032560	2.083854	4.995376	4.708662
22	H	3.237876	2.798921	2.198758	4.592958	4.740449
23	C	5.631723	5.308630	3.810078	3.891026	5.277216
24	C	5.542845	5.684519	4.472232	4.524112	5.899425
25	O	4.789863	4.436044	3.296097	4.478096	5.393169
26	H	5.297496	5.105878	3.451927	2.846766	4.348116
27	H	6.559952	5.916832	4.415083	4.672474	6.060994
28	H	6.433784	6.480096	5.367705	5.575074	6.983131
29	C	5.099979	5.911310	4.819629	4.169192	5.566885
30	H	4.891525	5.916743	5.124498	4.948035	6.057240
31	H	6.056738	6.967009	5.796836	4.542366	6.200945
32	H	4.421452	5.389926	4.233397	3.182377	4.533229

		16	17	18	19	20
16	C	0.000000				
17	C	1.326536	0.000000			
18	H	1.082892	2.122836	0.000000		
19	H	2.079885	1.081103	2.446865	0.000000	
20	H	2.126423	1.082592	3.100486	1.847119	0.000000
21	O	6.966001	8.111348	7.008868	9.008252	8.320595
22	H	7.214305	8.425413	7.110877	9.252968	8.746888
23	C	7.924114	9.210320	7.413647	9.773287	9.833085
24	C	8.675203	9.988416	8.212727	10.611750	10.565213
25	O	8.052282	9.325666	7.718783	10.020556	9.811746
26	H	6.972393	8.262607	6.401667	8.781049	8.939697
27	H	8.576542	9.826628	8.042486	10.343773	10.462856
28	H	9.750263	11.059917	9.286441	11.682003	11.627998
29	C	8.377951	9.700371	7.910689	10.326036	10.283365
30	H	8.833960	10.137384	8.471603	10.835215	10.634271
31	H	8.981653	10.303488	8.419847	10.853725	10.953400
32	H	7.333795	8.654957	6.860386	9.271714	9.254872

		21	22	23	24	25
21	O	0.000000				
22	H	0.977077	0.000000			
23	C	3.968928	3.026304	0.000000		
24	C	3.958878	3.009907	1.468107	0.000000	
25	O	2.783473	1.808853	1.450362	1.447830	0.000000
26	H	4.065383	3.233809	1.087382	2.208683	2.145607
27	H	4.678605	3.753874	1.086583	2.216522	2.133402
28	H	4.655055	3.720150	2.191640	1.088942	2.108831
29	C	4.213317	3.427364	2.601982	1.503849	2.520204
30	H	4.084129	3.433506	3.428325	2.149471	2.906345
31	H	5.305612	4.507893	3.166120	2.135898	3.425859
32	H	3.954578	3.275373	2.716999	2.151975	2.742496

		26	27	28	29	30
26	H	0.000000				
27	H	1.852547	0.000000			
28	H	3.120711	2.503356	0.000000		
29	C	2.812753	3.540952	2.208207	0.000000	
30	H	3.741662	4.339071	2.583398	1.094292	0.000000
31	H	3.336080	3.957911	2.531363	1.094415	1.769921
32	H	2.505146	3.772111	3.099819	1.091792	1.786806

		31	32
31	H	0.000000	
32	H	1.767928	0.000000

Stoichiometry C10H17BrN2O2
Framework group C1[X(C10H17BrN2O2)]
Deg. of freedom 90
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.710549	2.114657	-0.440047
2	6	0	-3.788253	1.349614	-0.130784
3	7	0	-3.320262	0.050194	0.038127
4	6	0	-1.988677	0.040427	-0.167172
5	7	0	-1.603110	1.280680	-0.462694
6	6	0	-0.200893	1.679746	-0.702752
7	6	0	0.455123	2.251578	0.566330
8	1	0	-2.637723	3.167635	-0.651381
9	1	0	-4.824262	1.614583	-0.024418

10	1	0	0.330517	0.786121	-1.033977
11	1	0	-0.195722	2.428048	-1.496327
12	1	0	-0.161731	3.066187	0.964271
13	1	0	0.510108	1.463285	1.326024
14	35	0	0.525370	-2.058879	-0.140750
15	1	0	-1.293625	-0.824757	-0.110783
16	6	0	-4.050989	-1.125247	0.363923
17	6	0	-5.361376	-1.169010	0.565587
18	1	0	-3.411034	-1.996269	0.430517
19	1	0	-5.825486	-2.114477	0.809465
20	1	0	-6.007115	-0.302581	0.499805
21	8	0	1.718943	2.776045	0.250000
22	1	0	2.403755	2.096672	0.405448
23	6	0	3.797622	-0.460135	1.229091
24	6	0	4.544132	0.009608	0.055463
25	8	0	3.722062	0.927865	0.815211
26	1	0	2.884260	-1.030076	1.076328
27	1	0	4.316715	-0.607115	2.172278
28	1	0	5.605242	0.214299	0.189409
29	6	0	4.108602	-0.303439	-1.349484
30	1	0	4.291613	0.549918	-2.009610
31	1	0	4.682986	-1.153489	-1.730590
32	1	0	3.050674	-0.571421	-1.380845

Rotational constants (GHZ): 0.5996872 0.2212997 0.1723265

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.

475 basis functions, 751 primitive gaussians, 492 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1307.2271495218 Hartrees.

NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 475 RedAO= T EigKep= 3.79D-06 NBF= 475

NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000021 0.000008 -0.000011 Ang= 0.00 deg.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3225.52371212 A.U. after 7 cycles
NFock= 7 Conv=0.66D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000001987	-0.000000993	0.000011331
2	6	-0.000000445	0.000000361	0.000007934
3	7	-0.000000480	-0.000001129	0.000004386
4	6	0.000002534	0.000003770	-0.000012543
5	7	-0.000002745	0.000002822	-0.000001378
6	6	-0.000000910	0.000001261	0.000008685
7	6	0.000009644	-0.000007601	0.000002407
8	1	-0.000000386	0.000000381	0.000005695
9	1	-0.000000275	-0.000000068	0.000004538
10	1	0.000000679	0.000001636	0.000002418
11	1	-0.000000881	0.000001734	0.000007392
12	1	-0.000001329	-0.000004789	0.000005055
13	1	-0.000001598	-0.000004344	-0.000000756
14	35	-0.000000867	0.000004873	-0.000002876
15	1	0.000003484	-0.000001831	-0.000002275
16	6	0.000000218	0.000003369	-0.000003268
17	6	0.000000428	0.000003156	-0.000004601
18	1	0.000000755	0.000002582	-0.000004384
19	1	0.000000595	0.000003080	-0.000005934
20	1	0.000000401	0.000001788	-0.000001150
21	8	-0.000011192	-0.000001930	0.000004079
22	1	0.000001768	-0.000005538	0.000007633
23	6	0.000007852	-0.000004255	-0.000013284
24	6	-0.000002490	0.000001308	0.000002676
25	8	-0.000002344	-0.000004508	0.000000087
26	1	-0.000000814	-0.000003264	-0.000004086
27	1	-0.000001369	-0.000003708	-0.000006797
28	1	-0.000000848	-0.000002367	-0.000003602
29	6	0.000002425	0.000001758	-0.000004841
30	1	-0.000000561	0.000003733	0.000002362
31	1	0.000000548	0.000005864	-0.000004196
32	1	0.000000191	0.000002848	-0.000000706

Cartesian Forces: Max 0.000013284 RMS 0.000004306

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000008280 RMS 0.000001662
Search for a local minimum.
Step number 40 out of a maximum of 177
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 24 25 26 27 28
29 30 31 32 33
34 35 36 37 38
39 40
DE= -1.63D-07 DEPred=-6.41D-09 R= 2.55D+01
Trust test= 2.55D+01 RLast= 1.20D-02 DXMaxT set to 1.21D-01
ITU= 0 -1 -1 -1 -1 0 0 1 1 0 1 1 1 1 1 1 1 1 1
ITU= 1 1 1 -1 1 1 1 1 1 1 1 1 1 1 0 1 0 1 0

Eigenvalues ---	0.00003	0.00036	0.00075	0.00206	0.00215
Eigenvalues ---	0.00237	0.00353	0.00680	0.00960	0.01195
Eigenvalues ---	0.01319	0.01428	0.01751	0.01884	0.02020
Eigenvalues ---	0.02137	0.02200	0.02251	0.02326	0.02402
Eigenvalues ---	0.03003	0.03062	0.03118	0.03474	0.03771
Eigenvalues ---	0.04073	0.04628	0.05159	0.05382	0.05430
Eigenvalues ---	0.05670	0.05898	0.06491	0.08869	0.09353
Eigenvalues ---	0.10355	0.11021	0.11476	0.11578	0.12860
Eigenvalues ---	0.13842	0.14131	0.14264	0.15099	0.15948
Eigenvalues ---	0.15992	0.16001	0.16002	0.16015	0.16019
Eigenvalues ---	0.16050	0.17040	0.18160	0.20116	0.22049
Eigenvalues ---	0.22829	0.23407	0.23872	0.24366	0.25032
Eigenvalues ---	0.27801	0.28376	0.30860	0.31954	0.33109
Eigenvalues ---	0.33198	0.34053	0.34209	0.34467	0.34844
Eigenvalues ---	0.35042	0.35684	0.35689	0.35857	0.36092
Eigenvalues ---	0.36435	0.36669	0.37184	0.37239	0.37544
Eigenvalues ---	0.38170	0.42183	0.42508	0.45115	0.45633
Eigenvalues ---	0.49341	0.53980	0.55036	0.55776	0.60392

Eigenvalue 1 is 3.33D-05 Eigenvector:

	D54	D52	D53	D55	D47
1	0.50762	-0.50295	0.49558	0.48680	0.03404
	D46	A58	A48	D65	D64
1	0.02804	-0.02651	-0.01940	0.01887	0.01855

En-DIIS/RFO-DIIS IScMMF= 0 using points: 40 39 38 37 36

RFO step: Lambda=-1.36933603D-09.

DidBck=F Rises=F RFO-DIIS coefs: 2.20005 -1.31677 -0.46116 0.84540 -0.26752

Iteration 1 RMS(Cart)= 0.00086599 RMS(Int)= 0.00000054

Iteration 2 RMS(Cart)= 0.00000143 RMS(Int)= 0.00000026

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000026

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56501	0.00000	0.00000	0.00000	0.00000	2.56501
R2	2.62015	0.00000	0.00000	0.00000	0.00000	2.62015
R3	2.03418	0.00000	0.00000	0.00000	0.00000	2.03418
R4	2.62939	0.00000	0.00000	0.00000	0.00000	2.62939
R5	2.03076	0.00000	0.00000	0.00000	0.00000	2.03076
R6	2.54613	0.00000	-0.00001	0.00000	0.00000	2.54613
R7	2.68698	0.00000	0.00001	0.00000	0.00000	2.68698
R8	2.51711	0.00000	-0.00002	0.00001	-0.00001	2.51710
R9	2.09991	0.00000	-0.00001	0.00002	0.00001	2.09992
R10	2.79213	0.00000	0.00000	-0.00001	0.00000	2.79212
R11	2.90792	0.00000	0.00000	0.00000	0.00000	2.90791
R12	2.06203	0.00000	0.00000	0.00000	0.00000	2.06203
R13	2.06123	0.00000	-0.00001	0.00000	0.00000	2.06122
R14	2.07221	0.00000	0.00000	0.00000	0.00000	2.07221
R15	2.07144	0.00000	-0.00001	0.00001	0.00000	2.07144
R16	2.65395	-0.00001	0.00001	-0.00001	0.00000	2.65395
R17	4.15426	0.00000	-0.00009	-0.00011	-0.00020	4.15406
R18	8.46237	0.00000	0.00030	-0.00005	0.00025	8.46263
R19	2.50679	0.00000	0.00000	0.00000	0.00000	2.50679
R20	2.04637	0.00000	0.00000	0.00000	0.00000	2.04637
R21	2.04299	0.00000	0.00000	0.00000	0.00000	2.04299
R22	2.04580	0.00000	0.00000	0.00000	0.00000	2.04580
R23	1.84641	0.00000	-0.00002	0.00001	-0.00001	1.84639
R24	3.41824	0.00000	0.00008	-0.00003	0.00005	3.41828
R25	2.77432	0.00000	0.00000	0.00000	0.00000	2.77432
R26	2.74079	0.00000	-0.00002	0.00001	-0.00001	2.74078
R27	2.05485	0.00000	0.00000	0.00001	0.00000	2.05486
R28	2.05334	0.00000	0.00000	0.00000	0.00000	2.05335
R29	2.73600	0.00000	-0.00002	0.00001	-0.00001	2.73599
R30	2.05780	0.00000	0.00000	0.00000	0.00000	2.05780
R31	2.84186	0.00000	-0.00001	0.00000	-0.00001	2.84185
R32	2.06791	0.00000	0.00000	0.00000	0.00000	2.06791
R33	2.06814	0.00000	0.00000	0.00000	0.00000	2.06815
R34	2.06319	0.00000	0.00000	0.00000	0.00000	2.06319
A1	1.87430	0.00000	-0.00001	0.00001	0.00000	1.87430

A2	2.27811	0.00000	0.00001	0.00000	0.00001	2.27812
A3	2.13073	0.00000	0.00000	0.00000	0.00000	2.13073
A4	1.86187	0.00000	0.00000	-0.00001	0.00000	1.86186
A5	2.27709	0.00000	0.00000	0.00000	0.00000	2.27709
A6	2.14421	0.00000	0.00000	0.00000	0.00000	2.14421
A7	1.89724	0.00000	0.00000	0.00001	0.00000	1.89724
A8	2.24847	0.00000	0.00002	0.00000	0.00001	2.24849
A9	2.13746	0.00000	-0.00001	0.00000	-0.00002	2.13744
A10	1.88929	0.00000	0.00000	0.00000	0.00000	1.88929
A11	2.23454	0.00000	-0.00004	0.00002	-0.00002	2.23452
A12	2.15935	0.00000	0.00003	-0.00001	0.00002	2.15938
A13	1.90206	0.00000	0.00001	0.00000	0.00000	1.90206
A14	2.21205	0.00000	0.00003	0.00001	0.00004	2.21209
A15	2.16789	0.00000	-0.00003	-0.00001	-0.00003	2.16786
A16	1.95084	0.00000	0.00000	0.00001	0.00002	1.95085
A17	1.86535	0.00000	0.00001	0.00001	0.00003	1.86537
A18	1.88388	0.00000	-0.00002	0.00000	-0.00002	1.88387
A19	1.92522	0.00000	0.00004	-0.00003	0.00001	1.92523
A20	1.92097	0.00000	-0.00002	0.00001	-0.00001	1.92096
A21	1.91631	0.00000	-0.00002	0.00000	-0.00002	1.91629
A22	1.91296	0.00000	0.00001	-0.00001	-0.00001	1.91296
A23	1.90257	0.00000	0.00003	-0.00002	0.00000	1.90257
A24	1.91416	0.00000	-0.00003	-0.00001	-0.00003	1.91413
A25	1.88698	0.00000	0.00001	-0.00001	-0.00001	1.88697
A26	1.88656	0.00000	0.00002	0.00002	0.00004	1.88660
A27	1.96008	0.00000	-0.00003	0.00003	0.00000	1.96007
A28	1.78578	-0.00001	-0.00066	-0.00005	-0.00071	1.78507
A29	2.83693	0.00001	0.00043	0.00001	0.00044	2.83737
A30	2.17701	0.00000	-0.00001	0.00000	-0.00001	2.17701
A31	1.95554	0.00000	-0.00001	0.00000	-0.00001	1.95553
A32	2.15063	0.00000	0.00002	0.00000	0.00002	2.15065
A33	2.07969	0.00000	0.00000	0.00000	0.00000	2.07969
A34	2.15744	0.00000	0.00000	0.00000	0.00000	2.15744
A35	2.04605	0.00000	0.00000	0.00000	0.00000	2.04605
A36	1.91264	0.00000	-0.00010	0.00006	-0.00004	1.91260
A37	3.05357	-0.00001	0.00011	-0.00001	0.00009	3.05366
A38	2.07431	0.00000	-0.00004	0.00000	-0.00004	2.07428
A39	2.08780	0.00000	0.00001	0.00002	0.00002	2.08783
A40	2.00177	0.00000	-0.00001	0.00000	-0.00001	2.00176
A41	1.98454	0.00000	0.00003	-0.00001	0.00002	1.98457
A42	2.04017	0.00000	0.00001	-0.00001	0.00000	2.04017
A43	2.04575	0.00000	-0.00001	0.00001	-0.00001	2.04575
A44	2.13291	0.00000	-0.00001	0.00002	0.00000	2.13291
A45	1.94929	0.00000	0.00004	-0.00004	-0.00001	1.94928

A46	2.04634	0.00000	0.00000	0.00001	0.00000	2.04635
A47	2.02223	0.00000	0.00001	0.00000	0.00001	2.02223
A48	1.43271	0.00000	0.00044	0.00002	0.00046	1.43316
A49	1.00014	0.00000	0.00001	0.00001	0.00002	1.00016
A50	2.37602	0.00000	0.00025	-0.00008	0.00017	2.37619
A51	2.35287	0.00000	0.00060	0.00019	0.00079	2.35366
A52	1.93136	0.00000	0.00001	0.00000	0.00002	1.93138
A53	1.91242	0.00000	0.00000	-0.00001	-0.00001	1.91241
A54	1.93752	0.00000	0.00002	-0.00001	0.00001	1.93753
A55	1.88374	0.00000	-0.00001	0.00001	0.00000	1.88374
A56	1.91361	0.00000	-0.00003	0.00001	-0.00002	1.91359
A57	1.88379	0.00000	0.00000	0.00000	0.00000	1.88378
A58	3.78558	0.00000	0.00104	0.00021	0.00124	3.78682
A59	5.04091	0.00000	-0.00021	0.00020	-0.00001	5.04090
D1	0.00435	0.00000	0.00003	-0.00002	0.00001	0.00436
D2	-3.13127	0.00000	0.00001	0.00002	0.00003	-3.13124
D3	3.13641	0.00000	0.00004	-0.00001	0.00003	3.13644
D4	0.00079	0.00000	0.00001	0.00003	0.00004	0.00083
D5	-0.00679	0.00000	-0.00001	-0.00001	-0.00003	-0.00682
D6	-3.09749	0.00000	-0.00013	-0.00003	-0.00015	-3.09765
D7	-3.13983	0.00000	-0.00002	-0.00003	-0.00004	-3.13987
D8	0.05265	0.00000	-0.00013	-0.00004	-0.00017	0.05248
D9	-0.00050	0.00000	-0.00004	0.00005	0.00001	-0.00049
D10	-3.13639	0.00000	0.00007	0.00000	0.00007	-3.13632
D11	3.13568	0.00000	-0.00002	0.00001	0.00000	3.13568
D12	-0.00020	0.00000	0.00009	-0.00003	0.00006	-0.00015
D13	-0.00373	0.00000	0.00003	-0.00006	-0.00003	-0.00375
D14	3.13763	0.00000	0.00022	0.00013	0.00035	3.13798
D15	3.13260	0.00000	-0.00007	-0.00001	-0.00008	3.13251
D16	-0.00923	0.00000	0.00012	0.00017	0.00029	-0.00894
D17	0.00252	0.00000	-0.00035	-0.00012	-0.00048	0.00204
D18	-3.13939	0.00000	-0.00037	-0.00011	-0.00048	-3.13986
D19	-3.13267	0.00000	-0.00023	-0.00018	-0.00041	-3.13308
D20	0.00861	0.00000	-0.00024	-0.00017	-0.00041	0.00820
D21	0.00648	0.00000	-0.00001	0.00004	0.00003	0.00651
D22	3.09876	0.00000	0.00010	0.00006	0.00016	3.09892
D23	-3.13490	0.00000	-0.00019	-0.00013	-0.00032	-3.13522
D24	-0.04261	0.00000	-0.00008	-0.00012	-0.00020	-0.04281
D25	-3.11458	0.00000	-0.00233	-0.00091	-0.00325	-3.11782
D26	0.02675	0.00000	-0.00212	-0.00070	-0.00282	0.02393
D27	1.41103	0.00000	0.00056	0.00021	0.00077	1.41180
D28	-2.76417	0.00000	0.00062	0.00019	0.00081	-2.76336
D29	-0.70383	0.00000	0.00060	0.00019	0.00079	-0.70305
D30	-1.67237	0.00000	0.00043	0.00020	0.00063	-1.67174

D31	0.43562	0.00000	0.00049	0.00018	0.00067	0.43628
D32	2.49595	0.00000	0.00047	0.00018	0.00064	2.49660
D33	-0.93902	0.00000	0.00001	0.00002	0.00003	-0.93899
D34	1.12313	0.00000	0.00003	-0.00001	0.00002	1.12315
D35	-3.00754	0.00000	0.00000	0.00000	0.00000	-3.00754
D36	-3.01179	0.00000	-0.00003	0.00001	-0.00002	-3.01181
D37	-0.94964	0.00000	-0.00001	-0.00002	-0.00003	-0.94967
D38	1.20288	0.00000	-0.00005	0.00000	-0.00005	1.20283
D39	1.15420	0.00000	-0.00002	0.00003	0.00001	1.15421
D40	-3.06683	0.00000	0.00000	0.00000	0.00000	-3.06683
D41	-0.91432	0.00000	-0.00004	0.00002	-0.00002	-0.91434
D42	-1.63709	0.00000	-0.00035	0.00011	-0.00024	-1.63733
D43	2.56130	0.00000	-0.00036	0.00012	-0.00024	2.56106
D44	0.48119	0.00000	-0.00036	0.00010	-0.00026	0.48094
D45	0.43752	0.00000	0.00262	0.00080	0.00343	0.44095
D46	-0.26721	0.00000	-0.00093	-0.00007	-0.00099	-0.26820
D47	2.57050	0.00000	-0.00142	-0.00035	-0.00176	2.56874
D48	-3.14150	0.00000	-0.00004	0.00001	-0.00003	-3.14153
D49	0.00062	0.00000	-0.00003	-0.00001	-0.00004	0.00058
D50	0.00044	0.00000	-0.00003	0.00000	-0.00002	0.00041
D51	-3.14063	0.00000	-0.00001	-0.00002	-0.00003	-3.14066
D52	-1.93623	0.00000	0.00738	0.00047	0.00785	-1.92838
D53	2.44131	0.00000	-0.00701	-0.00054	-0.00755	2.43376
D54	2.06940	0.00000	-0.00772	-0.00086	-0.00858	2.06082
D55	-2.59960	0.00000	-0.00680	-0.00074	-0.00754	-2.60714
D56	-2.72924	0.00000	0.00006	-0.00006	0.00000	-2.72924
D57	-0.03020	0.00000	0.00001	0.00000	0.00000	-0.03019
D58	-0.02167	0.00000	0.00002	-0.00004	-0.00002	-0.02169
D59	2.67737	0.00000	-0.00004	0.00002	-0.00002	2.67735
D60	-0.17042	0.00000	0.00004	-0.00012	-0.00008	-0.17050
D61	0.27154	0.00000	0.00093	0.00026	0.00119	0.27273
D62	-2.58268	0.00000	-0.00001	-0.00009	-0.00010	-2.58278
D63	-2.14072	0.00000	0.00087	0.00029	0.00117	-2.13956
D64	2.14155	0.00000	-0.00036	0.00007	-0.00028	2.14127
D65	-0.25175	0.00000	-0.00041	0.00012	-0.00029	-0.25204
D66	2.48844	0.00000	0.00021	0.00000	0.00020	2.48864
D67	-1.71957	0.00000	0.00020	0.00000	0.00021	-1.71936
D68	0.35946	0.00000	0.00021	-0.00001	0.00021	0.35966
D69	1.27235	0.00000	0.00021	-0.00001	0.00020	1.27255
D70	-2.93566	0.00000	0.00021	-0.00001	0.00021	-2.93545
D71	-0.85663	0.00000	0.00022	-0.00001	0.00021	-0.85642
D72	-1.09018	0.00000	0.00015	0.00005	0.00020	-1.08997
D73	0.98500	0.00000	0.00015	0.00006	0.00021	0.98520
D74	3.06403	0.00000	0.00016	0.00005	0.00021	3.06423

Item	Value	Threshold	Converged?
Maximum Force	0.000008	0.000450	YES
RMS Force	0.000002	0.000300	YES
Maximum Displacement	0.003885	0.001800	NO
RMS Displacement	0.000867	0.001200	YES

Predicted change in Energy=-1.185284D-08

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.376464	-1.910028	-0.256291
2	6	0	-2.507629	-1.169482	-0.136128
3	7	0	-2.108771	0.112177	0.230344
4	6	0	-0.765127	0.135316	0.327505
5	7	0	-0.305233	-1.081559	0.041293
6	6	0	1.127915	-1.437525	-0.008349
7	6	0	1.683017	-1.372186	-1.442051
8	1	0	-1.242929	-2.945749	-0.517405
9	1	0	-3.537931	-1.442700	-0.272759
10	1	0	1.652901	-0.728415	0.633698
11	1	0	1.237250	-2.447195	0.389586
12	1	0	1.063651	-1.988276	-2.104828
13	1	0	1.635165	-0.336046	-1.796575
14	35	0	1.650465	2.235130	1.023139
15	1	0	-0.112851	0.994013	0.595849
16	6	0	-2.912342	1.257084	0.485757
17	6	0	-4.236618	1.282570	0.412702
18	1	0	-2.316033	2.121113	0.751328
19	1	0	-4.758258	2.205153	0.626041
20	1	0	-4.838919	0.422598	0.148714
21	8	0	2.990598	-1.884044	-1.466522
22	1	0	3.630547	-1.152645	-1.365595
23	6	0	4.837527	1.611843	-1.120557
24	6	0	5.710529	0.751728	-0.312217
25	8	0	4.856601	0.176861	-1.330318
26	1	0	3.921145	1.993962	-0.677123
27	1	0	5.258060	2.179657	-1.946029
28	1	0	6.761264	0.703402	-0.594019
29	6	0	5.398999	0.412954	1.119468
30	1	0	5.677845	-0.621800	1.340841
31	1	0	5.972985	1.066124	1.784040

32	1	0	4.339106	0.561580	1.335217

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357344	0.000000			
3	N	2.205085	1.391416	0.000000		
4	C	2.213139	2.225706	1.347352	0.000000	
5	N	1.386526	2.211280	2.171059	1.331993	0.000000
6	C	2.560596	3.647651	3.596483	2.483996	1.477528
7	C	3.325016	4.394092	4.402033	3.375989	2.497581
8	H	1.076443	2.213586	3.264922	3.230345	2.160236
9	H	2.211471	1.074633	2.171002	3.246366	3.267933
10	H	3.371253	4.254079	3.875496	2.585854	2.076040
11	H	2.745397	3.991622	4.215637	3.268444	2.089383
12	H	3.062251	4.159357	4.464213	3.710838	2.702187
13	H	3.730926	4.540314	4.280930	3.239645	2.774652
14	Br	5.289761	5.497729	4.389454	3.275394	3.973562
15	H	3.279682	3.309300	2.212448	1.111230	2.156975
16	C	3.597243	2.537470	1.421891	2.427744	3.530413
17	C	4.338285	3.050111	2.435325	3.657144	4.602482
18	H	4.260069	3.413547	2.085715	2.555059	3.847672
19	H	5.399052	4.127274	3.399545	4.507599	5.565415
20	H	4.194493	2.837387	2.748951	4.087821	4.777901
21	O	4.531730	5.701847	5.733047	4.626210	3.712141
22	H	5.184047	6.260118	6.089874	4.883377	4.180281
23	C	7.194736	7.915566	7.233602	5.972164	5.920497
24	C	7.570572	8.441575	7.864150	6.536309	6.298834
25	O	6.660311	7.580938	7.138365	5.861222	5.487209
26	H	6.594157	7.185346	6.381575	5.140524	5.276099
27	H	7.974814	8.648607	7.954953	6.754781	6.747978
28	H	8.553754	9.467299	8.927858	7.603847	7.316084
29	C	7.293549	8.160601	7.566216	6.220991	5.994522
30	H	7.346675	8.335669	7.899577	6.565969	6.139822
31	H	8.187480	8.978073	8.284852	6.956295	6.860446
32	H	6.427245	7.213821	6.557273	5.220189	5.093528

		6	7	8	9	10
6	C	0.000000				
7	C	1.538801	0.000000			
8	H	2.855657	3.448512	0.000000		
9	H	4.673335	5.350749	2.754277	0.000000	
10	H	1.091179	2.173495	3.824583	5.317575	0.000000
11	H	1.090752	2.170080	2.687466	4.924435	1.785094
12	H	2.168567	1.096565	2.959220	4.982839	3.071480

13	H	2.160628	1.096159	4.090263	5.505236	2.461807
14	Br	3.850379	4.369318	6.130783	6.490395	2.989024
15	H	2.795878	3.602370	4.247132	4.292228	2.466996
16	C	4.881469	5.634432	4.632178	2.873246	4.980515
17	C	6.029463	6.747586	5.263644	2.895706	6.227306
18	H	5.010169	5.745124	5.332385	3.904171	4.887339
19	H	6.951158	7.652737	6.340094	3.950174	7.050450
20	H	6.252027	6.948916	4.971983	2.312909	6.610883
21	O	2.407330	1.404409	4.466631	6.651432	2.745148
22	H	2.861195	1.961355	5.261693	7.257099	2.843980
23	C	4.929186	4.354161	7.622820	8.955293	4.323894
24	C	5.087781	4.691310	7.878072	9.505319	4.421530
25	O	4.272814	3.533223	6.900419	8.614497	3.865304
26	H	4.474874	4.114034	7.148000	8.222649	3.778163
27	H	5.822088	5.064634	8.400811	9.658714	5.301797
28	H	6.054849	5.551200	8.797118	10.525321	5.445435
29	C	4.789405	4.853517	7.620725	9.233118	3.946131
30	H	4.815348	4.926074	7.533321	9.391917	4.087981
31	H	5.740698	5.895493	8.570950	10.048986	4.817341
32	H	4.014142	4.302031	6.847823	8.285555	3.061358

		11	12	13	14	15
11	H	0.000000				
12	H	2.542213	0.000000			
13	H	3.065059	1.775250	0.000000		
14	Br	4.743026	5.288259	3.816014	0.000000	
15	H	3.702327	4.191880	3.247816	2.198233	0.000000
16	C	5.563276	5.749088	5.331690	4.697292	2.813979
17	C	6.623814	6.717831	6.479094	5.994810	4.137906
18	H	5.798803	6.038789	5.304848	3.977434	2.479625
19	H	7.592520	7.677052	7.294013	6.421083	4.800790
20	H	6.724103	6.762478	6.802460	6.794262	4.781440
21	O	2.614672	2.032590	2.083850	4.996195	4.708289
22	H	3.237961	2.798874	2.198664	4.593886	4.740087
23	C	5.631902	5.307709	3.808725	3.891181	5.275794
24	C	5.543994	5.684589	4.471595	4.524133	5.898732
25	O	4.789931	4.435555	3.295166	4.478229	5.391967
26	H	5.297644	5.105079	3.450769	2.846935	4.346663
27	H	6.559709	5.915230	4.413215	4.672663	6.059173
28	H	6.434942	6.480005	5.366888	5.575093	6.982385
29	C	5.102288	5.912464	4.819829	4.169066	5.567072
30	H	4.894470	5.918671	5.125260	4.948007	6.057889
31	H	6.059298	6.968085	5.796858	4.541996	6.201160
32	H	4.423624	5.391129	4.233810	3.182287	4.533606

		16	17	18	19	20

16	C	0.000000				
17	C	1.326535	0.000000			
18	H	1.082893	2.122845	0.000000		
19	H	2.079885	1.081102	2.446880	0.000000	
20	H	2.126421	1.082593	3.100492	1.847120	0.000000
21	O	6.965829	8.111201	7.008601	9.008059	8.320513
22	H	7.214131	8.425253	7.110603	9.252755	8.746792
23	C	7.922535	9.208660	7.411932	9.771475	9.831529
24	C	8.674448	9.987645	8.211702	10.610762	10.564641
25	O	8.051179	9.324556	7.717516	10.019322	9.810761
26	H	6.970783	8.260926	6.399924	8.779230	8.938116
27	H	8.574391	9.824322	8.040277	10.341316	10.460602
28	H	9.749417	11.059039	9.285322	11.680890	11.627328
29	C	8.378098	9.700560	7.910440	10.325954	10.283843
30	H	8.834743	10.138276	8.471906	10.835813	10.635519
31	H	8.981705	10.303563	8.419460	10.853475	10.953798
32	H	7.334085	8.655282	6.860317	9.271801	9.255444

		21	22	23	24	25
21	O	0.000000				
22	H	0.977069	0.000000			
23	C	3.968886	3.026423	0.000000		
24	C	3.959512	3.010410	1.468109	0.000000	
25	O	2.783495	1.808878	1.450357	1.447824	0.000000
26	H	4.065464	3.234127	1.087385	2.208664	2.145599
27	H	4.678138	3.753657	1.086584	2.216540	2.133416
28	H	4.655541	3.720435	2.191637	1.088941	2.108821
29	C	4.214729	3.428420	2.601980	1.503842	2.520196
30	H	4.086054	3.434824	3.428378	2.149477	2.906439
31	H	5.307002	4.508897	3.166032	2.135889	3.425832
32	H	3.955918	3.276432	2.717040	2.151976	2.742424

		26	27	28	29	30
26	H	0.000000				
27	H	1.852551	0.000000			
28	H	3.120694	2.503374	0.000000		
29	C	2.812717	3.540956	2.208204	0.000000	
30	H	3.741709	4.339112	2.583339	1.094293	0.000000
31	H	3.335903	3.957838	2.531425	1.094416	1.769921
32	H	2.505179	3.772165	3.099825	1.091792	1.786797

		31	32
31	H	0.000000	
32	H	1.767927	0.000000

Stoichiometry C10H17BrN2O2

Framework group C1[X(C10H17BrN2O2)]

Deg. of freedom 90

Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.710938	2.114512	-0.440734
2	6	0	-3.788409	1.349262	-0.131165
3	7	0	-3.319982	0.050096	0.038487
4	6	0	-1.988375	0.040680	-0.166671
5	7	0	-1.603214	1.280897	-0.462843
6	6	0	-0.201120	1.680234	-0.703157
7	6	0	0.455077	2.252082	0.565821
8	1	0	-2.638443	3.167406	-0.652601
9	1	0	-4.824520	1.613930	-0.025051
10	1	0	0.330399	0.786755	-1.034602
11	1	0	-0.196268	2.428609	-1.496662
12	1	0	-0.161852	3.066532	0.963971
13	1	0	0.510387	1.463739	1.325439
14	35	0	0.525336	-2.059040	-0.141452
15	1	0	-1.293093	-0.824310	-0.110040
16	6	0	-4.050328	-1.125451	0.364768
17	6	0	-5.360656	-1.169492	0.566752
18	1	0	-3.410124	-1.996285	0.431436
19	1	0	-5.824473	-2.115016	0.810967
20	1	0	-6.006624	-0.303236	0.500923
21	8	0	1.718729	2.776780	0.249212
22	1	0	2.403684	2.097564	0.404667
23	6	0	3.796585	-0.459333	1.230100
24	6	0	4.544042	0.009421	0.056678
25	8	0	3.721458	0.928338	0.815059
26	1	0	2.883303	-1.029328	1.077042
27	1	0	4.314917	-0.605629	2.173813
28	1	0	5.605061	0.214139	0.191292
29	6	0	4.109581	-0.304705	-1.348353
30	1	0	4.293354	0.548032	-2.009068
31	1	0	4.684051	-1.155236	-1.728257
32	1	0	3.051607	-0.572430	-1.380363

Rotational constants (GHZ): 0.5995227 0.2213214 0.1723301
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.
475 basis functions, 751 primitive gaussians, 492 cartesian basis functions
71 alpha electrons 71 beta electrons
nuclear repulsion energy 1307.2104317328 Hartrees.
NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 475 RedAO= T EigKep= 3.79D-06 NBF= 475
NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475
Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 0.000069 0.000018 -0.000021 Ang= 0.01 deg.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3225.52371243 A.U. after 8 cycles
NFock= 8 Conv=0.50D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000000247	-0.000001178	0.000009915
2	6	0.000000116	0.000001308	0.000005341
3	7	-0.000000817	-0.000000160	0.000004975
4	6	-0.000001491	0.000003952	-0.000008549
5	7	-0.000000121	-0.000000597	-0.000000878
6	6	-0.000002812	0.000000969	0.000006061
7	6	0.000007461	-0.000007447	0.000005675
8	1	-0.000000661	-0.000000340	0.000007138
9	1	-0.000000141	0.000000005	0.000005278
10	1	0.000000174	0.000002719	0.000002859
11	1	-0.000000265	0.000001598	0.000007860
12	1	0.000000443	-0.000005905	0.000004886
13	1	-0.000000847	-0.000004357	-0.000001255
14	35	-0.000000740	0.000004004	-0.000004713
15	1	0.000003576	0.000002364	0.000000474
16	6	0.000000796	0.000002947	-0.000005284

17	6	0.000000086	0.000003172	-0.000004802
18	1	0.000000335	0.000002742	-0.000004400
19	1	0.000000480	0.000003151	-0.000005446
20	1	0.000000217	0.000001895	-0.000000911
21	8	-0.000008038	-0.000004874	0.000000283
22	1	-0.000001009	-0.000002051	0.000009540
23	6	0.000004893	-0.000003417	-0.000008431
24	6	-0.000001627	-0.000000537	0.000002438
25	8	-0.000001733	-0.000005478	-0.000006886
26	1	-0.000000034	-0.000002741	-0.000006041
27	1	-0.000000269	-0.000004919	-0.000006309
28	1	0.000000045	-0.000001540	-0.000003452
29	6	0.000001368	0.000001324	-0.000000677
30	1	0.000000054	0.000004186	0.000000869
31	1	0.000000421	0.000005425	-0.000004139
32	1	0.000000389	0.000003779	-0.000001419

Cartesian Forces: Max 0.000009915 RMS 0.000003905

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000007274 RMS 0.000001200
Search for a local minimum.
Step number 41 out of a maximum of 177
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 24 25 26 27 28
29 30 31 32 33
34 35 36 37 38
39 40 41
DE= -3.02D-07 DEPred=-1.19D-08 R= 2.55D+01
Trust test= 2.55D+01 RLast= 1.72D-02 DXMaxT set to 1.21D-01
ITU= 0 0 -1 -1 -1 -1 0 0 1 1 0 1 1 1 1 1 1 1 1 1
ITU= 1 1 1 1 -1 1 1 1 1 1 1 1 1 1 1 1 0 1 0 1
ITU= 0
Eigenvalues --- 0.00003 0.00033 0.00079 0.00177 0.00207
Eigenvalues --- 0.00236 0.00341 0.00669 0.00887 0.01155
Eigenvalues --- 0.01215 0.01443 0.01763 0.01888 0.01989
Eigenvalues --- 0.02102 0.02184 0.02263 0.02325 0.02400
Eigenvalues --- 0.03017 0.03061 0.03135 0.03467 0.03769

Eigenvalues --- 0.04086 0.04627 0.05174 0.05392 0.05424
Eigenvalues --- 0.05670 0.05883 0.06499 0.08948 0.09354
Eigenvalues --- 0.10329 0.11041 0.11473 0.11584 0.12850
Eigenvalues --- 0.13839 0.14022 0.14171 0.15087 0.15954
Eigenvalues --- 0.15994 0.15999 0.16001 0.16015 0.16019
Eigenvalues --- 0.16055 0.16780 0.18139 0.20050 0.22048
Eigenvalues --- 0.22845 0.23403 0.23861 0.24373 0.25027
Eigenvalues --- 0.27656 0.28374 0.30876 0.32021 0.33106
Eigenvalues --- 0.33220 0.34052 0.34207 0.34471 0.34844
Eigenvalues --- 0.35044 0.35684 0.35689 0.35856 0.36139
Eigenvalues --- 0.36435 0.36670 0.37190 0.37243 0.37592
Eigenvalues --- 0.38271 0.42180 0.42488 0.44676 0.45660
Eigenvalues --- 0.49349 0.54038 0.55075 0.55784 0.60394
Eigenvalue 1 is 3.45D-05 Eigenvector:

	D52	D54	D53	D55	D47
1	-0.50892	0.50253	0.49358	0.48782	0.04187
	D46	A58	A48	D65	D64
1	0.03768	-0.01983	-0.01614	0.01525	0.01486

En-DIIS/RFO-DIIS IScMMF= 0 using points: 41 40 39 38 37
RFO step: Lambda=-6.59631240D-10.
DidBck=F Rises=F RFO-DIIS coefs: 1.33293 -0.11105 -0.67639 0.52719 -0.07267
Iteration 1 RMS(Cart)= 0.00048121 RMS(Int)= 0.00000032
Iteration 2 RMS(Cart)= 0.00000021 RMS(Int)= 0.00000014

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56501	0.00000	0.00000	0.00000	0.00000	2.56501
R2	2.62015	0.00000	0.00000	0.00000	0.00000	2.62015
R3	2.03418	0.00000	0.00000	0.00000	0.00000	2.03418
R4	2.62939	0.00000	0.00000	0.00000	0.00000	2.62939
R5	2.03076	0.00000	0.00000	0.00000	0.00000	2.03076
R6	2.54613	0.00000	0.00000	0.00000	0.00000	2.54612
R7	2.68698	0.00000	0.00000	0.00000	0.00000	2.68699
R8	2.51710	0.00000	0.00000	0.00000	0.00000	2.51710
R9	2.09992	0.00000	0.00000	0.00001	0.00000	2.09992
R10	2.79212	0.00000	0.00001	-0.00001	0.00000	2.79212
R11	2.90791	0.00000	0.00000	0.00000	0.00000	2.90792
R12	2.06203	0.00000	0.00000	0.00000	0.00000	2.06203
R13	2.06122	0.00000	0.00000	0.00000	0.00000	2.06122
R14	2.07221	0.00000	0.00000	0.00000	0.00000	2.07221
R15	2.07144	0.00000	0.00000	0.00000	0.00000	2.07144
R16	2.65395	-0.00001	-0.00001	0.00000	-0.00001	2.65394
R17	4.15406	0.00000	0.00001	-0.00004	-0.00003	4.15403
R18	8.46263	0.00000	0.00025	0.00006	0.00030	8.46293

R19	2.50679	0.00000	0.00000	0.00000	0.00000	2.50679
R20	2.04637	0.00000	0.00000	0.00000	0.00000	2.04637
R21	2.04299	0.00000	0.00000	0.00000	0.00000	2.04299
R22	2.04580	0.00000	0.00000	0.00000	0.00000	2.04580
R23	1.84639	0.00000	0.00000	0.00000	0.00000	1.84639
R24	3.41828	0.00000	0.00003	0.00002	0.00004	3.41833
R25	2.77432	0.00000	0.00000	0.00000	0.00000	2.77432
R26	2.74078	0.00000	0.00000	0.00000	0.00000	2.74077
R27	2.05486	0.00000	0.00000	0.00000	0.00000	2.05486
R28	2.05335	0.00000	0.00000	0.00000	0.00000	2.05335
R29	2.73599	0.00000	0.00000	0.00001	0.00001	2.73600
R30	2.05780	0.00000	0.00000	0.00000	0.00000	2.05780
R31	2.84185	0.00000	-0.00001	0.00000	0.00000	2.84185
R32	2.06791	0.00000	0.00000	0.00000	0.00000	2.06791
R33	2.06815	0.00000	0.00000	0.00000	0.00000	2.06815
R34	2.06319	0.00000	0.00000	0.00000	0.00000	2.06319
A1	1.87430	0.00000	0.00000	0.00000	0.00000	1.87430
A2	2.27812	0.00000	0.00000	0.00000	0.00000	2.27812
A3	2.13073	0.00000	0.00000	0.00000	0.00000	2.13073
A4	1.86186	0.00000	0.00000	0.00000	0.00000	1.86187
A5	2.27709	0.00000	0.00000	0.00000	0.00000	2.27709
A6	2.14421	0.00000	0.00000	0.00000	0.00000	2.14421
A7	1.89724	0.00000	-0.00001	0.00000	0.00000	1.89724
A8	2.24849	0.00000	0.00001	0.00000	0.00001	2.24849
A9	2.13744	0.00000	0.00000	0.00000	-0.00001	2.13744
A10	1.88929	0.00000	0.00000	0.00000	0.00000	1.88929
A11	2.23452	0.00000	-0.00001	0.00001	0.00000	2.23452
A12	2.15938	0.00000	0.00001	0.00000	0.00000	2.15938
A13	1.90206	0.00000	0.00000	0.00000	0.00000	1.90206
A14	2.21209	0.00000	0.00001	0.00001	0.00002	2.21211
A15	2.16786	0.00000	-0.00001	-0.00001	-0.00002	2.16784
A16	1.95085	0.00000	0.00001	0.00000	0.00001	1.95086
A17	1.86537	0.00000	0.00000	0.00000	0.00000	1.86537
A18	1.88387	0.00000	-0.00001	0.00000	0.00000	1.88386
A19	1.92523	0.00000	0.00001	0.00000	0.00001	1.92524
A20	1.92096	0.00000	-0.00001	0.00000	0.00000	1.92096
A21	1.91629	0.00000	0.00000	-0.00001	-0.00001	1.91628
A22	1.91296	0.00000	0.00000	0.00001	0.00001	1.91297
A23	1.90257	0.00000	0.00001	0.00000	0.00001	1.90258
A24	1.91413	0.00000	-0.00001	0.00000	-0.00001	1.91412
A25	1.88697	0.00000	-0.00001	0.00000	-0.00001	1.88696
A26	1.88660	0.00000	0.00002	-0.00001	0.00001	1.88661
A27	1.96007	0.00000	0.00000	-0.00001	-0.00001	1.96006
A28	1.78507	0.00000	-0.00019	-0.00008	-0.00028	1.78480

A29	2.83737	0.00000	0.00006	0.00006	0.00012	2.83749
A30	2.17701	0.00000	0.00000	0.00000	0.00000	2.17700
A31	1.95553	0.00000	0.00000	0.00000	0.00000	1.95553
A32	2.15065	0.00000	0.00000	0.00000	0.00000	2.15065
A33	2.07969	0.00000	0.00000	0.00000	0.00000	2.07969
A34	2.15744	0.00000	0.00000	0.00000	0.00000	2.15744
A35	2.04605	0.00000	0.00000	0.00000	0.00000	2.04605
A36	1.91260	0.00000	-0.00002	-0.00002	-0.00003	1.91256
A37	3.05366	0.00000	-0.00006	0.00001	-0.00005	3.05361
A38	2.07428	0.00000	-0.00003	0.00001	-0.00002	2.07426
A39	2.08783	0.00000	0.00002	-0.00001	0.00001	2.08784
A40	2.00176	0.00000	0.00000	-0.00001	-0.00001	2.00175
A41	1.98457	0.00000	0.00002	0.00000	0.00002	1.98459
A42	2.04017	0.00000	0.00000	0.00000	0.00000	2.04017
A43	2.04575	0.00000	0.00000	-0.00002	-0.00002	2.04573
A44	2.13291	0.00000	0.00001	0.00001	0.00002	2.13293
A45	1.94928	0.00000	-0.00002	0.00001	0.00000	1.94928
A46	2.04635	0.00000	0.00001	0.00000	0.00002	2.04636
A47	2.02223	0.00000	0.00000	0.00000	0.00000	2.02223
A48	1.43316	0.00000	0.00008	0.00002	0.00010	1.43326
A49	1.00016	0.00000	0.00000	0.00001	0.00001	1.00017
A50	2.37619	0.00000	-0.00002	0.00005	0.00004	2.37623
A51	2.35366	0.00000	0.00020	-0.00004	0.00016	2.35382
A52	1.93138	0.00000	0.00001	-0.00001	0.00001	1.93138
A53	1.91241	0.00000	-0.00001	0.00000	-0.00001	1.91240
A54	1.93753	0.00000	0.00001	0.00001	0.00002	1.93754
A55	1.88374	0.00000	0.00000	0.00000	0.00000	1.88374
A56	1.91359	0.00000	-0.00001	0.00000	-0.00001	1.91358
A57	1.88378	0.00000	0.00000	0.00000	-0.00001	1.88378
A58	3.78682	0.00000	0.00028	-0.00002	0.00026	3.78708
A59	5.04090	0.00000	0.00011	-0.00010	0.00001	5.04092
D1	0.00436	0.00000	0.00000	0.00000	0.00000	0.00437
D2	-3.13124	0.00000	-0.00001	0.00002	0.00000	-3.13124
D3	3.13644	0.00000	0.00005	0.00000	0.00004	3.13648
D4	0.00083	0.00000	0.00003	0.00001	0.00004	0.00087
D5	-0.00682	0.00000	0.00000	0.00000	0.00000	-0.00682
D6	-3.09765	0.00000	-0.00012	-0.00002	-0.00014	-3.09779
D7	-3.13987	0.00000	-0.00004	0.00000	-0.00004	-3.13991
D8	0.05248	0.00000	-0.00016	-0.00002	-0.00017	0.05231
D9	-0.00049	0.00000	-0.00001	0.00000	-0.00001	-0.00050
D10	-3.13632	0.00000	0.00001	-0.00003	-0.00003	-3.13634
D11	3.13568	0.00000	0.00001	-0.00001	-0.00001	3.13567
D12	-0.00015	0.00000	0.00002	-0.00005	-0.00003	-0.00017
D13	-0.00375	0.00000	0.00001	0.00000	0.00001	-0.00375

D14	3.13798	0.00000	0.00017	0.00006	0.00023	3.13821
D15	3.13251	0.00000	0.00000	0.00003	0.00002	3.13254
D16	-0.00894	0.00000	0.00016	0.00009	0.00025	-0.00869
D17	0.00204	0.00000	-0.00025	-0.00009	-0.00034	0.00170
D18	-3.13986	0.00000	-0.00026	-0.00009	-0.00034	-3.14021
D19	-3.13308	0.00000	-0.00024	-0.00013	-0.00037	-3.13344
D20	0.00820	0.00000	-0.00024	-0.00012	-0.00037	0.00784
D21	0.00651	0.00000	-0.00001	0.00000	0.00000	0.00651
D22	3.09892	0.00000	0.00011	0.00002	0.00013	3.09905
D23	-3.13522	0.00000	-0.00016	-0.00006	-0.00022	-3.13543
D24	-0.04281	0.00000	-0.00004	-0.00004	-0.00008	-0.04289
D25	-3.11782	0.00000	-0.00086	-0.00030	-0.00115	-3.11898
D26	0.02393	0.00000	-0.00067	-0.00022	-0.00090	0.02303
D27	1.41180	0.00000	0.00019	0.00001	0.00020	1.41200
D28	-2.76336	0.00000	0.00020	0.00001	0.00022	-2.76315
D29	-0.70305	0.00000	0.00020	0.00000	0.00020	-0.70285
D30	-1.67174	0.00000	0.00005	-0.00001	0.00004	-1.67170
D31	0.43628	0.00000	0.00007	-0.00001	0.00006	0.43634
D32	2.49660	0.00000	0.00006	-0.00002	0.00004	2.49664
D33	-0.93899	0.00000	-0.00001	-0.00007	-0.00008	-0.93907
D34	1.12315	0.00000	-0.00002	-0.00006	-0.00008	1.12307
D35	-3.00754	0.00000	-0.00002	-0.00006	-0.00009	-3.00763
D36	-3.01181	0.00000	-0.00002	-0.00007	-0.00009	-3.01190
D37	-0.94967	0.00000	-0.00003	-0.00006	-0.00009	-0.94976
D38	1.20283	0.00000	-0.00003	-0.00007	-0.00010	1.20273
D39	1.15421	0.00000	-0.00002	-0.00006	-0.00008	1.15413
D40	-3.06683	0.00000	-0.00003	-0.00006	-0.00008	-3.06692
D41	-0.91434	0.00000	-0.00003	-0.00006	-0.00009	-0.91443
D42	-1.63733	0.00000	-0.00020	0.00002	-0.00017	-1.63750
D43	2.56106	0.00000	-0.00020	0.00002	-0.00018	2.56088
D44	0.48094	0.00000	-0.00020	0.00003	-0.00017	0.48077
D45	0.44095	0.00000	0.00100	0.00031	0.00131	0.44226
D46	-0.26820	0.00000	-0.00064	-0.00008	-0.00072	-0.26893
D47	2.56874	0.00000	-0.00089	0.00001	-0.00089	2.56785
D48	-3.14153	0.00000	-0.00003	0.00000	-0.00003	-3.14155
D49	0.00058	0.00000	-0.00002	-0.00001	-0.00003	0.00055
D50	0.00041	0.00000	-0.00002	0.00000	-0.00003	0.00039
D51	-3.14066	0.00000	-0.00002	-0.00001	-0.00003	-3.14069
D52	-1.92838	0.00000	0.00364	-0.00058	0.00306	-1.92532
D53	2.43376	0.00000	-0.00331	0.00065	-0.00266	2.43110
D54	2.06082	0.00000	-0.00362	0.00073	-0.00289	2.05794
D55	-2.60714	0.00000	-0.00342	0.00074	-0.00268	-2.60982
D56	-2.72924	0.00000	-0.00001	0.00001	0.00000	-2.72923
D57	-0.03019	0.00000	-0.00001	-0.00001	-0.00002	-0.03021

D58	-0.02169	0.00000	-0.00003	0.00001	-0.00002	-0.02171
D59	2.67735	0.00000	-0.00003	-0.00001	-0.00004	2.67732
D60	-0.17050	0.00000	-0.00006	0.00003	-0.00003	-0.17052
D61	0.27273	0.00000	0.00032	-0.00007	0.00025	0.27298
D62	-2.58278	0.00000	-0.00008	0.00004	-0.00004	-2.58282
D63	-2.13956	0.00000	0.00030	-0.00006	0.00024	-2.13932
D64	2.14127	0.00000	0.00001	-0.00005	-0.00004	2.14123
D65	-0.25204	0.00000	0.00002	-0.00007	-0.00005	-0.25209
D66	2.48864	0.00000	0.00011	0.00001	0.00012	2.48876
D67	-1.71936	0.00000	0.00011	0.00000	0.00012	-1.71925
D68	0.35966	0.00000	0.00011	0.00000	0.00012	0.35978
D69	1.27255	0.00000	0.00010	0.00001	0.00011	1.27267
D70	-2.93545	0.00000	0.00010	0.00000	0.00011	-2.93534
D71	-0.85642	0.00000	0.00010	0.00000	0.00011	-0.85632
D72	-1.08997	0.00000	0.00012	-0.00002	0.00010	-1.08988
D73	0.98520	0.00000	0.00012	-0.00002	0.00009	0.98530
D74	3.06423	0.00000	0.00011	-0.00002	0.00009	3.06432

Item	Value	Threshold	Converged?
Maximum Force	0.000007	0.000450	YES
RMS Force	0.000001	0.000300	YES
Maximum Displacement	0.002466	0.001800	NO
RMS Displacement	0.000481	0.001200	YES

Predicted change in Energy=-3.348831D-09

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.376676	-1.910079	-0.256430
2	6	0	-2.507758	-1.169411	-0.136228
3	7	0	-2.108757	0.112186	0.230301
4	6	0	-0.765111	0.135170	0.327464
5	7	0	-0.305354	-1.081740	0.041193
6	6	0	1.127755	-1.437877	-0.008303
7	6	0	1.683073	-1.372417	-1.441919
8	1	0	-1.243253	-2.945793	-0.517628
9	1	0	-3.538089	-1.442511	-0.272866
10	1	0	1.652740	-0.728929	0.633925
11	1	0	1.236906	-2.447614	0.389510
12	1	0	1.063777	-1.988403	-2.104861
13	1	0	1.635330	-0.336240	-1.796355
14	35	0	1.650471	2.234569	1.024443

15	1	0	-0.112754	0.993734	0.596041
16	6	0	-2.912192	1.257184	0.485744
17	6	0	-4.236442	1.282929	0.412305
18	1	0	-2.315799	2.121039	0.751693
19	1	0	-4.757977	2.205552	0.625730
20	1	0	-4.838820	0.423135	0.147915
21	8	0	2.990629	-1.884328	-1.466237
22	1	0	3.630571	-1.152928	-1.365294
23	6	0	4.836987	1.611876	-1.120527
24	6	0	5.710468	0.752020	-0.312432
25	8	0	4.856327	0.176888	-1.330212
26	1	0	3.920667	1.993792	-0.676788
27	1	0	5.257098	2.179762	-1.946164
28	1	0	6.761117	0.703947	-0.594600
29	6	0	5.399534	0.413259	1.119384
30	1	0	5.678815	-0.621377	1.340757
31	1	0	5.973518	1.066690	1.783700
32	1	0	4.339665	0.561530	1.335492

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357345	0.000000			
3	N	2.205087	1.391416	0.000000		
4	C	2.213139	2.225705	1.347351	0.000000	
5	N	1.386526	2.211277	2.171056	1.331990	0.000000
6	C	2.560608	3.647656	3.596476	2.483981	1.477527
7	C	3.325135	4.394213	4.402084	3.375965	2.497590
8	H	1.076443	2.213588	3.264924	3.230345	2.160237
9	H	2.211470	1.074633	2.171003	3.246365	3.267930
10	H	3.371232	4.254046	3.875467	2.585844	2.076040
11	H	2.745358	3.991580	4.215613	3.268439	2.089379
12	H	3.062457	4.159583	4.464352	3.710876	2.702241
13	H	3.731020	4.540416	4.280959	3.239591	2.774636
14	Br	5.289835	5.497737	4.389415	3.275407	3.973656
15	H	3.279685	3.309299	2.212447	1.111232	2.156976
16	C	3.597247	2.537475	1.421892	2.427740	3.530409
17	C	4.338291	3.050116	2.435325	3.657142	4.602481
18	H	4.260067	3.413548	2.085714	2.555049	3.847660
19	H	5.399058	4.127280	3.399545	4.507596	5.565413
20	H	4.194500	2.837392	2.748949	4.087819	4.777902
21	O	4.531848	5.701955	5.733066	4.626156	3.712142
22	H	5.184147	6.260189	6.089855	4.883303	4.180285
23	C	7.194473	7.915156	7.233061	5.971670	5.920206

24	C	7.570833	8.441693	7.864110	6.536291	6.299035
25	O	6.660238	7.580757	7.138052	5.860904	5.487063
26	H	6.593841	7.184894	6.381003	5.139991	5.275761
27	H	7.974269	8.647880	7.954100	6.754017	6.747434
28	H	8.554014	9.467398	8.927783	7.603803	7.316278
29	C	7.294366	8.161291	7.566740	6.221520	5.995271
30	H	7.347905	8.336774	7.900475	6.566834	6.140935
31	H	8.188323	8.978771	8.285367	6.956830	6.861219
32	H	6.428034	7.214521	6.557858	5.220789	5.094286

		6	7	8	9	10
6	C	0.000000				
7	C	1.538804	0.000000			
8	H	2.855678	3.448653	0.000000		
9	H	4.673341	5.350900	2.754276	0.000000	
10	H	1.091180	2.173505	3.824570	5.317535	0.000000
11	H	1.090751	2.170080	2.687427	4.924383	1.785088
12	H	2.168577	1.096566	2.959442	4.983109	3.071498
13	H	2.160640	1.096160	4.090372	5.505372	2.461862
14	Br	3.850540	4.369709	6.130886	6.490384	2.989118
15	H	2.795859	3.602353	4.247135	4.292227	2.466976
16	C	4.881455	5.634460	4.632183	2.873255	4.980482
17	C	6.029453	6.747567	5.263653	2.895718	6.227291
18	H	5.010144	5.745184	5.332383	3.904178	4.887278
19	H	6.951145	7.652722	6.340103	3.950186	7.050428
20	H	6.252023	6.948861	4.971994	2.312919	6.610886
21	O	2.407319	1.404403	4.466802	6.651578	2.745100
22	H	2.861242	1.961325	5.261850	7.257200	2.844023
23	C	4.929142	4.353903	7.622674	8.954871	4.323991
24	C	5.088163	4.691363	7.878462	9.505438	4.421986
25	O	4.272840	3.533040	6.900457	8.614329	3.865399
26	H	4.474772	4.113832	7.147789	8.222188	3.778183
27	H	5.821864	5.064178	8.400393	9.657956	5.301768
28	H	6.055239	5.551195	8.797526	10.525419	5.445909
29	C	4.790248	4.853967	7.621657	9.233816	3.946990
30	H	4.816511	4.926794	7.534688	9.393048	4.089065
31	H	5.741564	5.895913	8.571926	10.049688	4.818232
32	H	4.014945	4.302516	6.848674	8.286254	3.062196

		11	12	13	14	15
11	H	0.000000				
12	H	2.542191	0.000000			
13	H	3.065069	1.775244	0.000000		
14	Br	4.743102	5.288690	3.816568	0.000000	
15	H	3.702313	4.191926	3.247797	2.198218	0.000000
16	C	5.563254	5.749208	5.331691	4.697166	2.813969

17	C	6.623821	6.717891	6.479012	5.994671	4.137897
18	H	5.798748	6.038952	5.304921	3.977258	2.479607
19	H	7.592521	7.677123	7.293941	6.420905	4.800779
20	H	6.724137	6.762483	6.802312	6.794152	4.781433
21	O	2.614695	2.032592	2.083839	4.996481	4.708207
22	H	3.238083	2.798823	2.198586	4.594211	4.739987
23	C	5.632074	5.307357	3.808216	3.891340	5.275286
24	C	5.544650	5.684580	4.471363	4.524242	5.898615
25	O	4.790164	4.435313	3.294756	4.478389	5.391610
26	H	5.297703	5.104810	3.450398	2.847095	4.346112
27	H	6.559721	5.914620	4.412473	4.672823	6.058447
28	H	6.435660	6.479916	5.366554	5.575195	6.982242
29	C	5.103409	5.912911	4.820012	4.169131	5.567419
30	H	4.895975	5.919427	5.125675	4.948134	6.058503
31	H	6.060495	6.968505	5.796972	4.541932	6.201497
32	H	4.424585	5.391626	4.234133	3.182384	4.534051

		16	17	18	19	20
16	C	0.000000				
17	C	1.326535	0.000000			
18	H	1.082893	2.122847	0.000000		
19	H	2.079885	1.081102	2.446885	0.000000	
20	H	2.126420	1.082593	3.100494	1.847120	0.000000
21	O	6.965817	8.111164	7.008591	9.008015	8.320465
22	H	7.214064	8.425150	7.110542	9.252638	8.746677
23	C	7.921849	9.207872	7.411262	9.770630	9.830732
24	C	8.674246	9.987398	8.211427	10.610431	10.564448
25	O	8.050753	9.324063	7.717088	10.018784	9.810269
26	H	6.970081	8.260137	6.399238	8.778397	8.937321
27	H	8.573367	9.823136	8.039319	10.340070	10.459373
28	H	9.749159	11.058724	9.284991	11.680477	11.627069
29	C	8.378454	9.700944	7.910630	10.326231	10.284345
30	H	8.835464	10.139069	8.472407	10.836485	10.636471
31	H	8.982027	10.303920	8.419588	10.853704	10.954297
32	H	7.334536	8.655766	6.860618	9.272198	9.256029

		21	22	23	24	25
21	O	0.000000				
22	H	0.977068	0.000000			
23	C	3.968878	3.026465	0.000000		
24	C	3.959687	3.010534	1.468107	0.000000	
25	O	2.783513	1.808900	1.450356	1.447829	0.000000
26	H	4.065466	3.234199	1.087386	2.208652	2.145592
27	H	4.678038	3.753642	1.086584	2.216546	2.133429
28	H	4.655695	3.720520	2.191622	1.088941	2.108825
29	C	4.215111	3.428672	2.601988	1.503840	2.520212

30	H	4.086637	3.435194	3.428413	2.149478	2.906509
31	H	5.307375	4.509131	3.165986	2.135880	3.425830
32	H	3.956236	3.276649	2.717092	2.151986	2.742421

		26	27	28	29	30
26	H	0.000000				
27	H	1.852552	0.000000			
28	H	3.120675	2.503364	0.000000		
29	C	2.812715	3.540962	2.208200	0.000000	
30	H	3.741749	4.339134	2.583306	1.094293	0.000000
31	H	3.335824	3.957787	2.531443	1.094416	1.769921
32	H	2.505236	3.772218	3.099834	1.091792	1.786791

		31	32
31	H	0.000000	
32	H	1.767924	0.000000

Stoichiometry C10H17BrN2O2
Framework group C1[X(C10H17BrN2O2)]
Deg. of freedom 90
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.711113	2.114434	-0.440979
2	6	0	-3.788494	1.349121	-0.131253
3	7	0	-3.319916	0.050046	0.038677
4	6	0	-1.988308	0.040744	-0.166479
5	7	0	-1.603294	1.280942	-0.462910
6	6	0	-0.201257	1.680336	-0.703461
7	6	0	0.455082	2.252397	0.565350
8	1	0	-2.638735	3.167298	-0.653034
9	1	0	-4.824637	1.613691	-0.025201
10	1	0	0.330270	0.786849	-1.034874
11	1	0	-0.196562	2.428606	-1.497065
12	1	0	-0.161795	3.066919	0.963439
13	1	0	0.510477	1.464191	1.325105
14	35	0	0.525313	-2.059113	-0.141966
15	1	0	-1.292956	-0.824192	-0.109858
16	6	0	-4.050113	-1.125518	0.365232
17	6	0	-5.360377	-1.169604	0.567616
18	1	0	-3.409849	-1.996320	0.431743
19	1	0	-5.824086	-2.115140	0.811989

20	1	0	-6.006396	-0.303372	0.501972
21	8	0	1.718699	2.777019	0.248505
22	1	0	2.403654	2.097851	0.404161
23	6	0	3.796049	-0.458990	1.230774
24	6	0	4.544067	0.009358	0.057547
25	8	0	3.721173	0.928553	0.815264
26	1	0	2.882812	-1.028988	1.077456
27	1	0	4.313935	-0.605035	2.174772
28	1	0	5.605033	0.214057	0.192605
29	6	0	4.110267	-0.305195	-1.347589
30	1	0	4.294496	0.547280	-2.008514
31	1	0	4.684810	-1.155943	-1.726899
32	1	0	3.052272	-0.572783	-1.380056

Rotational constants (GHZ): 0.5994512 0.2213243 0.1723290

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 492 symmetry adapted cartesian basis functions of A symmetry.

There are 475 symmetry adapted basis functions of A symmetry.

475 basis functions, 751 primitive gaussians, 492 cartesian basis functions

71 alpha electrons 71 beta electrons

nuclear repulsion energy 1307.1965440362 Hartrees.

NAtoms= 32 NActive= 32 NUniq= 32 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 475 RedAO= T EigKep= 3.79D-06 NBF= 475

NBsUse= 475 1.00D-06 EigRej= -1.00D+00 NBFU= 475

Initial guess from the checkpoint file: "/home/suqian/liuwen/qianmengshijie/ohpo/ohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000033 0.000011 -0.000008 Ang= 0.00 deg.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3225.52371259 A.U. after 7 cycles

NFock= 7 Conv=0.53D-08 -V/T= 2.0018

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z

1	6	-0.000000046	0.000000216	0.000007419
2	6	-0.000000246	0.000001446	0.000002314
3	7	-0.000000835	0.000000222	0.000004369
4	6	-0.000002455	0.000003519	-0.000003622
5	7	0.000001502	-0.000002564	0.000002233
6	6	-0.000002295	0.000000688	0.000002531
7	6	0.000002497	-0.000006632	0.000006163
8	1	-0.000000745	-0.000000756	0.000008983
9	1	-0.000000325	0.000000211	0.000005545
10	1	0.000000497	0.000003237	0.000001945
11	1	-0.000000041	0.000001565	0.000007909
12	1	-0.000000749	-0.000005899	0.000006008
13	1	-0.000001169	-0.000004378	-0.000000128
14	35	-0.000000601	0.000003055	-0.000005489
15	1	0.000003581	0.000004505	-0.000002108
16	6	0.000000734	0.000002205	-0.000004546
17	6	-0.000000021	0.000002940	-0.000004325
18	1	0.000000288	0.000003062	-0.000004801
19	1	0.000000466	0.000003271	-0.000005566
20	1	0.000000119	0.000001913	-0.000000854
21	8	-0.000002151	-0.000004283	0.000000456
22	1	-0.000000491	-0.000002907	0.000009349
23	6	0.000000884	-0.000003312	-0.000004040
24	6	-0.000001045	-0.000000217	0.000000470
25	8	0.000000728	-0.000005375	-0.000007274
26	1	0.000000287	-0.000001641	-0.000007074
27	1	-0.000000022	-0.000006113	-0.000006590
28	1	0.000000023	-0.000002831	-0.000003339
29	6	0.000000743	0.000001725	0.000000155
30	1	0.000000198	0.000003807	0.000000556
31	1	0.000000603	0.000005132	-0.000004035
32	1	0.000000089	0.000004190	-0.000002617

Cartesian Forces: Max 0.000009349 RMS 0.000003523

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000003300 RMS 0.000000700
Search for a local minimum.
Step number 42 out of a maximum of 177

All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 24 25 26 27 28
29 30 31 32 33
34 35 36 37 38
39 40 41 42
DE= -1.62D-07 DEPred=-3.35D-09 R= 4.85D+01
Trust test= 4.85D+01 RLast= 6.22D-03 DXMaxT set to 1.21D-01
ITU= 0 0 0 -1 -1 -1 -1 0 0 1 1 0 1 1 1 1 1 1 1 1
ITU= 1 1 1 1 1 -1 1 1 1 1 1 1 1 1 1 1 0 1 0
ITU= 1 0
Eigenvalues --- 0.00003 0.00029 0.00083 0.00161 0.00217
Eigenvalues --- 0.00236 0.00340 0.00665 0.00839 0.01057
Eigenvalues --- 0.01215 0.01504 0.01764 0.01792 0.01898
Eigenvalues --- 0.02076 0.02178 0.02257 0.02325 0.02401
Eigenvalues --- 0.03018 0.03059 0.03118 0.03504 0.03778
Eigenvalues --- 0.04114 0.04624 0.05189 0.05404 0.05416
Eigenvalues --- 0.05670 0.05887 0.06505 0.08945 0.09357
Eigenvalues --- 0.10340 0.11036 0.11452 0.11610 0.12831
Eigenvalues --- 0.13593 0.13957 0.14123 0.15036 0.15969
Eigenvalues --- 0.15991 0.15997 0.16001 0.16009 0.16026
Eigenvalues --- 0.16054 0.16808 0.18081 0.20021 0.22047
Eigenvalues --- 0.22823 0.23402 0.23843 0.24380 0.25039
Eigenvalues --- 0.27486 0.28389 0.30673 0.31944 0.33104
Eigenvalues --- 0.33218 0.34018 0.34193 0.34470 0.34843
Eigenvalues --- 0.35040 0.35684 0.35689 0.35855 0.36109
Eigenvalues --- 0.36435 0.36671 0.37163 0.37239 0.37488
Eigenvalues --- 0.38069 0.42176 0.42502 0.44314 0.45613
Eigenvalues --- 0.49358 0.53814 0.55018 0.55829 0.60395
Eigenvalue 1 is 3.35D-05 Eigenvector:

	D54	D52	D53	D55	D47
1	0.50885	-0.50426	0.49347	0.48506	0.04013

	D46	A58	D65	D64	A48
1	0.03244	-0.02868	0.02127	0.02111	-0.02067

En-DIIS/RFO-DIIS IScMMF= 0 using points: 42 41 40 39 38
RFO step: Lambda=-2.83543984D-10.
DidBck=F Rises=F RFO-DIIS coefs: 1.55424 -0.48357 -0.37152 0.44517 -0.14432
Iteration 1 RMS(Cart)= 0.00015630 RMS(Int)= 0.00000009
Iteration 2 RMS(Cart)= 0.00000003 RMS(Int)= 0.00000009

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56501	0.00000	0.00000	0.00000	0.00000	2.56501

R2	2.62015	0.00000	0.00000	0.00000	0.00000	2.62015
R3	2.03418	0.00000	0.00000	0.00000	0.00000	2.03418
R4	2.62939	0.00000	0.00000	0.00000	0.00000	2.62939
R5	2.03076	0.00000	0.00000	0.00000	0.00000	2.03076
R6	2.54612	0.00000	0.00000	0.00000	0.00000	2.54612
R7	2.68699	0.00000	0.00000	0.00000	0.00000	2.68699
R8	2.51710	0.00000	0.00000	0.00001	0.00000	2.51710
R9	2.09992	0.00000	0.00000	0.00001	0.00001	2.09993
R10	2.79212	0.00000	0.00000	0.00000	0.00000	2.79212
R11	2.90792	0.00000	0.00000	0.00000	0.00000	2.90792
R12	2.06203	0.00000	0.00000	0.00000	0.00000	2.06204
R13	2.06122	0.00000	0.00000	0.00000	0.00000	2.06122
R14	2.07221	0.00000	0.00000	0.00000	0.00000	2.07221
R15	2.07144	0.00000	0.00000	0.00000	0.00001	2.07145
R16	2.65394	0.00000	-0.00001	0.00000	-0.00001	2.65393
R17	4.15403	0.00000	-0.00002	-0.00001	-0.00003	4.15400
R18	8.46293	0.00000	0.00008	0.00008	0.00016	8.46309
R19	2.50679	0.00000	0.00000	0.00000	0.00000	2.50679
R20	2.04637	0.00000	0.00000	0.00000	0.00000	2.04637
R21	2.04299	0.00000	0.00000	0.00000	0.00000	2.04299
R22	2.04580	0.00000	0.00000	0.00000	0.00000	2.04580
R23	1.84639	0.00000	0.00000	0.00000	0.00000	1.84639
R24	3.41833	0.00000	0.00001	-0.00001	0.00000	3.41833
R25	2.77432	0.00000	0.00000	0.00000	0.00000	2.77432
R26	2.74077	0.00000	0.00000	0.00000	0.00000	2.74078
R27	2.05486	0.00000	0.00000	0.00000	0.00000	2.05486
R28	2.05335	0.00000	0.00000	0.00000	0.00000	2.05335
R29	2.73600	0.00000	0.00001	0.00000	0.00001	2.73601
R30	2.05780	0.00000	0.00000	0.00000	0.00000	2.05780
R31	2.84185	0.00000	0.00000	0.00000	0.00000	2.84184
R32	2.06791	0.00000	0.00000	0.00000	0.00000	2.06791
R33	2.06815	0.00000	0.00000	0.00000	0.00000	2.06815
R34	2.06319	0.00000	0.00000	0.00000	0.00000	2.06319
A1	1.87430	0.00000	0.00000	0.00000	0.00000	1.87429
A2	2.27812	0.00000	0.00000	0.00000	0.00000	2.27812
A3	2.13073	0.00000	0.00000	0.00000	0.00000	2.13073
A4	1.86187	0.00000	0.00000	0.00000	0.00000	1.86187
A5	2.27709	0.00000	0.00000	0.00000	0.00000	2.27709
A6	2.14421	0.00000	0.00000	0.00000	0.00000	2.14421
A7	1.89724	0.00000	0.00000	0.00000	0.00000	1.89724
A8	2.24849	0.00000	0.00000	0.00000	0.00000	2.24849
A9	2.13744	0.00000	0.00000	0.00000	0.00000	2.13744
A10	1.88929	0.00000	0.00000	0.00000	0.00000	1.88929
A11	2.23452	0.00000	0.00001	0.00000	0.00001	2.23453

A12	2.15938	0.00000	0.00000	0.00000	-0.00001	2.15937
A13	1.90206	0.00000	0.00000	0.00000	0.00000	1.90206
A14	2.21211	0.00000	0.00001	0.00000	0.00001	2.21212
A15	2.16784	0.00000	-0.00001	0.00000	-0.00001	2.16783
A16	1.95086	0.00000	0.00000	0.00001	0.00001	1.95087
A17	1.86537	0.00000	0.00000	-0.00001	-0.00001	1.86537
A18	1.88386	0.00000	0.00000	0.00000	0.00000	1.88386
A19	1.92524	0.00000	0.00000	0.00000	0.00000	1.92524
A20	1.92096	0.00000	0.00000	0.00000	0.00000	1.92096
A21	1.91628	0.00000	0.00000	0.00000	-0.00001	1.91627
A22	1.91297	0.00000	0.00000	0.00000	0.00000	1.91297
A23	1.90258	0.00000	0.00000	0.00000	0.00000	1.90258
A24	1.91412	0.00000	0.00000	0.00001	0.00000	1.91412
A25	1.88696	0.00000	-0.00001	0.00000	-0.00001	1.88695
A26	1.88661	0.00000	0.00000	0.00000	0.00000	1.88661
A27	1.96006	0.00000	0.00000	0.00000	0.00000	1.96007
A28	1.78480	0.00000	-0.00006	-0.00004	-0.00010	1.78470
A29	2.83749	0.00000	0.00001	0.00001	0.00002	2.83751
A30	2.17700	0.00000	0.00000	0.00000	0.00000	2.17701
A31	1.95553	0.00000	0.00000	0.00000	0.00000	1.95553
A32	2.15065	0.00000	0.00000	0.00000	0.00000	2.15065
A33	2.07969	0.00000	0.00000	0.00000	0.00000	2.07969
A34	2.15744	0.00000	0.00000	0.00000	0.00000	2.15744
A35	2.04605	0.00000	0.00000	0.00000	0.00000	2.04605
A36	1.91256	0.00000	0.00000	0.00001	0.00001	1.91257
A37	3.05361	0.00000	-0.00004	-0.00002	-0.00005	3.05356
A38	2.07426	0.00000	0.00000	0.00000	0.00000	2.07425
A39	2.08784	0.00000	0.00001	0.00000	0.00001	2.08784
A40	2.00175	0.00000	-0.00001	0.00001	0.00000	2.00175
A41	1.98459	0.00000	0.00001	0.00000	0.00001	1.98460
A42	2.04017	0.00000	0.00000	0.00000	0.00000	2.04016
A43	2.04573	0.00000	-0.00001	0.00001	-0.00001	2.04572
A44	2.13293	0.00000	0.00001	0.00000	0.00001	2.13294
A45	1.94928	0.00000	-0.00001	-0.00001	-0.00002	1.94926
A46	2.04636	0.00000	0.00001	0.00000	0.00001	2.04637
A47	2.02223	0.00000	0.00000	0.00000	0.00000	2.02223
A48	1.43326	0.00000	0.00001	-0.00001	0.00000	1.43326
A49	1.00017	0.00000	0.00001	-0.00001	0.00000	1.00017
A50	2.37623	0.00000	0.00000	-0.00002	-0.00002	2.37621
A51	2.35382	0.00000	0.00002	0.00000	0.00002	2.35383
A52	1.93138	0.00000	0.00000	0.00000	0.00000	1.93138
A53	1.91240	0.00000	-0.00001	0.00000	-0.00001	1.91239
A54	1.93754	0.00000	0.00001	-0.00001	0.00000	1.93755
A55	1.88374	0.00000	0.00000	0.00000	0.00000	1.88374

A56	1.91358	0.00000	0.00000	0.00000	0.00000	1.91359
A57	1.88378	0.00000	0.00000	0.00000	0.00000	1.88378
A58	3.78708	0.00000	0.00003	-0.00001	0.00002	3.78710
A59	5.04092	0.00000	0.00002	0.00006	0.00008	5.04100
D1	0.00437	0.00000	-0.00001	0.00000	-0.00001	0.00436
D2	-3.13124	0.00000	0.00000	0.00002	0.00002	-3.13122
D3	3.13648	0.00000	0.00002	-0.00002	0.00001	3.13649
D4	0.00087	0.00000	0.00003	0.00001	0.00004	0.00091
D5	-0.00682	0.00000	0.00000	0.00000	0.00000	-0.00682
D6	-3.09779	0.00000	-0.00006	0.00000	-0.00007	-3.09785
D7	-3.13991	0.00000	-0.00003	0.00001	-0.00001	-3.13992
D8	0.05231	0.00000	-0.00009	0.00001	-0.00008	0.05223
D9	-0.00050	0.00000	0.00001	0.00000	0.00001	-0.00049
D10	-3.13634	0.00000	-0.00003	-0.00001	-0.00004	-3.13638
D11	3.13567	0.00000	0.00001	-0.00002	-0.00001	3.13566
D12	-0.00017	0.00000	-0.00003	-0.00004	-0.00006	-0.00024
D13	-0.00375	0.00000	-0.00001	0.00000	-0.00001	-0.00376
D14	3.13821	0.00000	0.00011	0.00004	0.00014	3.13836
D15	3.13254	0.00000	0.00002	0.00001	0.00003	3.13257
D16	-0.00869	0.00000	0.00014	0.00005	0.00019	-0.00850
D17	0.00170	0.00000	-0.00014	-0.00011	-0.00025	0.00145
D18	-3.14021	0.00000	-0.00013	-0.00012	-0.00025	-3.14046
D19	-3.13344	0.00000	-0.00018	-0.00013	-0.00030	-3.13374
D20	0.00784	0.00000	-0.00017	-0.00013	-0.00030	0.00754
D21	0.00651	0.00000	0.00001	0.00000	0.00001	0.00651
D22	3.09905	0.00000	0.00007	0.00000	0.00007	3.09912
D23	-3.13543	0.00000	-0.00010	-0.00004	-0.00014	-3.13557
D24	-0.04289	0.00000	-0.00004	-0.00003	-0.00007	-0.04297
D25	-3.11898	0.00000	-0.00029	-0.00040	-0.00069	-3.11966
D26	0.02303	0.00000	-0.00015	-0.00036	-0.00051	0.02252
D27	1.41200	0.00000	0.00001	0.00004	0.00005	1.41205
D28	-2.76315	0.00000	0.00001	0.00003	0.00005	-2.76310
D29	-0.70285	0.00000	0.00001	0.00003	0.00004	-0.70281
D30	-1.67170	0.00000	-0.00006	0.00003	-0.00003	-1.67172
D31	0.43634	0.00000	-0.00006	0.00003	-0.00003	0.43631
D32	2.49664	0.00000	-0.00006	0.00003	-0.00004	2.49660
D33	-0.93907	0.00000	-0.00004	-0.00002	-0.00006	-0.93913
D34	1.12307	0.00000	-0.00005	-0.00002	-0.00007	1.12299
D35	-3.00763	0.00000	-0.00005	-0.00002	-0.00007	-3.00770
D36	-3.01190	0.00000	-0.00004	-0.00001	-0.00006	-3.01196
D37	-0.94976	0.00000	-0.00005	-0.00002	-0.00007	-0.94983
D38	1.20273	0.00000	-0.00005	-0.00002	-0.00006	1.20266
D39	1.15413	0.00000	-0.00004	-0.00001	-0.00005	1.15408
D40	-3.06692	0.00000	-0.00005	-0.00001	-0.00006	-3.06698

D41	-0.91443	0.00000	-0.00004	-0.00001	-0.00006	-0.91448
D42	-1.63750	0.00000	0.00000	0.00007	0.00007	-1.63743
D43	2.56088	0.00000	-0.00001	0.00007	0.00006	2.56094
D44	0.48077	0.00000	0.00000	0.00007	0.00008	0.48084
D45	0.44226	0.00000	0.00029	0.00040	0.00069	0.44295
D46	-0.26893	0.00000	-0.00023	-0.00004	-0.00027	-0.26920
D47	2.56785	0.00000	-0.00027	-0.00007	-0.00034	2.56752
D48	-3.14155	0.00000	0.00000	-0.00002	-0.00002	-3.14158
D49	0.00055	0.00000	-0.00001	-0.00001	-0.00002	0.00053
D50	0.00039	0.00000	-0.00001	-0.00001	-0.00002	0.00036
D51	-3.14069	0.00000	-0.00002	0.00000	-0.00002	-3.14072
D52	-1.92532	0.00000	0.00065	-0.00043	0.00023	-1.92509
D53	2.43110	0.00000	-0.00050	0.00041	-0.00009	2.43101
D54	2.05794	0.00000	-0.00055	0.00039	-0.00016	2.05778
D55	-2.60982	0.00000	-0.00053	0.00036	-0.00017	-2.60999
D56	-2.72923	0.00000	-0.00001	0.00000	-0.00001	-2.72924
D57	-0.03021	0.00000	-0.00002	0.00002	0.00000	-0.03021
D58	-0.02171	0.00000	-0.00001	-0.00001	-0.00002	-0.02173
D59	2.67732	0.00000	-0.00002	0.00001	-0.00001	2.67730
D60	-0.17052	0.00000	-0.00002	-0.00004	-0.00006	-0.17059
D61	0.27298	0.00000	0.00003	0.00000	0.00002	0.27300
D62	-2.58282	0.00000	-0.00002	-0.00004	-0.00006	-2.58288
D63	-2.13932	0.00000	0.00003	-0.00001	0.00002	-2.13930
D64	2.14123	0.00000	0.00001	0.00002	0.00003	2.14126
D65	-0.25209	0.00000	0.00001	0.00003	0.00004	-0.25205
D66	2.48876	0.00000	0.00004	-0.00002	0.00002	2.48878
D67	-1.71925	0.00000	0.00004	-0.00002	0.00002	-1.71923
D68	0.35978	0.00000	0.00004	-0.00002	0.00002	0.35980
D69	1.27267	0.00000	0.00003	-0.00002	0.00001	1.27268
D70	-2.93534	0.00000	0.00003	-0.00002	0.00001	-2.93533
D71	-0.85632	0.00000	0.00003	-0.00002	0.00001	-0.85631
D72	-1.08988	0.00000	0.00003	0.00000	0.00003	-1.08985
D73	0.98530	0.00000	0.00003	0.00000	0.00003	0.98533
D74	3.06432	0.00000	0.00002	0.00000	0.00003	3.06435

Item	Value	Threshold	Converged?
Maximum Force	0.000003	0.000450	YES
RMS Force	0.000001	0.000300	YES
Maximum Displacement	0.000964	0.001800	YES
RMS Displacement	0.000156	0.001200	YES

Predicted change in Energy=-1.365943D-09

Optimization completed.

-- Stationary point found.

! Optimized Parameters !

! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.		!
! R1	R(1,2)	1.3573	-DE/DX =	0.0	!
! R2	R(1,5)	1.3865	-DE/DX =	0.0	!
! R3	R(1,8)	1.0764	-DE/DX =	0.0	!
! R4	R(2,3)	1.3914	-DE/DX =	0.0	!
! R5	R(2,9)	1.0746	-DE/DX =	0.0	!
! R6	R(3,4)	1.3474	-DE/DX =	0.0	!
! R7	R(3,16)	1.4219	-DE/DX =	0.0	!
! R8	R(4,5)	1.332	-DE/DX =	0.0	!
! R9	R(4,15)	1.1112	-DE/DX =	0.0	!
! R10	R(5,6)	1.4775	-DE/DX =	0.0	!
! R11	R(6,7)	1.5388	-DE/DX =	0.0	!
! R12	R(6,10)	1.0912	-DE/DX =	0.0	!
! R13	R(6,11)	1.0908	-DE/DX =	0.0	!
! R14	R(7,12)	1.0966	-DE/DX =	0.0	!
! R15	R(7,13)	1.0962	-DE/DX =	0.0	!
! R16	R(7,21)	1.4044	-DE/DX =	0.0	!
! R17	R(14,15)	2.1982	-DE/DX =	0.0	!
! R18	R(14,25)	4.4784	-DE/DX =	0.0	!
! R19	R(16,17)	1.3265	-DE/DX =	0.0	!
! R20	R(16,18)	1.0829	-DE/DX =	0.0	!
! R21	R(17,19)	1.0811	-DE/DX =	0.0	!
! R22	R(17,20)	1.0826	-DE/DX =	0.0	!
! R23	R(21,22)	0.9771	-DE/DX =	0.0	!
! R24	R(22,25)	1.8089	-DE/DX =	0.0	!
! R25	R(23,24)	1.4681	-DE/DX =	0.0	!
! R26	R(23,25)	1.4504	-DE/DX =	0.0	!
! R27	R(23,26)	1.0874	-DE/DX =	0.0	!
! R28	R(23,27)	1.0866	-DE/DX =	0.0	!
! R29	R(24,25)	1.4478	-DE/DX =	0.0	!
! R30	R(24,28)	1.0889	-DE/DX =	0.0	!
! R31	R(24,29)	1.5038	-DE/DX =	0.0	!
! R32	R(29,30)	1.0943	-DE/DX =	0.0	!
! R33	R(29,31)	1.0944	-DE/DX =	0.0	!
! R34	R(29,32)	1.0918	-DE/DX =	0.0	!
! A1	A(2,1,5)	107.3892	-DE/DX =	0.0	!
! A2	A(2,1,8)	130.5267	-DE/DX =	0.0	!
! A3	A(5,1,8)	122.0819	-DE/DX =	0.0	!
! A4	A(1,2,3)	106.677	-DE/DX =	0.0	!
! A5	A(1,2,9)	130.4676	-DE/DX =	0.0	!
! A6	A(3,2,9)	122.8545	-DE/DX =	0.0	!

! A7	A(2,3,4)	108.704	-DE/DX =	0.0	!
! A8	A(2,3,16)	128.8291	-DE/DX =	0.0	!
! A9	A(4,3,16)	122.4661	-DE/DX =	0.0	!
! A10	A(3,4,5)	108.2481	-DE/DX =	0.0	!
! A11	A(3,4,15)	128.0284	-DE/DX =	0.0	!
! A12	A(5,4,15)	123.7234	-DE/DX =	0.0	!
! A13	A(1,5,4)	108.9802	-DE/DX =	0.0	!
! A14	A(1,5,6)	126.7445	-DE/DX =	0.0	!
! A15	A(4,5,6)	124.208	-DE/DX =	0.0	!
! A16	A(5,6,7)	111.7763	-DE/DX =	0.0	!
! A17	A(5,6,10)	106.8779	-DE/DX =	0.0	!
! A18	A(5,6,11)	107.9373	-DE/DX =	0.0	!
! A19	A(7,6,10)	110.3081	-DE/DX =	0.0	!
! A20	A(7,6,11)	110.0629	-DE/DX =	0.0	!
! A21	A(10,6,11)	109.7946	-DE/DX =	0.0	!
! A22	A(6,7,12)	109.6049	-DE/DX =	0.0	!
! A23	A(6,7,13)	109.0101	-DE/DX =	0.0	!
! A24	A(6,7,21)	109.6709	-DE/DX =	0.0	!
! A25	A(12,7,13)	108.1149	-DE/DX =	0.0	!
! A26	A(12,7,21)	108.0947	-DE/DX =	0.0	!
! A27	A(13,7,21)	112.3034	-DE/DX =	0.0	!
! A28	A(15,14,25)	102.2612	-DE/DX =	0.0	!
! A29	A(4,15,14)	162.5762	-DE/DX =	0.0	!
! A30	A(3,16,17)	124.7332	-DE/DX =	0.0	!
! A31	A(3,16,18)	112.0434	-DE/DX =	0.0	!
! A32	A(17,16,18)	123.2234	-DE/DX =	0.0	!
! A33	A(16,17,19)	119.1576	-DE/DX =	0.0	!
! A34	A(16,17,20)	123.6123	-DE/DX =	0.0	!
! A35	A(19,17,20)	117.2301	-DE/DX =	0.0	!
! A36	A(7,21,22)	109.5818	-DE/DX =	0.0	!
! A37	A(21,22,25)	174.959	-DE/DX =	0.0	!
! A38	A(24,23,26)	118.8462	-DE/DX =	0.0	!
! A39	A(24,23,27)	119.6243	-DE/DX =	0.0	!
! A40	A(25,23,26)	114.6918	-DE/DX =	0.0	!
! A41	A(25,23,27)	113.7086	-DE/DX =	0.0	!
! A42	A(26,23,27)	116.893	-DE/DX =	0.0	!
! A43	A(23,24,28)	117.2114	-DE/DX =	0.0	!
! A44	A(23,24,29)	122.2077	-DE/DX =	0.0	!
! A45	A(25,24,28)	111.6854	-DE/DX =	0.0	!
! A46	A(25,24,29)	117.2479	-DE/DX =	0.0	!
! A47	A(28,24,29)	115.8653	-DE/DX =	0.0	!
! A48	A(14,25,22)	82.1198	-DE/DX =	0.0	!
! A49	A(14,25,23)	57.3054	-DE/DX =	0.0	!
! A50	A(22,25,23)	136.1479	-DE/DX =	0.0	!

! A51	A(22,25,24)	134.8639	-DE/DX =	0.0	!
! A52	A(24,29,30)	110.6602	-DE/DX =	0.0	!
! A53	A(24,29,31)	109.5725	-DE/DX =	0.0	!
! A54	A(24,29,32)	111.0131	-DE/DX =	0.0	!
! A55	A(30,29,31)	107.9304	-DE/DX =	0.0	!
! A56	A(30,29,32)	109.6402	-DE/DX =	0.0	!
! A57	A(31,29,32)	107.9326	-DE/DX =	0.0	!
! A58	L(14,25,24,22,-1)	216.9837	-DE/DX =	0.0	!
! A59	L(14,25,24,22,-2)	288.8232	-DE/DX =	0.0	!
! D1	D(5,1,2,3)	0.2502	-DE/DX =	0.0	!
! D2	D(5,1,2,9)	-179.4069	-DE/DX =	0.0	!
! D3	D(8,1,2,3)	179.7071	-DE/DX =	0.0	!
! D4	D(8,1,2,9)	0.0501	-DE/DX =	0.0	!
! D5	D(2,1,5,4)	-0.3907	-DE/DX =	0.0	!
! D6	D(2,1,5,6)	-177.49	-DE/DX =	0.0	!
! D7	D(8,1,5,4)	-179.9035	-DE/DX =	0.0	!
! D8	D(8,1,5,6)	2.9971	-DE/DX =	0.0	!
! D9	D(1,2,3,4)	-0.0286	-DE/DX =	0.0	!
! D10	D(1,2,3,16)	-179.6992	-DE/DX =	0.0	!
! D11	D(9,2,3,4)	179.6608	-DE/DX =	0.0	!
! D12	D(9,2,3,16)	-0.0098	-DE/DX =	0.0	!
! D13	D(2,3,4,5)	-0.2147	-DE/DX =	0.0	!
! D14	D(2,3,4,15)	179.8064	-DE/DX =	0.0	!
! D15	D(16,3,4,5)	179.4812	-DE/DX =	0.0	!
! D16	D(16,3,4,15)	-0.4978	-DE/DX =	0.0	!
! D17	D(2,3,16,17)	0.0972	-DE/DX =	0.0	!
! D18	D(2,3,16,18)	-179.9207	-DE/DX =	0.0	!
! D19	D(4,3,16,17)	-179.533	-DE/DX =	0.0	!
! D20	D(4,3,16,18)	0.4491	-DE/DX =	0.0	!
! D21	D(3,4,5,1)	0.3729	-DE/DX =	0.0	!
! D22	D(3,4,5,6)	177.5624	-DE/DX =	0.0	!
! D23	D(15,4,5,1)	-179.6471	-DE/DX =	0.0	!
! D24	D(15,4,5,6)	-2.4575	-DE/DX =	0.0	!
! D25	D(3,4,15,14)	-178.7043	-DE/DX =	0.0	!
! D26	D(5,4,15,14)	1.3198	-DE/DX =	0.0	!
! D27	D(1,5,6,7)	80.9016	-DE/DX =	0.0	!
! D28	D(1,5,6,10)	-158.3167	-DE/DX =	0.0	!
! D29	D(1,5,6,11)	-40.2702	-DE/DX =	0.0	!
! D30	D(4,5,6,7)	-95.7812	-DE/DX =	0.0	!
! D31	D(4,5,6,10)	25.0005	-DE/DX =	0.0	!
! D32	D(4,5,6,11)	143.047	-DE/DX =	0.0	!
! D33	D(5,6,7,12)	-53.8048	-DE/DX =	0.0	!
! D34	D(5,6,7,13)	64.3469	-DE/DX =	0.0	!
! D35	D(5,6,7,21)	-172.3245	-DE/DX =	0.0	!

! D36	D(10,6,7,12)	-172.5691	-DE/DX =	0.0 !
! D37	D(10,6,7,13)	-54.4174	-DE/DX =	0.0 !
! D38	D(10,6,7,21)	68.9112	-DE/DX =	0.0 !
! D39	D(11,6,7,12)	66.1269	-DE/DX =	0.0 !
! D40	D(11,6,7,13)	-175.7214	-DE/DX =	0.0 !
! D41	D(11,6,7,21)	-52.3928	-DE/DX =	0.0 !
! D42	D(6,7,21,22)	-93.8219	-DE/DX =	0.0 !
! D43	D(12,7,21,22)	146.7276	-DE/DX =	0.0 !
! D44	D(13,7,21,22)	27.5459	-DE/DX =	0.0 !
! D45	D(25,14,15,4)	25.3394	-DE/DX =	0.0 !
! D46	D(15,14,25,22)	-15.4083	-DE/DX =	0.0 !
! D47	D(15,14,25,23)	147.1271	-DE/DX =	0.0 !
! D48	D(3,16,17,19)	-179.9978	-DE/DX =	0.0 !
! D49	D(3,16,17,20)	0.0316	-DE/DX =	0.0 !
! D50	D(18,16,17,19)	0.0221	-DE/DX =	0.0 !
! D51	D(18,16,17,20)	-179.9485	-DE/DX =	0.0 !
! D52	D(7,21,22,25)	-110.3126	-DE/DX =	0.0 !
! D53	D(21,22,25,14)	139.2917	-DE/DX =	0.0 !
! D54	D(21,22,25,23)	117.9112	-DE/DX =	0.0 !
! D55	D(21,22,25,24)	-149.5315	-DE/DX =	0.0 !
! D56	D(26,23,24,28)	-156.3734	-DE/DX =	0.0 !
! D57	D(26,23,24,29)	-1.7308	-DE/DX =	0.0 !
! D58	D(27,23,24,28)	-1.2436	-DE/DX =	0.0 !
! D59	D(27,23,24,29)	153.399	-DE/DX =	0.0 !
! D60	D(26,23,25,14)	-9.7703	-DE/DX =	0.0 !
! D61	D(26,23,25,22)	15.6404	-DE/DX =	0.0 !
! D62	D(27,23,25,14)	-147.9848	-DE/DX =	0.0 !
! D63	D(27,23,25,22)	-122.5741	-DE/DX =	0.0 !
! D64	D(28,24,25,22)	122.6837	-DE/DX =	0.0 !
! D65	D(29,24,25,22)	-14.4438	-DE/DX =	0.0 !
! D66	D(23,24,29,30)	142.5956	-DE/DX =	0.0 !
! D67	D(23,24,29,31)	-98.5056	-DE/DX =	0.0 !
! D68	D(23,24,29,32)	20.6139	-DE/DX =	0.0 !
! D69	D(25,24,29,30)	72.9183	-DE/DX =	0.0 !
! D70	D(25,24,29,31)	-168.1828	-DE/DX =	0.0 !
! D71	D(25,24,29,32)	-49.0634	-DE/DX =	0.0 !
! D72	D(28,24,29,30)	-62.4454	-DE/DX =	0.0 !
! D73	D(28,24,29,31)	56.4534	-DE/DX =	0.0 !
! D74	D(28,24,29,32)	175.5729	-DE/DX =	0.0 !

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.376676	-1.910079	-0.256430
2	6	0	-2.507758	-1.169411	-0.136228
3	7	0	-2.108757	0.112186	0.230301
4	6	0	-0.765111	0.135170	0.327464
5	7	0	-0.305354	-1.081740	0.041193
6	6	0	1.127755	-1.437877	-0.008303
7	6	0	1.683073	-1.372417	-1.441919
8	1	0	-1.243253	-2.945793	-0.517628
9	1	0	-3.538089	-1.442511	-0.272866
10	1	0	1.652740	-0.728929	0.633925
11	1	0	1.236906	-2.447614	0.389510
12	1	0	1.063777	-1.988403	-2.104861
13	1	0	1.635330	-0.336240	-1.796355
14	35	0	1.650471	2.234569	1.024443
15	1	0	-0.112754	0.993734	0.596041
16	6	0	-2.912192	1.257184	0.485744
17	6	0	-4.236442	1.282929	0.412305
18	1	0	-2.315799	2.121039	0.751693
19	1	0	-4.757977	2.205552	0.625730
20	1	0	-4.838820	0.423135	0.147915
21	8	0	2.990629	-1.884328	-1.466237
22	1	0	3.630571	-1.152928	-1.365294
23	6	0	4.836987	1.611876	-1.120527
24	6	0	5.710468	0.752020	-0.312432
25	8	0	4.856327	0.176888	-1.330212
26	1	0	3.920667	1.993792	-0.676788
27	1	0	5.257098	2.179762	-1.946164
28	1	0	6.761117	0.703947	-0.594600
29	6	0	5.399534	0.413259	1.119384
30	1	0	5.678815	-0.621377	1.340757
31	1	0	5.973518	1.066690	1.783700
32	1	0	4.339665	0.561530	1.335492

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357345	0.000000			
3	N	2.205087	1.391416	0.000000		
4	C	2.213139	2.225705	1.347351	0.000000	
5	N	1.386526	2.211277	2.171056	1.331990	0.000000
6	C	2.560608	3.647656	3.596476	2.483981	1.477527

7	C	3.325135	4.394213	4.402084	3.375965	2.497590
8	H	1.076443	2.213588	3.264924	3.230345	2.160237
9	H	2.211470	1.074633	2.171003	3.246365	3.267930
10	H	3.371232	4.254046	3.875467	2.585844	2.076040
11	H	2.745358	3.991580	4.215613	3.268439	2.089379
12	H	3.062457	4.159583	4.464352	3.710876	2.702241
13	H	3.731020	4.540416	4.280959	3.239591	2.774636
14	Br	5.289835	5.497737	4.389415	3.275407	3.973656
15	H	3.279685	3.309299	2.212447	1.111232	2.156976
16	C	3.597247	2.537475	1.421892	2.427740	3.530409
17	C	4.338291	3.050116	2.435325	3.657142	4.602481
18	H	4.260067	3.413548	2.085714	2.555049	3.847660
19	H	5.399058	4.127280	3.399545	4.507596	5.565413
20	H	4.194500	2.837392	2.748949	4.087819	4.777902
21	O	4.531848	5.701955	5.733066	4.626156	3.712142
22	H	5.184147	6.260189	6.089855	4.883303	4.180285
23	C	7.194473	7.915156	7.233061	5.971670	5.920206
24	C	7.570833	8.441693	7.864110	6.536291	6.299035
25	O	6.660238	7.580757	7.138052	5.860904	5.487063
26	H	6.593841	7.184894	6.381003	5.139991	5.275761
27	H	7.974269	8.647880	7.954100	6.754017	6.747434
28	H	8.554014	9.467398	8.927783	7.603803	7.316278
29	C	7.294366	8.161291	7.566740	6.221520	5.995271
30	H	7.347905	8.336774	7.900475	6.566834	6.140935
31	H	8.188323	8.978771	8.285367	6.956830	6.861219
32	H	6.428034	7.214521	6.557858	5.220789	5.094286

		6	7	8	9	10
6	C	0.000000				
7	C	1.538804	0.000000			
8	H	2.855678	3.448653	0.000000		
9	H	4.673341	5.350900	2.754276	0.000000	
10	H	1.091180	2.173505	3.824570	5.317535	0.000000
11	H	1.090751	2.170080	2.687427	4.924383	1.785088
12	H	2.168577	1.096566	2.959442	4.983109	3.071498
13	H	2.160640	1.096160	4.090372	5.505372	2.461862
14	Br	3.850540	4.369709	6.130886	6.490384	2.989118
15	H	2.795859	3.602353	4.247135	4.292227	2.466976
16	C	4.881455	5.634460	4.632183	2.873255	4.980482
17	C	6.029453	6.747567	5.263653	2.895718	6.227291
18	H	5.010144	5.745184	5.332383	3.904178	4.887278
19	H	6.951145	7.652722	6.340103	3.950186	7.050428
20	H	6.252023	6.948861	4.971994	2.312919	6.610886
21	O	2.407319	1.404403	4.466802	6.651578	2.745100
22	H	2.861242	1.961325	5.261850	7.257200	2.844023

23	C	4.929142	4.353903	7.622674	8.954871	4.323991
24	C	5.088163	4.691363	7.878462	9.505438	4.421986
25	O	4.272840	3.533040	6.900457	8.614329	3.865399
26	H	4.474772	4.113832	7.147789	8.222188	3.778183
27	H	5.821864	5.064178	8.400393	9.657956	5.301768
28	H	6.055239	5.551195	8.797526	10.525419	5.445909
29	C	4.790248	4.853967	7.621657	9.233816	3.946990
30	H	4.816511	4.926794	7.534688	9.393048	4.089065
31	H	5.741564	5.895913	8.571926	10.049688	4.818232
32	H	4.014945	4.302516	6.848674	8.286254	3.062196

		11	12	13	14	15
11	H	0.000000				
12	H	2.542191	0.000000			
13	H	3.065069	1.775244	0.000000		
14	Br	4.743102	5.288690	3.816568	0.000000	
15	H	3.702313	4.191926	3.247797	2.198218	0.000000
16	C	5.563254	5.749208	5.331691	4.697166	2.813969
17	C	6.623821	6.717891	6.479012	5.994671	4.137897
18	H	5.798748	6.038952	5.304921	3.977258	2.479607
19	H	7.592521	7.677123	7.293941	6.420905	4.800779
20	H	6.724137	6.762483	6.802312	6.794152	4.781433
21	O	2.614695	2.032592	2.083839	4.996481	4.708207
22	H	3.238083	2.798823	2.198586	4.594211	4.739987
23	C	5.632074	5.307357	3.808216	3.891340	5.275286
24	C	5.544650	5.684580	4.471363	4.524242	5.898615
25	O	4.790164	4.435313	3.294756	4.478389	5.391610
26	H	5.297703	5.104810	3.450398	2.847095	4.346112
27	H	6.559721	5.914620	4.412473	4.672823	6.058447
28	H	6.435660	6.479916	5.366554	5.575195	6.982242
29	C	5.103409	5.912911	4.820012	4.169131	5.567419
30	H	4.895975	5.919427	5.125675	4.948134	6.058503
31	H	6.060495	6.968505	5.796972	4.541932	6.201497
32	H	4.424585	5.391626	4.234133	3.182384	4.534051

		16	17	18	19	20
16	C	0.000000				
17	C	1.326535	0.000000			
18	H	1.082893	2.122847	0.000000		
19	H	2.079885	1.081102	2.446885	0.000000	
20	H	2.126420	1.082593	3.100494	1.847120	0.000000
21	O	6.965817	8.111164	7.008591	9.008015	8.320465
22	H	7.214064	8.425150	7.110542	9.252638	8.746677
23	C	7.921849	9.207872	7.411262	9.770630	9.830732
24	C	8.674246	9.987398	8.211427	10.610431	10.564448
25	O	8.050753	9.324063	7.717088	10.018784	9.810269

26	H	6.970081	8.260137	6.399238	8.778397	8.937321
27	H	8.573367	9.823136	8.039319	10.340070	10.459373
28	H	9.749159	11.058724	9.284991	11.680477	11.627069
29	C	8.378454	9.700944	7.910630	10.326231	10.284345
30	H	8.835464	10.139069	8.472407	10.836485	10.636471
31	H	8.982027	10.303920	8.419588	10.853704	10.954297
32	H	7.334536	8.655766	6.860618	9.272198	9.256029

		21	22	23	24	25
21	O	0.000000				
22	H	0.977068	0.000000			
23	C	3.968878	3.026465	0.000000		
24	C	3.959687	3.010534	1.468107	0.000000	
25	O	2.783513	1.808900	1.450356	1.447829	0.000000
26	H	4.065466	3.234199	1.087386	2.208652	2.145592
27	H	4.678038	3.753642	1.086584	2.216546	2.133429
28	H	4.655695	3.720520	2.191622	1.088941	2.108825
29	C	4.215111	3.428672	2.601988	1.503840	2.520212
30	H	4.086637	3.435194	3.428413	2.149478	2.906509
31	H	5.307375	4.509131	3.165986	2.135880	3.425830
32	H	3.956236	3.276649	2.717092	2.151986	2.742421

		26	27	28	29	30
26	H	0.000000				
27	H	1.852552	0.000000			
28	H	3.120675	2.503364	0.000000		
29	C	2.812715	3.540962	2.208200	0.000000	
30	H	3.741749	4.339134	2.583306	1.094293	0.000000
31	H	3.335824	3.957787	2.531443	1.094416	1.769921
32	H	2.505236	3.772218	3.099834	1.091792	1.786791

		31	32
31	H	0.000000	
32	H	1.767924	0.000000

Stoichiometry C10H17BrN2O2
Framework group C1[X(C10H17BrN2O2)]
Deg. of freedom 90
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.711113	2.114434	-0.440979
2	6	0	-3.788494	1.349121	-0.131253

3	7	0	-3.319916	0.050046	0.038677
4	6	0	-1.988308	0.040744	-0.166479
5	7	0	-1.603294	1.280942	-0.462910
6	6	0	-0.201257	1.680336	-0.703461
7	6	0	0.455082	2.252397	0.565350
8	1	0	-2.638735	3.167298	-0.653034
9	1	0	-4.824637	1.613691	-0.025201
10	1	0	0.330270	0.786849	-1.034874
11	1	0	-0.196562	2.428606	-1.497065
12	1	0	-0.161795	3.066919	0.963439
13	1	0	0.510477	1.464191	1.325105
14	35	0	0.525313	-2.059113	-0.141966
15	1	0	-1.292956	-0.824192	-0.109858
16	6	0	-4.050113	-1.125518	0.365232
17	6	0	-5.360377	-1.169604	0.567616
18	1	0	-3.409849	-1.996320	0.431743
19	1	0	-5.824086	-2.115140	0.811989
20	1	0	-6.006396	-0.303372	0.501972
21	8	0	1.718699	2.777019	0.248505
22	1	0	2.403654	2.097851	0.404161
23	6	0	3.796049	-0.458990	1.230774
24	6	0	4.544067	0.009358	0.057547
25	8	0	3.721173	0.928553	0.815264
26	1	0	2.882812	-1.028988	1.077456
27	1	0	4.313935	-0.605035	2.174772
28	1	0	5.605033	0.214057	0.192605
29	6	0	4.110267	-0.305195	-1.347589
30	1	0	4.294496	0.547280	-2.008514
31	1	0	4.684810	-1.155943	-1.726899
32	1	0	3.052272	-0.572783	-1.380056

Rotational constants (GHZ): 0.5994512 0.2213243 0.1723290

****

Population analysis using the SCF density.

****

Orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A)

The electronic state is 1-A.

Alpha occ. eigenvalues -- -482.69901 -62.35241 -56.17020 -56.17009 -56.17006
Alpha occ. eigenvalues -- -19.13299 -19.11271 -14.45380 -14.44198 -10.29564
Alpha occ. eigenvalues -- -10.27333 -10.27242 -10.27039 -10.23843 -10.23283
Alpha occ. eigenvalues -- -10.22203 -10.22168 -10.20689 -10.15291 -8.56153
Alpha occ. eigenvalues -- -6.38486 -6.38418 -6.38407 -2.49727 -2.49704
Alpha occ. eigenvalues -- -2.49694 -2.49642 -2.49642 -1.11700 -1.06477
Alpha occ. eigenvalues -- -1.02158 -1.00144 -0.85615 -0.82567 -0.78276

Alpha occ. eigenvalues -- -0.73829 -0.71401 -0.68816 -0.65787 -0.65418
Alpha occ. eigenvalues -- -0.63577 -0.63410 -0.58864 -0.58571 -0.54369
Alpha occ. eigenvalues -- -0.53766 -0.52266 -0.51918 -0.50194 -0.49657
Alpha occ. eigenvalues -- -0.49462 -0.48351 -0.46702 -0.45740 -0.44716
Alpha occ. eigenvalues -- -0.43719 -0.41800 -0.40709 -0.39508 -0.39128
Alpha occ. eigenvalues -- -0.36736 -0.35797 -0.33691 -0.32119 -0.30400
Alpha occ. eigenvalues -- -0.30121 -0.28064 -0.27343 -0.20342 -0.19834
Alpha occ. eigenvalues -- -0.19649
Alpha virt. eigenvalues -- -0.08377 -0.04680 -0.03103 -0.01426 -0.00829
Alpha virt. eigenvalues -- -0.00457 0.00845 0.00889 0.01038 0.01497
Alpha virt. eigenvalues -- 0.02483 0.02838 0.03419 0.04013 0.04171
Alpha virt. eigenvalues -- 0.04796 0.05352 0.05672 0.05729 0.06359
Alpha virt. eigenvalues -- 0.06844 0.07204 0.07844 0.07919 0.08120
Alpha virt. eigenvalues -- 0.08628 0.08758 0.09261 0.09464 0.09842
Alpha virt. eigenvalues -- 0.09888 0.10154 0.10621 0.10960 0.11070
Alpha virt. eigenvalues -- 0.11813 0.11989 0.12539 0.12693 0.12846
Alpha virt. eigenvalues -- 0.12969 0.13189 0.13477 0.13841 0.14235
Alpha virt. eigenvalues -- 0.14728 0.14947 0.15057 0.15220 0.15730
Alpha virt. eigenvalues -- 0.16038 0.16140 0.16474 0.16642 0.17072
Alpha virt. eigenvalues -- 0.17822 0.17913 0.17983 0.18493 0.18629
Alpha virt. eigenvalues -- 0.19136 0.19455 0.19820 0.20439 0.20762
Alpha virt. eigenvalues -- 0.20816 0.21533 0.21688 0.22085 0.22277
Alpha virt. eigenvalues -- 0.22778 0.23131 0.23301 0.23937 0.24174
Alpha virt. eigenvalues -- 0.24340 0.24803 0.25105 0.26191 0.26246
Alpha virt. eigenvalues -- 0.26641 0.27424 0.27728 0.28049 0.28687
Alpha virt. eigenvalues -- 0.29119 0.29467 0.29977 0.30227 0.30458
Alpha virt. eigenvalues -- 0.30861 0.31394 0.32395 0.32918 0.34271
Alpha virt. eigenvalues -- 0.34427 0.35348 0.35943 0.36342 0.36428
Alpha virt. eigenvalues -- 0.36748 0.37462 0.38346 0.39041 0.39923
Alpha virt. eigenvalues -- 0.40304 0.41089 0.41770 0.44194 0.44244
Alpha virt. eigenvalues -- 0.45845 0.47258 0.47946 0.48568 0.50262
Alpha virt. eigenvalues -- 0.50754 0.51579 0.52508 0.52732 0.53157
Alpha virt. eigenvalues -- 0.53587 0.54086 0.55055 0.55605 0.56559
Alpha virt. eigenvalues -- 0.57679 0.58059 0.58487 0.59567 0.60520
Alpha virt. eigenvalues -- 0.61019 0.61891 0.62416 0.62890 0.63309
Alpha virt. eigenvalues -- 0.63646 0.65056 0.65539 0.65800 0.66387
Alpha virt. eigenvalues -- 0.66776 0.67254 0.68047 0.68772 0.69391
Alpha virt. eigenvalues -- 0.69847 0.70258 0.71079 0.71293 0.72316
Alpha virt. eigenvalues -- 0.72642 0.74094 0.74591 0.75050 0.75792
Alpha virt. eigenvalues -- 0.76278 0.77376 0.78955 0.79001 0.79634
Alpha virt. eigenvalues -- 0.80312 0.81550 0.82008 0.82555 0.82836
Alpha virt. eigenvalues -- 0.85744 0.86335 0.86974 0.88249 0.89882
Alpha virt. eigenvalues -- 0.90563 0.92658 0.94203 0.95764 0.97903
Alpha virt. eigenvalues -- 0.98397 0.99892 1.01017 1.01792 1.02467

Alpha virt. eigenvalues --	1.02993	1.03433	1.04742	1.06109	1.08943
Alpha virt. eigenvalues --	1.09236	1.10257	1.10629	1.11797	1.13239
Alpha virt. eigenvalues --	1.15756	1.16693	1.17106	1.19319	1.20525
Alpha virt. eigenvalues --	1.21846	1.24276	1.26007	1.28137	1.30785
Alpha virt. eigenvalues --	1.32830	1.33200	1.36670	1.37424	1.38423
Alpha virt. eigenvalues --	1.42396	1.43953	1.45088	1.47237	1.47624
Alpha virt. eigenvalues --	1.48373	1.49222	1.50397	1.50768	1.51210
Alpha virt. eigenvalues --	1.51797	1.53699	1.55040	1.57050	1.57364
Alpha virt. eigenvalues --	1.57695	1.59141	1.59694	1.60068	1.61212
Alpha virt. eigenvalues --	1.61494	1.62169	1.62986	1.63309	1.65720
Alpha virt. eigenvalues --	1.66249	1.67917	1.68570	1.68995	1.69536
Alpha virt. eigenvalues --	1.71442	1.71912	1.72677	1.72876	1.73901
Alpha virt. eigenvalues --	1.75378	1.76946	1.79645	1.80089	1.81041
Alpha virt. eigenvalues --	1.81945	1.83858	1.84810	1.85966	1.86920
Alpha virt. eigenvalues --	1.90192	1.90688	1.92115	1.94872	1.96744
Alpha virt. eigenvalues --	1.97801	1.98998	2.00860	2.04175	2.04882
Alpha virt. eigenvalues --	2.05521	2.07705	2.09191	2.09990	2.11338
Alpha virt. eigenvalues --	2.12101	2.12484	2.14133	2.14537	2.16143
Alpha virt. eigenvalues --	2.18915	2.19839	2.21261	2.22418	2.24543
Alpha virt. eigenvalues --	2.25177	2.27324	2.29053	2.30553	2.35290
Alpha virt. eigenvalues --	2.37059	2.39425	2.40767	2.42405	2.44906
Alpha virt. eigenvalues --	2.46167	2.46530	2.49619	2.50120	2.50635
Alpha virt. eigenvalues --	2.51320	2.52042	2.53922	2.55359	2.56410
Alpha virt. eigenvalues --	2.56557	2.57064	2.58629	2.59551	2.61398
Alpha virt. eigenvalues --	2.62215	2.64913	2.65106	2.69244	2.69970
Alpha virt. eigenvalues --	2.71163	2.71702	2.71998	2.72575	2.74381
Alpha virt. eigenvalues --	2.74580	2.75808	2.76804	2.77809	2.80205
Alpha virt. eigenvalues --	2.81236	2.81880	2.82682	2.84649	2.85122
Alpha virt. eigenvalues --	2.85624	2.87869	2.87900	2.89235	2.91122
Alpha virt. eigenvalues --	2.93504	2.95325	2.97694	3.00793	3.09435
Alpha virt. eigenvalues --	3.10039	3.12515	3.12898	3.15312	3.17943
Alpha virt. eigenvalues --	3.22038	3.24602	3.27048	3.31570	3.31822
Alpha virt. eigenvalues --	3.36782	3.38094	3.49548	3.55294	3.58490
Alpha virt. eigenvalues --	3.63830	3.65643	3.70282	3.72191	3.75197
Alpha virt. eigenvalues --	3.76166	3.81006	3.81703	3.82058	3.83220
Alpha virt. eigenvalues --	3.84529	3.85974	3.87926	3.89768	3.94543
Alpha virt. eigenvalues --	4.04854	4.05830	4.08602	4.12519	4.20180
Alpha virt. eigenvalues --	4.28470	4.28953	4.30954	4.33976	4.45664
Alpha virt. eigenvalues --	4.52000	4.69330	4.90127	5.02227	5.10565
Alpha virt. eigenvalues --	5.12518	5.22283	5.43100	5.49049	5.59630
Alpha virt. eigenvalues --	5.76408	6.76957	7.68901	7.74657	7.79222
Alpha virt. eigenvalues --	23.69802	23.74590	23.82893	23.85718	23.87451
Alpha virt. eigenvalues --	23.88260	23.90806	23.99467	24.13588	24.22273
Alpha virt. eigenvalues --	35.43511	35.56816	48.05536	49.90780	49.94929

Alpha virt. eigenvalues -- 289.89764 289.95333 289.993051020.84461

Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	7.461763	-1.404750	0.304417	-0.286925	-0.110806	0.096507
2	C	-1.404750	6.847315	-0.116134	0.338196	0.371118	-0.363381
3	N	0.304417	-0.116134	6.791912	0.012592	-0.353433	-0.114693
4	C	-0.286925	0.338196	0.012592	7.544860	0.677716	-0.788951
5	N	-0.110806	0.371118	-0.353433	0.677716	6.864018	-0.088600
6	C	0.096507	-0.363381	-0.114693	-0.788951	-0.088600	8.044437
7	C	-0.157210	0.207968	-0.024680	0.188280	0.077577	-0.786820
8	H	0.522631	-0.117734	0.035670	0.013457	-0.065873	-0.039914
9	H	-0.116033	0.505830	-0.086026	0.014678	0.030773	0.009517
10	H	0.097057	-0.084624	0.025269	0.052135	-0.058012	0.267107
11	H	-0.030995	0.030801	-0.004416	-0.036668	-0.044766	0.474969
12	H	-0.001866	-0.056855	0.015953	-0.007843	-0.038884	0.009891
13	H	-0.011165	0.031063	-0.012457	0.025899	0.036956	-0.078695
14	Br	-0.031544	0.016697	0.001839	-0.155217	-0.028139	-0.031539
15	H	-0.140959	-0.081432	0.108032	-0.892673	-0.173241	0.181749
16	C	0.355544	-0.383881	0.281394	-0.185745	-0.156658	-0.215299
17	C	-0.280740	0.202639	-0.002757	-0.388161	-0.070448	-0.091543
18	H	-0.000761	0.019605	-0.095375	0.171157	0.023318	0.000544
19	H	-0.003246	0.005714	0.023339	-0.012661	-0.000008	0.000286
20	H	-0.006794	0.013606	-0.034194	0.004392	-0.000545	-0.005927
21	O	-0.009657	0.006196	0.000497	0.024601	0.021591	-0.266875
22	H	0.002962	0.001219	-0.000063	0.015023	0.013766	-0.067586
23	C	-0.002496	0.001116	0.000600	0.015324	0.001271	-0.090523
24	C	0.008911	-0.002447	0.000207	-0.012512	0.004707	0.071114
25	O	-0.004736	0.000591	-0.000034	-0.005249	-0.006947	0.005284
26	H	0.000841	0.000808	-0.001307	0.018030	0.003445	-0.019303
27	H	-0.000211	0.000116	0.000031	0.000672	-0.000396	0.000926
28	H	0.000041	0.000010	-0.000001	0.000288	0.000283	0.000319
29	C	-0.007921	0.001876	-0.000574	-0.009006	-0.003368	-0.005339
30	H	0.000839	-0.000528	0.000010	-0.002472	-0.000464	0.006808
31	H	-0.000289	0.000154	-0.000014	0.000653	-0.000104	-0.000820
32	H	-0.004021	0.002823	0.000173	0.013728	-0.003485	0.006098

		7	8	9	10	11	12
1	C	-0.157210	0.522631	-0.116033	0.097057	-0.030995	-0.001866
2	C	0.207968	-0.117734	0.505830	-0.084624	0.030801	-0.056855
3	N	-0.024680	0.035670	-0.086026	0.025269	-0.004416	0.015953
4	C	0.188280	0.013457	0.014678	0.052135	-0.036668	-0.007843
5	N	0.077577	-0.065873	0.030773	-0.058012	-0.044766	-0.038884
6	C	-0.786820	-0.039914	0.009517	0.267107	0.474969	0.009891
7	C	6.073851	0.007630	0.000233	-0.142410	-0.156018	0.388539
8	H	0.007630	0.486629	-0.009254	0.005704	-0.016129	-0.006697

9	H	0.000233	-0.009254	0.498707	-0.000913	0.001848	-0.000745
10	H	-0.142410	0.005704	-0.000913	0.670610	-0.056150	0.011099
11	H	-0.156018	-0.016129	0.001848	-0.056150	0.627643	-0.019061
12	H	0.388539	-0.006697	-0.000745	0.011099	-0.019061	0.699509
13	H	0.359747	0.000628	0.000704	-0.028341	0.020587	-0.104615
14	Br	-0.018699	-0.002271	-0.000184	0.035299	0.012467	0.003671
15	H	-0.105614	-0.009777	-0.007770	-0.021655	0.014745	0.032790
16	C	0.009165	0.009207	-0.004934	0.019302	-0.003678	0.000612
17	C	0.007570	-0.004178	-0.013504	-0.005782	0.000716	-0.001003
18	H	0.003822	0.000693	0.002901	0.001262	-0.001416	-0.001078
19	H	-0.000189	-0.000172	-0.000995	-0.000132	0.000066	0.000050
20	H	0.000904	0.000592	0.004968	0.000166	-0.000212	-0.000251
21	O	0.378063	0.000478	-0.000052	-0.004514	0.014710	-0.088265
22	H	-0.013592	0.000735	-0.000128	0.023565	-0.009565	0.015695
23	C	0.014510	-0.000028	-0.000046	0.012889	-0.010142	-0.000398
24	C	-0.003087	0.000304	0.000024	0.017932	0.008631	0.000549
25	O	0.017788	-0.000272	0.000016	-0.022844	0.004650	-0.002099
26	H	0.008251	0.000227	-0.000012	0.010066	-0.002102	-0.001214
27	H	-0.002517	-0.000022	0.000006	-0.002151	0.000044	-0.000721
28	H	-0.000420	0.000009	0.000000	-0.002192	0.000567	0.000136
29	C	0.005830	-0.000345	-0.000019	-0.009689	0.000656	0.001416
30	H	-0.002949	0.000039	0.000006	0.005179	-0.000764	-0.000044
31	H	-0.000170	-0.000017	0.000000	-0.001344	0.000262	-0.000107
32	H	0.009212	-0.000089	0.000018	-0.042368	0.000030	-0.000531

		13	14	15	16	17	18
1	C	-0.011165	-0.031544	-0.140959	0.355544	-0.280740	-0.000761
2	C	0.031063	0.016697	-0.081432	-0.383881	0.202639	0.019605
3	N	-0.012457	0.001839	0.108032	0.281394	-0.002757	-0.095375
4	C	0.025899	-0.155217	-0.892673	-0.185745	-0.388161	0.171157
5	N	0.036956	-0.028139	-0.173241	-0.156658	-0.070448	0.023318
6	C	-0.078695	-0.031539	0.181749	-0.215299	-0.091543	0.000544
7	C	0.359747	-0.018699	-0.105614	0.009165	0.007570	0.003822
8	H	0.000628	-0.002271	-0.009777	0.009207	-0.004178	0.000693
9	H	0.000704	-0.000184	-0.007770	-0.004934	-0.013504	0.002901
10	H	-0.028341	0.035299	-0.021655	0.019302	-0.005782	0.001262
11	H	0.020587	0.012467	0.014745	-0.003678	0.000716	-0.001416
12	H	-0.104615	0.003671	0.032790	0.000612	-0.001003	-0.001078
13	H	0.627838	-0.012029	-0.062523	0.001288	0.000400	0.001366
14	Br	-0.012029	35.689938	0.253080	0.032214	0.034547	-0.005430
15	H	-0.062523	0.253080	1.740373	-0.059540	0.190774	-0.086181
16	C	0.001288	0.032214	-0.059540	6.313160	-0.447579	0.406218
17	C	0.000400	0.034547	0.190774	-0.447579	6.659902	-0.110732
18	H	0.001366	-0.005430	-0.086181	0.406218	-0.110732	0.464180
19	H	-0.000036	-0.000372	0.007349	-0.094625	0.449605	-0.008854

20	H	0.000081	0.000316	0.000666	0.072586	0.310932	0.001928
21	O	-0.008283	-0.006050	-0.007710	0.000668	0.000108	0.000035
22	H	-0.010436	-0.007454	-0.001773	0.000778	0.000318	0.000086
23	C	-0.006838	-0.104772	0.010195	0.001989	0.000288	-0.000495
24	C	-0.005701	0.111876	-0.005851	-0.000595	-0.000145	0.000378
25	O	0.012459	0.000393	-0.000687	-0.000159	-0.000011	-0.000030
26	H	-0.005363	0.015058	-0.022575	0.000132	0.000197	0.000624
27	H	0.003717	-0.002326	-0.001652	0.000048	-0.000027	0.000007
28	H	0.000335	0.002212	-0.000862	-0.000010	0.000000	0.000011
29	C	0.001665	-0.057856	0.011498	-0.000325	0.000165	-0.000183
30	H	-0.000334	0.004276	0.000338	-0.000174	-0.000049	0.000002
31	H	0.000491	-0.000318	-0.000322	0.000093	0.000023	-0.000005
32	H	0.005724	-0.010114	-0.008702	-0.000144	-0.000067	-0.000046

		19	20	21	22	23	24
1	C	-0.003246	-0.006794	-0.009657	0.002962	-0.002496	0.008911
2	C	0.005714	0.013606	0.006196	0.001219	0.001116	-0.002447
3	N	0.023339	-0.034194	0.000497	-0.000063	0.000600	0.000207
4	C	-0.012661	0.004392	0.024601	0.015023	0.015324	-0.012512
5	N	-0.000008	-0.000545	0.021591	0.013766	0.001271	0.004707
6	C	0.000286	-0.005927	-0.266875	-0.067586	-0.090523	0.071114
7	C	-0.000189	0.000904	0.378063	-0.013592	0.014510	-0.003087
8	H	-0.000172	0.000592	0.000478	0.000735	-0.000028	0.000304
9	H	-0.000995	0.004968	-0.000052	-0.000128	-0.000046	0.000024
10	H	-0.000132	0.000166	-0.004514	0.023565	0.012889	0.017932
11	H	0.000066	-0.000212	0.014710	-0.009565	-0.010142	0.008631
12	H	0.000050	-0.000251	-0.088265	0.015695	-0.000398	0.000549
13	H	-0.000036	0.000081	-0.008283	-0.010436	-0.006838	-0.005701
14	Br	-0.000372	0.000316	-0.006050	-0.007454	-0.104772	0.111876
15	H	0.007349	0.000666	-0.007710	-0.001773	0.010195	-0.005851
16	C	-0.094625	0.072586	0.000668	0.000778	0.001989	-0.000595
17	C	0.449605	0.310932	0.000108	0.000318	0.000288	-0.000145
18	H	-0.008854	0.001928	0.000035	0.000086	-0.000495	0.000378
19	H	0.460913	-0.020022	-0.000001	-0.000003	0.000009	-0.000005
20	H	-0.020022	0.533259	0.000008	0.000024	0.000004	-0.000001
21	O	-0.000001	0.000008	7.978970	0.269043	0.011506	-0.064264
22	H	-0.000003	0.000024	0.269043	0.394357	0.018595	0.020573
23	C	0.000009	0.000004	0.011506	0.018595	6.734418	-1.305769
24	C	-0.000005	-0.000001	-0.064264	0.020573	-1.305769	7.045866
25	O	0.000000	-0.000001	0.064777	-0.083909	0.102278	0.041199
26	H	-0.000018	0.000019	-0.001353	0.012206	0.325087	0.080397
27	H	0.000000	-0.000001	0.003265	-0.009039	0.347854	-0.002639
28	H	0.000000	0.000000	0.001836	0.000532	-0.027192	0.284756
29	C	0.000000	0.000004	0.031682	-0.005972	0.178088	-0.170962
30	H	0.000000	-0.000002	-0.004818	-0.005469	0.027082	-0.006710

31	H	0.000000	0.000001	0.000731	-0.000625	-0.008405	-0.076075
32	H	0.000010	-0.000007	0.008858	-0.003428	-0.007469	-0.120338
		25	26	27	28	29	30
1	C	-0.004736	0.000841	-0.000211	0.000041	-0.007921	0.000839
2	C	0.000591	0.000808	0.000116	0.000010	0.001876	-0.000528
3	N	-0.000034	-0.001307	0.000031	-0.000001	-0.000574	0.000010
4	C	-0.005249	0.018030	0.000672	0.000288	-0.009006	-0.002472
5	N	-0.006947	0.003445	-0.000396	0.000283	-0.003368	-0.000464
6	C	0.005284	-0.019303	0.000926	0.000319	-0.005339	0.006808
7	C	0.017788	0.008251	-0.002517	-0.000420	0.005830	-0.002949
8	H	-0.000272	0.000227	-0.000022	0.000009	-0.000345	0.000039
9	H	0.000016	-0.000012	0.000006	0.000000	-0.000019	0.000006
10	H	-0.022844	0.010066	-0.002151	-0.002192	-0.009689	0.005179
11	H	0.004650	-0.002102	0.000044	0.000567	0.000656	-0.000764
12	H	-0.002099	-0.001214	-0.000721	0.000136	0.001416	-0.000044
13	H	0.012459	-0.005363	0.003717	0.000335	0.001665	-0.000334
14	Br	0.000393	0.015058	-0.002326	0.002212	-0.057856	0.004276
15	H	-0.000687	-0.022575	-0.001652	-0.000862	0.011498	0.000338
16	C	-0.000159	0.000132	0.000048	-0.000010	-0.000325	-0.000174
17	C	-0.000011	0.000197	-0.000027	0.000000	0.000165	-0.000049
18	H	-0.000030	0.000624	0.000007	0.000011	-0.000183	0.000002
19	H	0.000000	-0.000018	0.000000	0.000000	0.000000	0.000000
20	H	-0.000001	0.000019	-0.000001	0.000000	0.000004	-0.000002
21	O	0.064777	-0.001353	0.003265	0.001836	0.031682	-0.004818
22	H	-0.083909	0.012206	-0.009039	0.000532	-0.005972	-0.005469
23	C	0.102278	0.325087	0.347854	-0.027192	0.178088	0.027082
24	C	0.041199	0.080397	-0.002639	0.284756	-0.170962	-0.006710
25	O	8.293370	-0.053266	-0.036217	-0.010684	-0.068359	-0.024429
26	H	-0.053266	0.530333	-0.033616	0.010018	-0.031433	-0.006872
27	H	-0.036217	-0.033616	0.572578	-0.000858	0.005352	0.001939
28	H	-0.010684	0.010018	-0.000858	0.559649	-0.013407	-0.011125
29	C	-0.068359	-0.031433	0.005352	-0.013407	5.508164	0.363555
30	H	-0.024429	-0.006872	0.001939	-0.011125	0.363555	0.610942
31	H	0.017243	0.000486	-0.000017	0.001618	0.432892	-0.049405
32	H	0.020358	-0.000789	0.002867	0.019467	0.394317	-0.052811
		31	32				
1	C	-0.000289	-0.004021				
2	C	0.000154	0.002823				
3	N	-0.000014	0.000173				
4	C	0.000653	0.013728				
5	N	-0.000104	-0.003485				
6	C	-0.000820	0.006098				
7	C	-0.000170	0.009212				
8	H	-0.000017	-0.000089				

9	H	0.000000	0.000018
10	H	-0.001344	-0.042368
11	H	0.000262	0.000030
12	H	-0.000107	-0.000531
13	H	0.000491	0.005724
14	Br	-0.000318	-0.010114
15	H	-0.000322	-0.008702
16	C	0.000093	-0.000144
17	C	0.000023	-0.000067
18	H	-0.000005	-0.000046
19	H	0.000000	0.000010
20	H	0.000001	-0.000007
21	O	0.000731	0.008858
22	H	-0.000625	-0.003428
23	C	-0.008405	-0.007469
24	C	-0.076075	-0.120338
25	O	0.017243	0.020358
26	H	0.000486	-0.000789
27	H	-0.000017	0.002867
28	H	0.001618	0.019467
29	C	0.432892	0.394317
30	H	-0.049405	-0.052811
31	H	0.573706	-0.019976
32	H	-0.019976	0.621045

Mulliken charges:

		1
1	C	-0.238385
2	C	0.006304
3	N	0.244223
4	C	-0.347599
5	N	0.077638
6	C	-0.119751
7	C	-0.344565
8	H	0.188138
9	H	0.170386
10	H	0.228481
11	H	0.178691
12	H	0.152369
13	H	0.215866
14	Br	-0.739571
15	H	0.139912
16	C	0.048950
17	C	-0.441457
18	H	0.212450

19	H	0.193999
20	H	0.123501
21	O	-0.355782
22	H	0.429565
23	C	-0.238530
24	C	0.079677
25	O	-0.260475
26	H	0.162998
27	H	0.152986
28	H	0.184665
29	C	-0.552404
30	H	0.148404
31	H	0.129659
32	H	0.169658

Sum of Mulliken charges = 0.00000

Mulliken charges with hydrogens summed into heavy atoms:

		1
1	C	-0.050247
2	C	0.176690
3	N	0.244223
4	C	-0.207687
5	N	0.077638
6	C	0.287422
7	C	0.023670
14	Br	-0.739571
16	C	0.261400
17	C	-0.123958
21	O	0.073783
23	C	0.077454
24	C	0.264342
25	O	-0.260475
29	C	-0.104682

Electronic spatial extent (au): <R**2>= 6085.9469

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= -8.9875 Y= 5.0057 Z= -0.0991 Tot= 10.2879

Quadrupole moment (field-independent basis, Debye-Ang):

XX= -63.8843 YY= -119.9986 ZZ= -107.2250

XY= -9.5949 XZ= -2.2476 YZ= -6.1613

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

XX= 33.1517 YY= -22.9626 ZZ= -10.1891

XY= -9.5949 XZ= -2.2476 YZ= -6.1613

Octapole moment (field-independent basis, Debye-Ang**2):

XXX= -83.8975 YYY= -17.8947 ZZZ= 1.0570
XYY= -60.1105
XXY= -39.1584 XXZ= 9.1366 XZZ= 24.1610
YZZ= -10.1168
YYZ= -4.0828 XYZ= 1.9760
Hexadecapole moment (field-independent basis, Debye-Ang**3):
XXXX= -4706.3923 YYYY= -1828.3705 ZZZZ= -411.1814
XXXY= -73.8182
XXXZ= -89.0634 YYYX= -95.0363 YYYZ= -30.9743
ZZZX= 33.5365
ZZZY= 4.6175 XXYY= -1198.8964 XXZZ= -1076.2428
YYZZ= -360.3491
XXYZ= -62.1079 YYXZ= -9.5578 ZZXY= -11.9854
N-N= 1.307196544036D+03 E-N=-1.028726439868D+04 KE= 3.219705190211D+03
1\1\GINC-NODE12\FOpt\RB3LYP\6-311++G(d,p)\C10H17Br1N2O2\SUQIAN\22-Jul-
2024\0\\# opt b3lyp/6-311++g(d,p)\\oh\\0,1\C,-1.3766755869,-1.91007880
27,-0.2564301242\C,-2.5077580369,-1.1694113582,-0.1362276955\N,-2.1087
571911,0.112186305,0.2303012262\C,-0.7651110361,0.1351698938,0.3274640
947\N,-0.3053543934,-1.0817403065,0.0411926471\C,1.1277550784,-1.43787
7287,-0.0083032571\C,1.6830727774,-1.3724169247,-1.4419189857\H,-1.243
2527924,-2.9457926882,-0.5176275404\H,-3.5380892155,-1.442511432,-0.27
28663522\H,1.6527399808,-0.7289287231,0.6339249238\H,1.2369059013,-2.4
47614485,0.3895096183\H,1.0637774618,-1.9884028595,-2.1048611861\H,1.6
353298825,-0.3362401786,-1.7963546081\Br,1.6504711291,2.2345688306,1.0
244434033\H,-0.1127538749,0.9937342965,0.5960414531\C,-2.9121915208,1.
257183592,0.4857444444\C,-4.2364418825,1.2829290828,0.4123053374\H,-2.
3157987819,2.1210385358,0.7516927258\H,-4.7579772764,2.2055516172,0.62
57303412\H,-4.8388201642,0.4231351609,0.1479146661\O,2.9906287605,-1.8
843275006,-1.4662370463\H,3.6305713048,-1.1529278785,-1.365293533\C,4.
8369873255,1.6118760139,-1.120526775\C,5.7104681645,0.7520195972,-0.31
24316255\O,4.8563272852,0.1768884256,-1.3302123534\H,3.9206666602,1.99
37921552,-0.6767882496\H,5.2570982575,2.179762432,-1.9461644567\H,6.76
11169239,0.7039473403,-0.5945995057\C,5.3995338211,0.413259078,1.11938
40503\H,5.6788145724,-0.6213773325,1.3407574882\H,5.9735183261,1.06669
01493,1.7837002312\H,4.3396646097,0.5615304107,1.3354924833\\Version=E
M64L-G09RevD.01\State=1-A\HF=-3225.5237126\RMSD=5.316e-09\RMSF=3.523e-
06\Dipole=-3.4362801,-2.0648827,-0.5578579\Quadrupole=24.085684,-10.80
57538,-13.2799302,8.0047286,2.4487033,-6.7927865\PG=C01 [X(C10H17Br1N2
O2)]\\@

NECESSARY EVIL: ONE WE LIKE TOO MUCH TO RELINQUISH.
Job cpu time: 1 days 1 hours 17 minutes 34.3 seconds.
File lengths (MBytes): RWF= 135 Int= 0 D2E= 0 Chk= 17 Scr= 1

Normal termination of Gaussian 09 at Mon Jul 22 07:45:43 2024.

Entering Gaussian System, Link 0=g09
Input=oh.gjf
Output=oh.log
Initial command:
/apps/gaussian/09_D01/g09/l1.exe "/scr/tmp/sywang/91397/Gau-1046.inp" -scrdir="/scr/tmp/sywang/91397/"
Entering Link 1 = /apps/gaussian/09_D01/g09/l1.exe PID= 1047.

Warning -- This program may not be used in any manner that
competes with the business of Gaussian, Inc. or will provide
assistance to any competitor of Gaussian, Inc. The licensee
of this program is prohibited from giving any competitor of
Gaussian, Inc. access to this program. By using this program,
the user acknowledges that Gaussian, Inc. is engaged in the
business of creating and licensing software in the field of
computational chemistry and represents and warrants to the
licensee that it is not a competitor of Gaussian, Inc. and that
it will not use this program in any manner prohibited above.

Cite this work as:
Gaussian 09, Revision D.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci,
G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian,
A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada,
M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima,
Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr.,
J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers,
K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand,
K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi,
M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross,
V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,
O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,
R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth,
P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels,
O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski,
and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

****
Gaussian 09: EM64L-G09RevD.01 24-Apr-2013
                17-Jul-2024
****
%chk=.\oh.chk
%mem=40000MB
%nprocl=1
Will use up to 1 processors via Linda.
%nprocs=28

Will use up to 28 processors via shared memory.

---

opt b3lyp/6-311++g(d,p)

1/14=-1,18=20,19=15,26=3,38=1/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=4,6=6,7=1111,11=2,16=1,25=1,30=1,71=1,74=-5/1,2,3;
4//1;
5/5=2,38=5/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(2);
2/9=110/2;
99//99;
2/9=110/2;
3/5=4,6=6,7=1111,11=2,16=1,25=1,30=1,71=1,74=-5/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;

--

oh

--

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	-0.42168	-1.85955	-1.23032
C	-1.73784	-1.55011	-1.34941
N	-2.14352	-1.00466	-0.14423
C	-1.06727	-0.89019	0.66667
N	-0.02662	-1.48548	0.04411
C	1.36706	-1.51631	0.51578
C	2.25431	-0.50621	-0.22394
H	0.26355	-2.30392	-1.93306
H	-2.41539	-1.6626	-2.17975
H	1.35298	-1.30522	1.58654
H	1.73293	-2.54193	0.3935
H	2.35166	-0.81305	-1.27423
H	1.74501	0.46557	-0.22669
Br	-0.63112	1.91315	-0.19863
H	-1.08973	-0.55539	1.68269
C	-3.40627	-0.27939	0.05662

C	-4.44575	-0.41174	-0.75579
H	-3.41894	0.38099	0.93407
H	-5.38917	0.13014	-0.60574
H	-4.43309	-1.07212	-1.63324
O	3.55259	-0.40664	0.36721
H	4.12665	0.10777	-0.20501

Add virtual bond connecting atoms Br14 and H13 Dist= 5.26D+00.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.

! Initial Parameters !
! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.	!
! R1	R(1,2)	1.3573	estimate D2E/DX2	!
! R2	R(1,5)	1.3857	estimate D2E/DX2	!
! R3	R(1,8)	1.0774	estimate D2E/DX2	!
! R4	R(2,3)	1.3837	estimate D2E/DX2	!
! R5	R(2,9)	1.0776	estimate D2E/DX2	!
! R6	R(3,4)	1.3524	estimate D2E/DX2	!
! R7	R(3,16)	1.47	estimate D2E/DX2	!
! R8	R(4,5)	1.3509	estimate D2E/DX2	!
! R9	R(4,15)	1.07	estimate D2E/DX2	!
! R10	R(5,6)	1.4717	estimate D2E/DX2	!
! R11	R(6,7)	1.5345	estimate D2E/DX2	!
! R12	R(6,10)	1.0915	estimate D2E/DX2	!
! R13	R(6,11)	1.0958	estimate D2E/DX2	!
! R14	R(7,12)	1.0985	estimate D2E/DX2	!
! R15	R(7,13)	1.0972	estimate D2E/DX2	!
! R16	R(7,21)	1.43	estimate D2E/DX2	!
! R17	R(13,14)	2.7825	estimate D2E/DX2	!
! R18	R(16,17)	1.3259	estimate D2E/DX2	!
! R19	R(16,18)	1.0983	estimate D2E/DX2	!
! R20	R(17,19)	1.0983	estimate D2E/DX2	!
! R21	R(17,20)	1.0983	estimate D2E/DX2	!
! R22	R(21,22)	0.96	estimate D2E/DX2	!
! A1	A(2,1,5)	107.1943	estimate D2E/DX2	!
! A2	A(2,1,8)	130.8073	estimate D2E/DX2	!
! A3	A(5,1,8)	121.9977	estimate D2E/DX2	!
! A4	A(1,2,3)	107.323	estimate D2E/DX2	!

! A5	A(1,2,9)	130.8079	estimate D2E/DX2	!
! A6	A(3,2,9)	121.8677	estimate D2E/DX2	!
! A7	A(2,3,4)	108.8017	estimate D2E/DX2	!
! A8	A(2,3,16)	124.4271	estimate D2E/DX2	!
! A9	A(4,3,16)	124.0504	estimate D2E/DX2	!
! A10	A(3,4,5)	107.4229	estimate D2E/DX2	!
! A11	A(3,4,15)	125.3898	estimate D2E/DX2	!
! A12	A(5,4,15)	126.2746	estimate D2E/DX2	!
! A13	A(1,5,4)	108.8551	estimate D2E/DX2	!
! A14	A(1,5,6)	123.9942	estimate D2E/DX2	!
! A15	A(4,5,6)	126.2317	estimate D2E/DX2	!
! A16	A(5,6,7)	112.2888	estimate D2E/DX2	!
! A17	A(5,6,10)	107.3471	estimate D2E/DX2	!
! A18	A(5,6,11)	107.4599	estimate D2E/DX2	!
! A19	A(7,6,10)	110.6751	estimate D2E/DX2	!
! A20	A(7,6,11)	111.6701	estimate D2E/DX2	!
! A21	A(10,6,11)	107.1461	estimate D2E/DX2	!
! A22	A(6,7,12)	109.1639	estimate D2E/DX2	!
! A23	A(6,7,13)	108.4117	estimate D2E/DX2	!
! A24	A(6,7,21)	111.8083	estimate D2E/DX2	!
! A25	A(12,7,13)	106.6273	estimate D2E/DX2	!
! A26	A(12,7,21)	109.5258	estimate D2E/DX2	!
! A27	A(13,7,21)	111.1495	estimate D2E/DX2	!
! A28	A(7,13,14)	149.0011	estimate D2E/DX2	!
! A29	A(3,16,17)	122.7159	estimate D2E/DX2	!
! A30	A(3,16,18)	114.5661	estimate D2E/DX2	!
! A31	A(17,16,18)	122.718	estimate D2E/DX2	!
! A32	A(16,17,19)	122.7159	estimate D2E/DX2	!
! A33	A(16,17,20)	122.718	estimate D2E/DX2	!
! A34	A(19,17,20)	114.5661	estimate D2E/DX2	!
! A35	A(7,21,22)	109.5	estimate D2E/DX2	!
! D1	D(5,1,2,3)	-0.7123	estimate D2E/DX2	!
! D2	D(5,1,2,9)	178.8452	estimate D2E/DX2	!
! D3	D(8,1,2,3)	179.6081	estimate D2E/DX2	!
! D4	D(8,1,2,9)	-0.8344	estimate D2E/DX2	!
! D5	D(2,1,5,4)	-3.2728	estimate D2E/DX2	!
! D6	D(2,1,5,6)	-172.8844	estimate D2E/DX2	!
! D7	D(8,1,5,4)	176.4413	estimate D2E/DX2	!
! D8	D(8,1,5,6)	6.8297	estimate D2E/DX2	!
! D9	D(1,2,3,4)	4.449	estimate D2E/DX2	!
! D10	D(1,2,3,16)	166.335	estimate D2E/DX2	!
! D11	D(9,2,3,4)	-175.1566	estimate D2E/DX2	!
! D12	D(9,2,3,16)	-13.2707	estimate D2E/DX2	!
! D13	D(2,3,4,5)	-6.4599	estimate D2E/DX2	!

! D14	D(2,3,4,15)	-176.0646	estimate D2E/DX2	!
! D15	D(16,3,4,5)	-168.4295	estimate D2E/DX2	!
! D16	D(16,3,4,15)	21.9658	estimate D2E/DX2	!
! D17	D(2,3,16,17)	20.8072	estimate D2E/DX2	!
! D18	D(2,3,16,18)	-159.1916	estimate D2E/DX2	!
! D19	D(4,3,16,17)	180.0	estimate D2E/DX2	!
! D20	D(4,3,16,18)	0.0013	estimate D2E/DX2	!
! D21	D(3,4,5,1)	6.0135	estimate D2E/DX2	!
! D22	D(3,4,5,6)	175.3324	estimate D2E/DX2	!
! D23	D(15,4,5,1)	175.5003	estimate D2E/DX2	!
! D24	D(15,4,5,6)	-15.1808	estimate D2E/DX2	!
! D25	D(1,5,6,7)	65.9316	estimate D2E/DX2	!
! D26	D(1,5,6,10)	-172.2114	estimate D2E/DX2	!
! D27	D(1,5,6,11)	-57.249	estimate D2E/DX2	!
! D28	D(4,5,6,7)	-101.8551	estimate D2E/DX2	!
! D29	D(4,5,6,10)	20.0019	estimate D2E/DX2	!
! D30	D(4,5,6,11)	134.9643	estimate D2E/DX2	!
! D31	D(5,6,7,12)	-67.0241	estimate D2E/DX2	!
! D32	D(5,6,7,13)	48.7588	estimate D2E/DX2	!
! D33	D(5,6,7,21)	171.6319	estimate D2E/DX2	!
! D34	D(10,6,7,12)	173.0353	estimate D2E/DX2	!
! D35	D(10,6,7,13)	-71.1818	estimate D2E/DX2	!
! D36	D(10,6,7,21)	51.6913	estimate D2E/DX2	!
! D37	D(11,6,7,12)	53.7596	estimate D2E/DX2	!
! D38	D(11,6,7,13)	169.5425	estimate D2E/DX2	!
! D39	D(11,6,7,21)	-67.5844	estimate D2E/DX2	!
! D40	D(6,7,13,14)	-29.1187	estimate D2E/DX2	!
! D41	D(12,7,13,14)	88.3001	estimate D2E/DX2	!
! D42	D(21,7,13,14)	-152.3898	estimate D2E/DX2	!
! D43	D(6,7,21,22)	169.9704	estimate D2E/DX2	!
! D44	D(12,7,21,22)	48.8358	estimate D2E/DX2	!
! D45	D(13,7,21,22)	-68.727	estimate D2E/DX2	!
! D46	D(3,16,17,19)	-179.9988	estimate D2E/DX2	!
! D47	D(3,16,17,20)	0.0016	estimate D2E/DX2	!
! D48	D(18,16,17,19)	-0.0002	estimate D2E/DX2	!
! D49	D(18,16,17,20)	-179.9998	estimate D2E/DX2	!

Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-06

Number of steps in this run= 116 maximum allowed number of steps= 132.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-0.421676	-1.859550	-1.230320
2	6	0	-1.737840	-1.550108	-1.349412
3	7	0	-2.143524	-1.004664	-0.144230
4	6	0	-1.067273	-0.890191	0.666669
5	7	0	-0.026615	-1.485482	0.044106
6	6	0	1.367061	-1.516307	0.515781
7	6	0	2.254309	-0.506214	-0.223935
8	1	0	0.263552	-2.303918	-1.933064
9	1	0	-2.415386	-1.662601	-2.179752
10	1	0	1.352979	-1.305219	1.586538
11	1	0	1.732930	-2.541925	0.393495
12	1	0	2.351663	-0.813053	-1.274227
13	1	0	1.745007	0.465569	-0.226685
14	35	0	-0.631122	1.913147	-0.198626
15	1	0	-1.089731	-0.555386	1.682691
16	6	0	-3.406271	-0.279385	0.056620
17	6	0	-4.445754	-0.411741	-0.755790
18	1	0	-3.418941	0.380995	0.934071
19	1	0	-5.389171	0.130144	-0.605742
20	1	0	-4.433086	-1.072124	-1.633238
21	8	0	3.552589	-0.406639	0.367211
22	1	0	4.126650	0.107775	-0.205007

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357286	0.000000			
3	N	2.207981	1.383673	0.000000		
4	C	2.225987	2.224800	1.352397	0.000000	
5	N	1.385699	2.207795	2.178981	1.350898	0.000000
6	C	2.523146	3.622223	3.608545	2.518089	1.471652
7	C	3.163104	4.277110	4.426708	3.460278	2.496683
8	H	1.077427	2.216856	3.268333	3.244739	2.159453
9	H	2.217000	1.077584	2.156418	3.242860	3.268508
10	H	3.375111	4.270004	3.912982	2.622218	2.077227
11	H	2.782937	4.008450	4.204666	3.262512	2.081860
12	H	2.964539	4.156072	4.638999	3.932194	2.801137
13	H	3.332863	4.177762	4.158011	3.247320	2.649259
14	Br	3.916823	3.813564	3.286935	2.966086	3.460495
15	H	3.260794	3.256251	2.156379	1.070000	2.163390
16	C	3.613993	2.524940	1.470000	2.493222	3.588440
17	C	4.302852	2.996843	2.454756	3.696815	4.617526

18	H	4.322988	3.430678	2.170131	2.686588	3.972864
19	H	5.387484	4.087605	3.469151	4.619406	5.638223
20	H	4.107772	2.751977	2.731994	4.080609	4.733005
21	O	4.523034	5.678288	5.750210	4.654742	3.752200
22	H	5.060524	6.200845	6.368382	5.360279	4.455349

		6	7	8	9	10
6	C	0.000000				
7	C	1.534496	0.000000			
8	H	2.799090	3.180562	0.000000		
9	H	4.646957	5.193121	2.765656	0.000000	
10	H	1.091456	2.174538	3.817309	5.339779	0.000000
11	H	1.095767	2.190245	2.761991	4.960175	1.759874
12	H	2.160587	1.098518	2.648953	4.926100	3.069784
13	H	2.149868	1.097159	3.574423	5.064825	2.564596
14	Br	4.032898	3.765589	4.646757	4.460317	4.181070
15	H	2.884593	3.849707	4.238210	4.231046	2.557015
16	C	4.952323	5.672066	4.639523	2.810071	5.103278
17	C	6.051924	6.721803	5.209978	2.777537	6.317445
18	H	5.165320	5.857805	5.384233	3.857369	5.102964
19	H	7.043812	7.679422	6.296008	3.812459	7.233460
20	H	6.201394	6.857670	4.864732	2.172200	6.625696
21	O	2.455600	1.430000	4.439448	6.609175	2.670672
22	H	3.282150	1.970533	4.870931	7.059184	3.591578

		11	12	13	14	15
11	H	0.000000				
12	H	2.480549	0.000000			
13	H	3.070796	1.760753	0.000000		
14	Br	5.078092	4.181637	2.782491	0.000000	
15	H	3.684533	4.544552	3.567044	3.137408	0.000000
16	C	5.625296	5.933781	5.212570	3.545956	2.843702
17	C	6.635863	6.828961	6.274962	4.501883	4.150869
18	H	5.947895	6.293027	5.293473	3.376748	2.619629
19	H	7.672206	7.826686	7.152111	5.097438	4.918543
20	H	6.654902	6.799178	6.520102	5.042310	4.737133
21	O	2.805583	2.074057	2.093039	4.817159	4.827396
22	H	3.620636	2.267539	2.408466	5.088792	5.586933

		16	17	18	19	20
16	C	0.000000				
17	C	1.325916	0.000000			
18	H	1.098263	2.130353	0.000000		
19	H	2.130336	1.098267	2.513117	0.000000	
20	H	2.130353	1.098263	3.119474	1.848052	0.000000
21	O	6.966950	8.076797	7.038745	9.010541	8.259278
22	H	7.547399	8.605775	7.635973	9.524281	8.757915

		21	22
21	O	0.000000	
22	H	0.960000	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.116637	-1.884609	-0.893774
2	6	0	-1.221655	-1.658393	-0.888518
3	7	0	-1.529899	-1.037803	0.309149
4	6	0	-0.382550	-0.797900	0.983697
5	7	0	0.621187	-1.385111	0.296222
6	6	0	2.056438	-1.300608	0.610346
7	6	0	2.793771	-0.308458	-0.298860
8	1	0	0.749569	-2.347689	-1.632559
9	1	0	-1.975592	-1.876183	-1.626986
10	1	0	2.143564	-1.002506	1.656682
11	1	0	2.471346	-2.311339	0.526783
12	1	0	2.797523	-0.695597	-1.326892
13	1	0	2.226585	0.630504	-0.319056
14	35	0	-0.219798	1.943601	-0.136727
15	1	0	-0.317420	-0.381689	1.967275
16	6	0	-2.807317	-0.368349	0.593638
17	6	0	-3.917212	-0.624166	-0.085144
18	1	0	-2.767905	0.360866	1.413926
19	1	0	-4.871592	-0.123990	0.127392
20	1	0	-3.956625	-1.353384	-0.905430
21	8	0	4.138880	-0.089495	0.134310
22	1	0	4.614747	0.406232	-0.536068

Rotational constants (GHZ): 0.9554452 0.5504519 0.3819944
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 358 symmetry adapted cartesian basis functions of A symmetry.
There are 345 symmetry adapted basis functions of A symmetry.
345 basis functions, 553 primitive gaussians, 358 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 878.3387205814 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 345 RedAO= T EigKep= 4.38D-06 NBF= 345
NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.32570154 A.U. after 15 cycles
NFock= 15 Conv=0.59D-08 -V/T= 2.0017

****

Population analysis using the SCF density.

****

Orbital symmetries:
Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A)
Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A)

The electronic state is 1-A.

Alpha occ. eigenvalues -- -482.69321 -62.34644 -56.16448 -56.16404 -56.16398
Alpha occ. eigenvalues -- -19.13885 -14.43304 -14.43002 -10.30781 -10.25858
Alpha occ. eigenvalues -- -10.25619 -10.25508 -10.25344 -10.23437 -10.20807
Alpha occ. eigenvalues -- -8.55541 -6.37926 -6.37784 -6.37760 -2.49149
Alpha occ. eigenvalues -- -2.49117 -2.49098 -2.48984 -2.48984 -1.09803
Alpha occ. eigenvalues -- -1.03830 -0.98340 -0.83853 -0.81444 -0.78120
Alpha occ. eigenvalues -- -0.69279 -0.68602 -0.64400 -0.63172 -0.62242
Alpha occ. eigenvalues -- -0.58035 -0.54358 -0.52236 -0.51291 -0.50429
Alpha occ. eigenvalues -- -0.50140 -0.49111 -0.47367 -0.46488 -0.44886
Alpha occ. eigenvalues -- -0.41575 -0.40973 -0.38027 -0.35556 -0.30255
Alpha occ. eigenvalues -- -0.29439 -0.29000 -0.19127 -0.18983 -0.18898
Alpha virt. eigenvalues -- -0.06864 -0.03714 -0.02120 -0.01382 -0.00550
Alpha virt. eigenvalues -- -0.00257 0.00244 0.00806 0.01465 0.02244
Alpha virt. eigenvalues -- 0.03512 0.04149 0.04758 0.05563 0.05840
Alpha virt. eigenvalues -- 0.06376 0.06946 0.07449 0.08159 0.08675
Alpha virt. eigenvalues -- 0.08946 0.09142 0.09732 0.09895 0.10060
Alpha virt. eigenvalues -- 0.10534 0.10943 0.11128 0.11563 0.12143
Alpha virt. eigenvalues -- 0.12477 0.12740 0.13213 0.13664 0.14391
Alpha virt. eigenvalues -- 0.14597 0.14821 0.15416 0.15544 0.16400
Alpha virt. eigenvalues -- 0.16620 0.17262 0.17750 0.17976 0.18502
Alpha virt. eigenvalues -- 0.19311 0.19582 0.20059 0.20341 0.21175
Alpha virt. eigenvalues -- 0.21395 0.21615 0.22462 0.23366 0.24690

Alpha virt. eigenvalues --	0.24995	0.25261	0.25918	0.26462	0.27031
Alpha virt. eigenvalues --	0.27874	0.27905	0.28497	0.28630	0.29486
Alpha virt. eigenvalues --	0.30426	0.30830	0.31249	0.32088	0.33067
Alpha virt. eigenvalues --	0.33910	0.34787	0.35416	0.36634	0.38698
Alpha virt. eigenvalues --	0.39320	0.39637	0.40250	0.42647	0.45162
Alpha virt. eigenvalues --	0.46398	0.47868	0.49186	0.49829	0.50696
Alpha virt. eigenvalues --	0.51821	0.52682	0.53269	0.54532	0.56145
Alpha virt. eigenvalues --	0.56838	0.58521	0.59347	0.59910	0.60607
Alpha virt. eigenvalues --	0.62331	0.63349	0.64291	0.65303	0.65561
Alpha virt. eigenvalues --	0.66133	0.66779	0.67484	0.68351	0.69009
Alpha virt. eigenvalues --	0.69727	0.70294	0.72116	0.73786	0.75255
Alpha virt. eigenvalues --	0.75499	0.76736	0.77811	0.78491	0.79491
Alpha virt. eigenvalues --	0.80725	0.81621	0.82625	0.83551	0.85095
Alpha virt. eigenvalues --	0.86881	0.88408	0.89757	0.90480	0.93700
Alpha virt. eigenvalues --	0.95151	0.97823	0.98573	0.99993	1.01552
Alpha virt. eigenvalues --	1.01921	1.04448	1.04761	1.06875	1.09213
Alpha virt. eigenvalues --	1.10954	1.11290	1.12293	1.15533	1.16988
Alpha virt. eigenvalues --	1.19037	1.20842	1.22352	1.25511	1.30239
Alpha virt. eigenvalues --	1.32559	1.35702	1.37642	1.39932	1.43528
Alpha virt. eigenvalues --	1.45553	1.48028	1.50934	1.51616	1.52182
Alpha virt. eigenvalues --	1.53688	1.55360	1.56121	1.57666	1.58501
Alpha virt. eigenvalues --	1.59505	1.62040	1.62525	1.62666	1.63670
Alpha virt. eigenvalues --	1.66014	1.66487	1.68780	1.70328	1.71275
Alpha virt. eigenvalues --	1.73161	1.74454	1.75099	1.78080	1.79888
Alpha virt. eigenvalues --	1.80933	1.81876	1.86122	1.88744	1.90068
Alpha virt. eigenvalues --	1.90793	1.95640	1.98798	2.01408	2.03477
Alpha virt. eigenvalues --	2.05226	2.06954	2.08007	2.08636	2.11464
Alpha virt. eigenvalues --	2.12641	2.13535	2.15586	2.17115	2.18453
Alpha virt. eigenvalues --	2.20610	2.23542	2.25944	2.26972	2.31760
Alpha virt. eigenvalues --	2.34376	2.36192	2.42318	2.45035	2.45373
Alpha virt. eigenvalues --	2.47666	2.47985	2.49972	2.52231	2.54519
Alpha virt. eigenvalues --	2.55923	2.56431	2.58216	2.58626	2.59837
Alpha virt. eigenvalues --	2.61427	2.63044	2.68087	2.70691	2.72622
Alpha virt. eigenvalues --	2.74437	2.74916	2.77488	2.78668	2.79442
Alpha virt. eigenvalues --	2.81646	2.83466	2.84283	2.87098	2.89729
Alpha virt. eigenvalues --	2.92869	2.93883	2.95449	2.99235	3.08269
Alpha virt. eigenvalues --	3.10060	3.11876	3.19245	3.21485	3.24103
Alpha virt. eigenvalues --	3.33047	3.38651	3.47753	3.54072	3.54949
Alpha virt. eigenvalues --	3.60522	3.64843	3.71181	3.74036	3.76196
Alpha virt. eigenvalues --	3.80287	3.83554	3.85381	3.88462	3.93693
Alpha virt. eigenvalues --	3.98060	4.03728	4.08693	4.18760	4.27630
Alpha virt. eigenvalues --	4.30699	4.33470	4.37705	4.44671	4.69125
Alpha virt. eigenvalues --	4.89779	4.96819	5.04812	5.22504	5.36583
Alpha virt. eigenvalues --	5.65341	6.79632	7.68866	7.73180	7.76191

Alpha virt. eigenvalues -- 23.68243 23.73909 23.81174 23.85527 23.85900
Alpha virt. eigenvalues -- 24.15523 24.22610 35.43963 35.56434 48.07753
Alpha virt. eigenvalues -- 49.90429 289.89601 289.94049 289.964741020.87034
Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	7.054411	-1.134197	0.414817	-0.122093	-0.285269	-0.154198
2	C	-1.134197	6.706233	-0.086936	-0.312854	0.513254	0.055094
3	N	0.414817	-0.086936	6.677760	0.183476	-0.295688	-0.132647
4	C	-0.122093	-0.312854	0.183476	6.259537	0.187645	-0.343635
5	N	-0.285269	0.513254	-0.295688	0.187645	6.880375	0.255939
6	C	-0.154198	0.055094	-0.132647	-0.343635	0.255939	6.627643
7	C	-0.082695	0.119779	0.028481	0.081002	-0.029295	-0.640556
8	H	0.518526	-0.120927	0.064451	0.006285	-0.103539	-0.045430
9	H	-0.162327	0.558153	-0.096982	-0.000331	0.042867	0.017758
10	H	0.069035	-0.057050	0.035540	0.051278	-0.083984	0.379211
11	H	-0.084921	0.070150	-0.033898	-0.033901	0.007574	0.379414
12	H	0.058726	-0.078166	0.016884	0.026440	-0.054469	0.056814
13	H	-0.094074	0.066575	-0.041004	-0.018518	0.068864	-0.025457
14	Br	0.085759	-0.064205	0.025590	-0.017337	0.009190	0.125450
15	H	0.005482	0.029038	-0.032388	0.367861	-0.021990	-0.009334
16	C	0.233065	-0.281471	0.164073	0.047208	-0.116067	-0.080875
17	C	0.015513	0.013360	0.036355	-0.281374	-0.042293	-0.038399
18	H	0.002623	-0.010069	-0.074767	0.059299	-0.007088	-0.005292
19	H	-0.000854	0.003215	0.015015	0.002728	-0.000177	0.000177
20	H	0.005646	0.003584	-0.029167	-0.013812	-0.001502	-0.003596
21	O	0.010047	-0.004000	0.000642	0.009146	0.011448	-0.173193
22	H	-0.001105	0.001647	0.000116	-0.001087	-0.002279	0.005854

		7	8	9	10	11	12
1	C	-0.082695	0.518526	-0.162327	0.069035	-0.084921	0.058726
2	C	0.119779	-0.120927	0.558153	-0.057050	0.070150	-0.078166
3	N	0.028481	0.064451	-0.096982	0.035540	-0.033898	0.016884
4	C	0.081002	0.006285	-0.000331	0.051278	-0.033901	0.026440
5	N	-0.029295	-0.103539	0.042867	-0.083984	0.007574	-0.054469
6	C	-0.640556	-0.045430	0.017758	0.379211	0.379414	0.056814
7	C	6.015517	0.004485	-0.003950	-0.069112	-0.019314	0.271038
8	H	0.004485	0.509832	-0.014102	0.009222	-0.021220	0.014705
9	H	-0.003950	-0.014102	0.523578	-0.000372	0.000414	0.000824
10	H	-0.069112	0.009222	-0.000372	0.592865	-0.096800	0.042999
11	H	-0.019314	-0.021220	0.000414	-0.096800	0.636173	-0.070558
12	H	0.271038	0.014705	0.000824	0.042999	-0.070558	0.776549
13	H	0.336791	-0.013371	0.000239	-0.059874	0.051684	-0.118927
14	Br	-0.153478	0.002744	-0.000937	-0.001583	0.000423	-0.001111
15	H	-0.002191	-0.000019	0.000359	-0.016102	0.009601	-0.003879
16	C	0.030921	0.011873	-0.012284	0.019997	-0.015012	0.007423

17	C	0.013033	0.006848	-0.006493	0.001494	0.000584	-0.000803
18	H	0.002484	0.000101	-0.000448	0.001742	-0.000896	0.000453
19	H	-0.000149	-0.000076	0.000377	-0.000002	-0.000014	0.000012
20	H	0.001783	0.001884	0.001216	0.000180	-0.000115	-0.000036
21	O	0.309187	-0.000403	-0.000108	0.010169	0.022977	-0.060595
22	H	0.009152	-0.000400	0.000061	0.000555	-0.001104	-0.004476

		13	14	15	16	17	18
1	C	-0.094074	0.085759	0.005482	0.233065	0.015513	0.002623
2	C	0.066575	-0.064205	0.029038	-0.281471	0.013360	-0.010069
3	N	-0.041004	0.025590	-0.032388	0.164073	0.036355	-0.074767
4	C	-0.018518	-0.017337	0.367861	0.047208	-0.281374	0.059299
5	N	0.068864	0.009190	-0.021990	-0.116067	-0.042293	-0.007088
6	C	-0.025457	0.125450	-0.009334	-0.080875	-0.038399	-0.005292
7	C	0.336791	-0.153478	-0.002191	0.030921	0.013033	0.002484
8	H	-0.013371	0.002744	-0.000019	0.011873	0.006848	0.000101
9	H	0.000239	-0.000937	0.000359	-0.012284	-0.006493	-0.000448
10	H	-0.059874	-0.001583	-0.016102	0.019997	0.001494	0.001742
11	H	0.051684	0.000423	0.009601	-0.015012	0.000584	-0.000896
12	H	-0.118927	-0.001111	-0.003879	0.007423	-0.000803	0.000453
13	H	0.664134	0.055598	0.007678	-0.020924	-0.005421	-0.001364
14	Br	0.055598	35.611223	-0.003527	-0.066345	0.046378	0.010279
15	H	0.007678	-0.003527	0.458020	-0.010900	0.006431	-0.005773
16	C	-0.020924	-0.066345	-0.010900	5.446478	0.226535	0.420766
17	C	-0.005421	0.046378	0.006431	0.226535	5.656502	-0.052464
18	H	-0.001364	0.010279	-0.005773	0.420766	-0.052464	0.477190
19	H	0.000053	0.002289	-0.000144	-0.043539	0.399017	-0.005388
20	H	-0.000454	-0.001518	-0.000125	0.025541	0.350955	0.005550
21	O	-0.075364	0.000816	-0.000723	0.000128	-0.000022	0.000096
22	H	-0.007622	-0.000474	-0.000179	0.000123	0.000066	-0.000005

		19	20	21	22
1	C	-0.000854	0.005646	0.010047	-0.001105
2	C	0.003215	0.003584	-0.004000	0.001647
3	N	0.015015	-0.029167	0.000642	0.000116
4	C	0.002728	-0.013812	0.009146	-0.001087
5	N	-0.000177	-0.001502	0.011448	-0.002279
6	C	0.000177	-0.003596	-0.173193	0.005854
7	C	-0.000149	0.001783	0.309187	0.009152
8	H	-0.000076	0.001884	-0.000403	-0.000400
9	H	0.000377	0.001216	-0.000108	0.000061
10	H	-0.000002	0.000180	0.010169	0.000555
11	H	-0.000014	-0.000115	0.022977	-0.001104
12	H	0.000012	-0.000036	-0.060595	-0.004476
13	H	0.000053	-0.000454	-0.075364	-0.007622
14	Br	0.002289	-0.001518	0.000816	-0.000474

15	H	-0.000144	-0.000125	-0.000723	-0.000179
16	C	-0.043539	0.025541	0.000128	0.000123
17	C	0.399017	0.350955	-0.000022	0.000066
18	H	-0.005388	0.005550	0.000096	-0.000005
19	H	0.471105	-0.034267	0.000002	0.000000
20	H	-0.034267	0.575380	-0.000005	0.000006
21	O	0.000002	-0.000005	7.996492	0.240468
22	H	0.000000	0.000006	0.240468	0.490303

Mulliken charges:

		1
1	C	-0.351917
2	C	0.009793
3	N	0.160277
4	C	-0.136964
5	N	0.066485
6	C	-0.250741
7	C	-0.222913
8	H	0.168530
9	H	0.152489
10	H	0.170591
11	H	0.198761
12	H	0.120154
13	H	0.230757
14	Br	-0.665225
15	H	0.222803
16	C	0.013285
17	C	-0.345802
18	H	0.182970
19	H	0.190621
20	H	0.112871
21	O	-0.297205
22	H	0.270380

Sum of Mulliken charges = 0.00000

Mulliken charges with hydrogens summed into heavy atoms:

		1
1	C	-0.183388
2	C	0.162282
3	N	0.160277
4	C	0.085839
5	N	0.066485
6	C	0.118610
7	C	0.127999
14	Br	-0.665225
16	C	0.196255

17 C -0.042310

21 O -0.026825

Electronic spatial extent (au): <R**2>= 2823.6477

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= -1.2876 Y= -9.0282 Z= -0.0888 Tot= 9.1200

Quadrupole moment (field-independent basis, Debye-Ang):

XX= -66.3236 YY= -91.5734 ZZ= -73.5090

XY= 3.1554 XZ= -6.1440 YZ= 4.5643

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

XX= 10.8117 YY= -14.4380 ZZ= 3.6263

XY= 3.1554 XZ= -6.1440 YZ= 4.5643

Octapole moment (field-independent basis, Debye-Ang**2):

XXX= -36.1207 YYY= 12.0633 ZZZ= 2.5551 XYY= 15.3435

XXY= 26.2880 XXZ= -36.8065 XZZ= 3.9104 YZZ= 4.3125

YYZ= -10.2422 XYZ= -12.5179

Hexadecapole moment (field-independent basis, Debye-Ang**3):

XXXX= -2048.1309 YYYY= -1102.4571 ZZZZ= -252.8162 XXXY= 75.7762

XXXZ= -125.7871 YYYX= -25.1074 YYYZ= 11.9322 ZZZX= 0.0594

ZZZY= 7.4670 XXYY= -548.6433 XXZZ= -406.3423 YYZZ= -208.1943

XXYZ= 17.0032 YYXZ= 8.4985 ZZXY= -4.4454

N-N= 8.783387205814D+02 E-N=-8.978679142029D+03 KE= 3.027075206880D+03

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.005914250	0.001126378	0.000384416
2	6	0.003262105	-0.004205771	-0.002157029
3	7	-0.023120519	0.018794569	0.004603255
4	6	0.003110723	-0.003431796	-0.018111028
5	7	0.002270720	0.003372816	0.004293616
6	6	0.006096997	-0.004822957	0.008626212
7	6	-0.001586603	0.013240655	-0.013198070
8	1	-0.001022802	0.000525917	0.000865048
9	1	0.002911109	0.000155773	0.001512918

10	1	0.001023251	0.001747958	-0.000539357
11	1	0.000494861	0.002074573	0.000175261
12	1	-0.001129678	-0.002124082	0.000127218
13	1	-0.000557675	-0.001025952	0.001928161
14	35	0.000462653	-0.000838601	0.003160618
15	1	0.001635608	0.003540243	0.002023711
16	6	0.013196234	-0.007160644	0.007942216
17	6	-0.008891440	-0.005683506	-0.009584197
18	1	0.005196420	-0.007432009	-0.009423375
19	1	0.012313289	-0.002599943	0.002386724
20	1	0.000477775	0.005618053	0.007823442
21	8	-0.007770902	-0.012788790	0.008670426
22	1	-0.002457877	0.001917116	-0.001510186

Cartesian Forces: Max 0.023120519 RMS 0.006901382

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.027795801 RMS 0.005093083

Search for a local minimum.

Step number 1 out of a maximum of 116

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Second derivative matrix not updated -- first step.

ITU= 0

Eigenvalues ---	0.00230	0.00310	0.00744	0.00766	0.01295
Eigenvalues ---	0.01558	0.01846	0.01895	0.02007	0.02102
Eigenvalues ---	0.02166	0.02333	0.02391	0.02414	0.03069
Eigenvalues ---	0.03069	0.04134	0.04517	0.05242	0.05604
Eigenvalues ---	0.08680	0.09511	0.12817	0.13458	0.15578
Eigenvalues ---	0.15999	0.16000	0.16000	0.16000	0.16000
Eigenvalues ---	0.16000	0.18403	0.21941	0.22000	0.22672
Eigenvalues ---	0.23176	0.23392	0.24357	0.25000	0.29012
Eigenvalues ---	0.33847	0.33875	0.33875	0.33875	0.33998
Eigenvalues ---	0.34155	0.34645	0.35543	0.35740	0.36288
Eigenvalues ---	0.36307	0.37230	0.40989	0.42965	0.45774
Eigenvalues ---	0.49262	0.53438	0.54073	0.55473	0.60481

RFO step: Lambda=-1.89355569D-02 EMin= 2.30000000D-03

Linear search not attempted -- first point.

Iteration 1 RMS(Cart)= 0.18914693 RMS(Int)= 0.01327995

Iteration 2 RMS(Cart)= 0.01821417 RMS(Int)= 0.00070427

Iteration 3 RMS(Cart)= 0.00016552 RMS(Int)= 0.00070073

Iteration 4 RMS(Cart)= 0.00000011 RMS(Int)= 0.00070073

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56490	-0.00399	0.00000	-0.00595	-0.00591	2.55899
R2	2.61859	0.00089	0.00000	0.00177	0.00169	2.62028
R3	2.03604	-0.00143	0.00000	-0.00374	-0.00374	2.03231
R4	2.61476	0.00114	0.00000	0.00309	0.00320	2.61796
R5	2.03634	-0.00301	0.00000	-0.00788	-0.00788	2.02846
R6	2.55566	-0.00390	0.00000	-0.00760	-0.00757	2.54809
R7	2.77790	-0.02780	0.00000	-0.07386	-0.07386	2.70404
R8	2.55283	-0.01045	0.00000	-0.01969	-0.01980	2.53303
R9	2.02201	0.00299	0.00000	0.00765	0.00765	2.02965
R10	2.78102	-0.00270	0.00000	-0.00722	-0.00722	2.77380
R11	2.89978	-0.00820	0.00000	-0.02654	-0.02654	2.87323
R12	2.06255	-0.00021	0.00000	-0.00058	-0.00058	2.06197
R13	2.07070	-0.00179	0.00000	-0.00498	-0.00498	2.06572
R14	2.07590	0.00037	0.00000	0.00103	0.00103	2.07693
R15	2.07333	-0.00161	0.00000	-0.00448	-0.00448	2.06885
R16	2.70231	-0.00708	0.00000	-0.01652	-0.01652	2.68579
R17	5.25815	-0.00079	0.00000	-0.02118	-0.02118	5.23696
R18	2.50562	-0.00318	0.00000	-0.00509	-0.00509	2.50052
R19	2.07542	-0.01206	0.00000	-0.03372	-0.03372	2.04170
R20	2.07542	-0.01154	0.00000	-0.03225	-0.03225	2.04317
R21	2.07542	-0.00962	0.00000	-0.02690	-0.02690	2.04852
R22	1.81414	0.00046	0.00000	0.00080	0.00080	1.81494
A1	1.87089	0.00199	0.00000	0.00899	0.00839	1.87928
A2	2.28302	-0.00113	0.00000	-0.00514	-0.00524	2.27777
A3	2.12926	-0.00086	0.00000	-0.00363	-0.00375	2.12551
A4	1.87314	-0.00177	0.00000	-0.00525	-0.00541	1.86773
A5	2.28303	-0.00040	0.00000	-0.00451	-0.00443	2.27859
A6	2.12699	0.00216	0.00000	0.00974	0.00981	2.13680
A7	1.89895	-0.00291	0.00000	-0.01063	-0.01091	1.88804
A8	2.17166	0.00778	0.00000	0.03349	0.03357	2.20523
A9	2.16509	-0.00456	0.00000	-0.01582	-0.01587	2.14922
A10	1.87488	0.00577	0.00000	0.01737	0.01686	1.89174
A11	2.18846	-0.00196	0.00000	-0.00555	-0.00548	2.18298
A12	2.20391	-0.00403	0.00000	-0.01648	-0.01638	2.18752
A13	1.89988	-0.00330	0.00000	-0.01645	-0.01691	1.88297
A14	2.16411	0.00352	0.00000	0.01539	0.01560	2.17971
A15	2.20316	-0.00017	0.00000	0.00149	0.00175	2.20491
A16	1.95981	-0.00807	0.00000	-0.03658	-0.03663	1.92318
A17	1.87356	0.00654	0.00000	0.03554	0.03485	1.90841
A18	1.87553	0.00037	0.00000	-0.00308	-0.00291	1.87262
A19	1.93165	-0.00302	0.00000	-0.02991	-0.02965	1.90200
A20	1.94901	0.00509	0.00000	0.02820	0.02829	1.97730

A21	1.87005	-0.00043	0.00000	0.00886	0.00889	1.87895
A22	1.90527	0.00330	0.00000	0.01944	0.02057	1.92584
A23	1.89214	-0.00261	0.00000	-0.04167	-0.04297	1.84917
A24	1.95142	-0.01455	0.00000	-0.09049	-0.09151	1.85991
A25	1.86100	0.00323	0.00000	0.06293	0.06233	1.92333
A26	1.91158	0.00456	0.00000	0.03699	0.03610	1.94768
A27	1.93992	0.00686	0.00000	0.01968	0.01443	1.95436
A28	2.60056	-0.00289	0.00000	-0.01075	-0.01075	2.58981
A29	2.14180	0.00440	0.00000	0.01840	0.01837	2.16017
A30	1.99956	-0.00723	0.00000	-0.03732	-0.03734	1.96221
A31	2.14183	0.00283	0.00000	0.01892	0.01889	2.16072
A32	2.14180	-0.00717	0.00000	-0.04007	-0.04010	2.10170
A33	2.14183	0.00293	0.00000	0.01639	0.01636	2.15819
A34	1.99956	0.00424	0.00000	0.02367	0.02364	2.02319
A35	1.91114	-0.00553	0.00000	-0.03092	-0.03092	1.88021
D1	-0.01243	0.00112	0.00000	0.03111	0.03125	0.01881
D2	3.12144	0.00070	0.00000	0.02775	0.02776	-3.13398
D3	3.13475	-0.00044	0.00000	-0.01265	-0.01244	3.12232
D4	-0.01456	-0.00085	0.00000	-0.01601	-0.01592	-0.03048
D5	-0.05712	-0.00200	0.00000	-0.05633	-0.05615	-0.11327
D6	-3.01740	-0.00213	0.00000	-0.05844	-0.05832	-3.07573
D7	3.07948	-0.00061	0.00000	-0.01729	-0.01709	3.06239
D8	0.11920	-0.00075	0.00000	-0.01940	-0.01926	0.09994
D9	0.07765	-0.00003	0.00000	0.00437	0.00416	0.08181
D10	2.90309	-0.00022	0.00000	0.02275	0.02281	2.92590
D11	-3.05706	0.00035	0.00000	0.00744	0.00736	-3.04970
D12	-0.23162	0.00016	0.00000	0.02581	0.02601	-0.20561
D13	-0.11275	-0.00172	0.00000	-0.04091	-0.04122	-0.15396
D14	-3.07291	-0.00014	0.00000	-0.01318	-0.01331	-3.08622
D15	-2.93965	-0.00427	0.00000	-0.07015	-0.07007	-3.00972
D16	0.38338	-0.00270	0.00000	-0.04242	-0.04217	0.34121
D17	0.36315	0.00069	0.00000	0.02787	0.02795	0.39110
D18	-2.77842	0.00121	0.00000	0.04127	0.04114	-2.73727
D19	-3.14159	0.00127	0.00000	0.05190	0.05203	-3.08956
D20	0.00002	0.00179	0.00000	0.06531	0.06523	0.06525
D21	0.10495	0.00235	0.00000	0.06004	0.06006	0.16501
D22	3.06013	0.00296	0.00000	0.06397	0.06404	3.12417
D23	3.06306	0.00104	0.00000	0.03350	0.03353	3.09659
D24	-0.26495	0.00165	0.00000	0.03743	0.03751	-0.22745
D25	1.15072	0.00553	0.00000	0.15285	0.15320	1.30392
D26	-3.00566	0.00116	0.00000	0.11682	0.11651	-2.88914
D27	-0.99918	0.00406	0.00000	0.14307	0.14308	-0.85610
D28	-1.77771	0.00559	0.00000	0.15180	0.15211	-1.62559
D29	0.34910	0.00122	0.00000	0.11577	0.11543	0.46453

D30	2.35557	0.00412	0.00000	0.14202	0.14200	2.49757
D31	-1.16979	0.00137	0.00000	0.09425	0.09464	-1.07515
D32	0.85100	0.00555	0.00000	0.15663	0.15553	1.00653
D33	2.99554	0.00286	0.00000	0.09336	0.09510	3.09064
D34	3.02004	0.00056	0.00000	0.09425	0.09399	3.11403
D35	-1.24236	0.00473	0.00000	0.15663	0.15488	-1.08748
D36	0.90218	0.00204	0.00000	0.09336	0.09445	0.99664
D37	0.93828	-0.00022	0.00000	0.08456	0.08457	1.02285
D38	2.95907	0.00395	0.00000	0.14694	0.14546	3.10453
D39	-1.17957	0.00127	0.00000	0.08367	0.08503	-1.09454
D40	-0.50822	-0.00373	0.00000	0.08056	0.08038	-0.42783
D41	1.54113	0.00051	0.00000	0.11545	0.11437	1.65549
D42	-2.65970	0.01184	0.00000	0.20967	0.21094	-2.44876
D43	2.96654	0.00303	0.00000	0.05946	0.05912	3.02566
D44	0.85235	0.00531	0.00000	0.06908	0.06990	0.92225
D45	-1.19951	-0.00562	0.00000	-0.04313	-0.04362	-1.24313
D46	-3.14157	0.00108	0.00000	0.02327	0.02336	-3.11821
D47	0.00003	0.00028	0.00000	0.00725	0.00734	0.00737
D48	0.00000	0.00051	0.00000	0.00878	0.00868	0.00868
D49	-3.14159	-0.00028	0.00000	-0.00724	-0.00734	3.13426

Item	Value	Threshold	Converged?
Maximum Force	0.027796	0.000450	NO
RMS Force	0.005093	0.000300	NO
Maximum Displacement	1.391131	0.001800	NO
RMS Displacement	0.194765	0.001200	NO

Predicted change in Energy=-1.311278D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.435568	-1.953352	-1.239460
2	6	0	-1.750210	-1.658620	-1.375845
3	7	0	-2.127823	-0.956321	-0.242960
4	6	0	-1.027603	-0.745732	0.507591
5	7	0	-0.016954	-1.454035	-0.015499
6	6	0	1.364065	-1.495263	0.480106
7	6	0	2.211817	-0.459969	-0.241870
8	1	0	0.229001	-2.497896	-1.886308
9	1	0	-2.435339	-1.876905	-2.172818
10	1	0	1.371114	-1.276646	1.549108
11	1	0	1.726117	-2.518271	0.348518

12	1	0	2.243193	-0.675762	-1.319083
13	1	0	1.725407	0.504485	-0.063569
14	35	0	-0.589200	1.904941	0.537529
15	1	0	-1.018813	-0.267995	1.469498
16	6	0	-3.348960	-0.232896	-0.061300
17	6	0	-4.452877	-0.468079	-0.751930
18	1	0	-3.264518	0.535335	0.693682
19	1	0	-5.340187	0.126748	-0.585036
20	1	0	-4.533036	-1.235258	-1.513592
21	8	0	3.506630	-0.518491	0.341238
22	1	0	4.084092	0.053104	-0.170848

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.354161	0.000000			
3	N	2.202455	1.385367	0.000000		
4	C	2.204776	2.214240	1.348392	0.000000	
5	N	1.386591	2.212820	2.180648	1.340421	0.000000
6	C	2.530896	3.629043	3.606462	2.506517	1.467834
7	C	3.199066	4.291890	4.367934	3.337244	2.450883
8	H	1.075450	2.209578	3.260624	3.221783	2.156401
9	H	2.208186	1.073413	2.160183	3.232007	3.268246
10	H	3.390891	4.294639	3.944196	2.668421	2.099094
11	H	2.741111	3.974579	4.200284	3.278746	2.074464
12	H	2.968895	4.112968	4.510270	3.746964	2.722738
13	H	3.477571	4.298954	4.124745	3.077066	2.621819
14	Br	4.250614	4.208077	3.341160	2.686850	3.451960
15	H	3.243309	3.250347	2.153186	1.074046	2.148402
16	C	3.582720	2.513308	1.430916	2.444450	3.549020
17	C	4.310741	3.018453	2.429672	3.660053	4.603461
18	H	4.234803	3.374834	2.096286	2.584483	3.873914
19	H	5.367529	4.086667	3.407247	4.533590	5.582119
20	H	4.168939	2.818213	2.734476	4.075890	4.763102
21	O	4.483119	5.646471	5.681553	4.542971	3.663079
22	H	5.059163	6.198476	6.293809	5.218031	4.371976

		6	7	8	9	10
6	C	0.000000				
7	C	1.520449	0.000000			
8	H	2.809548	3.284643	0.000000		
9	H	4.649637	5.228033	2.750714	0.000000	
10	H	1.091150	2.140408	3.820728	5.357437	0.000000
11	H	1.093134	2.195692	2.690022	4.907770	1.763257
12	H	2.163684	1.099062	2.774687	4.905127	3.057467

13	H	2.103603	1.094787	3.817840	5.237534	2.428720
14	Br	3.921725	3.747794	5.092093	5.005654	3.871514
15	H	2.857130	3.660957	4.217930	4.226299	2.595278
16	C	4.909104	5.568340	4.611148	2.827715	5.095285
17	C	6.034056	6.684188	5.227518	2.841508	6.314066
18	H	5.058926	5.644124	5.297312	3.837090	5.050160
19	H	6.979430	7.582530	6.292687	3.869601	7.180922
20	H	6.230428	6.907343	4.940665	2.290550	6.651378
21	O	2.358803	1.421260	4.429769	6.593388	2.567914
22	H	3.196831	1.942602	4.930733	7.087722	3.476598

		11	12	13	14	15
11	H	0.000000				
12	H	2.538325	0.000000			
13	H	3.050716	1.799278	0.000000		
14	Br	4.996121	4.257873	2.771281	0.000000	
15	H	3.722228	4.310817	3.236937	2.403078	0.000000
16	C	5.580977	5.748941	5.127664	3.541924	2.788218
17	C	6.602593	6.723254	6.292131	4.714014	4.094822
18	H	5.860895	5.987726	5.047151	3.009574	2.508071
19	H	7.602651	7.660972	7.094873	5.195575	4.801167
20	H	6.655116	6.802070	6.655628	5.442590	4.710009
21	O	2.677573	2.092289	2.093587	4.763127	4.670691
22	H	3.527287	2.288798	2.403882	5.076491	5.369682

		16	17	18	19	20
16	C	0.000000				
17	C	1.323220	0.000000			
18	H	1.080420	2.123400	0.000000		
19	H	2.090126	1.081199	2.471935	0.000000	
20	H	2.125068	1.084028	3.100999	1.835420	0.000000
21	O	6.873334	8.034383	6.861722	8.918547	8.281931
22	H	7.439359	8.572580	7.414987	9.433664	8.815766

		21	22
21	O	0.000000	
22	H	0.960424	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)		
Number	Number	Type	X	Y	Z

1	6	0	0.006709	-2.205639	-0.547039
2	6	0	-1.323601	-1.962820	-0.618225
3	7	0	-1.593353	-0.923494	0.257147
4	6	0	-0.422871	-0.485181	0.763124
5	7	0	0.544402	-1.333688	0.387425
6	6	0	1.973036	-1.219214	0.704342
7	6	0	2.700923	-0.486107	-0.411230
8	1	0	0.611159	-2.937847	-1.052118
9	1	0	-2.086821	-2.426724	-1.213628
10	1	0	2.093435	-0.660362	1.633749
11	1	0	2.350193	-2.230994	0.874625
12	1	0	2.617672	-1.045279	-1.353745
13	1	0	2.207374	0.486705	-0.503992
14	35	0	-0.068052	2.023831	-0.130253
15	1	0	-0.321003	0.282960	1.506869
16	6	0	-2.808578	-0.171774	0.332411
17	6	0	-3.975208	-0.613516	-0.108893
18	1	0	-2.664068	0.801817	0.777996
19	1	0	-4.856485	0.009506	-0.044205
20	1	0	-4.116250	-1.588347	-0.561584
21	8	0	4.054340	-0.358476	0.003443
22	1	0	4.552100	0.008063	-0.731607

Rotational constants (GHZ): 0.9068064 0.5736435 0.3724779

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 882.3931666386 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 4.43D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Initial guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.998995 0.037985 -0.000480 0.023779 Ang= 5.14 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.33172231 A.U. after 15 cycles
NFock= 15 Conv=0.20D-08 -V/T= 2.0016
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.003166454	-0.006591672	-0.003588083
2	6	0.005082323	-0.004673894	-0.004888225
3	7	-0.010980342	0.013373676	-0.004384521
4	6	-0.000015461	-0.004579558	0.018363268
5	7	0.002322527	0.002843360	-0.001234563
6	6	-0.003081934	-0.003827644	0.001011127
7	6	-0.001755860	0.001717539	0.002083207
8	1	-0.000048073	-0.000489634	-0.000481504
9	1	0.000102150	0.000136375	-0.000768251
10	1	-0.002578412	0.000095350	-0.000510682
11	1	0.002257906	0.001583034	-0.000845024
12	1	-0.000027895	0.000768447	0.000902382
13	1	0.002576899	0.002565545	-0.004544927
14	35	0.002490948	0.011675221	-0.002705970
15	1	-0.001224603	-0.006940928	0.000447305
16	6	0.007091045	-0.007009810	0.003603990
17	6	-0.005306079	-0.002028392	-0.004319111
18	1	0.000922618	0.001443702	0.000000416
19	1	0.001063340	0.001221177	0.001522744
20	1	0.000912928	-0.000194771	0.000736022

21	8	0.001486595	-0.002758843	-0.002094877
22	1	0.001875837	0.001671720	0.001695278

Cartesian Forces: Max 0.018363268 RMS 0.004459658

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.059742140 RMS 0.010489947

Search for a local minimum.

Step number 2 out of a maximum of 116

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 1 2

DE= -6.02D-03 DEPred=-1.31D-02 R= 4.59D-01

Trust test= 4.59D-01 RLast= 6.22D-01 DXMaxT set to 3.00D-01

ITU= 0 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00245	0.00310	0.00754	0.01086	0.01276
Eigenvalues ---	0.01510	0.01822	0.01855	0.02036	0.02115
Eigenvalues ---	0.02198	0.02336	0.02410	0.02464	0.03060
Eigenvalues ---	0.03069	0.04214	0.04796	0.05328	0.05743
Eigenvalues ---	0.08342	0.09083	0.11335	0.13178	0.15324
Eigenvalues ---	0.15471	0.15983	0.15999	0.15999	0.16000
Eigenvalues ---	0.16038	0.17530	0.21692	0.22440	0.22742
Eigenvalues ---	0.23144	0.23544	0.24348	0.27840	0.30199
Eigenvalues ---	0.33839	0.33865	0.33875	0.33892	0.34151
Eigenvalues ---	0.34581	0.34646	0.35541	0.36279	0.36305
Eigenvalues ---	0.37197	0.40780	0.42960	0.45574	0.48376
Eigenvalues ---	0.53160	0.53341	0.55465	0.60070	0.70554

RFO step: Lambda=-2.39542645D-02 EMin= 2.45176711D-03

Quartic linear search produced a step of -0.28326.

Maximum step size (0.300) exceeded in Quadratic search.

-- Step size scaled by 0.915

Iteration 1 RMS(Cart)= 0.18567310 RMS(Int)= 0.01704051

Iteration 2 RMS(Cart)= 0.05859751 RMS(Int)= 0.00184204

Iteration 3 RMS(Cart)= 0.00199067 RMS(Int)= 0.00124622

Iteration 4 RMS(Cart)= 0.00000515 RMS(Int)= 0.00124622

Iteration 5 RMS(Cart)= 0.00000002 RMS(Int)= 0.00124622

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55899	-0.00203	0.00167	-0.01038	-0.00882	2.55017
R2	2.62028	0.00627	-0.00048	0.00788	0.00745	2.62773

R3	2.03231	0.00051	0.00106	-0.00452	-0.00346	2.02885
R4	2.61796	0.00804	-0.00091	0.01182	0.01081	2.62878
R5	2.02846	0.00048	0.00223	-0.01025	-0.00802	2.02044
R6	2.54809	0.00734	0.00214	-0.00404	-0.00181	2.54628
R7	2.70404	-0.00712	0.02092	-0.11023	-0.08931	2.61473
R8	2.53303	0.00209	0.00561	-0.02552	-0.01982	2.51321
R9	2.02965	-0.00270	-0.00217	0.00733	0.00516	2.03481
R10	2.77380	0.00099	0.00204	-0.00868	-0.00664	2.76716
R11	2.87323	0.01654	0.00752	-0.01154	-0.00403	2.86921
R12	2.06197	-0.00050	0.00016	-0.00143	-0.00127	2.06071
R13	2.06572	-0.00063	0.00141	-0.00763	-0.00622	2.05950
R14	2.07693	-0.00104	-0.00029	0.00006	-0.00023	2.07670
R15	2.06885	0.00911	0.00127	0.00558	0.00685	2.07570
R16	2.68579	0.00295	0.00468	-0.01960	-0.01492	2.67087
R17	5.23696	0.00324	0.00600	0.01470	0.02070	5.25766
R18	2.50052	0.00403	0.00144	-0.00409	-0.00265	2.49788
R19	2.04170	0.00110	0.00955	-0.04483	-0.03528	2.00642
R20	2.04317	0.00003	0.00914	-0.04419	-0.03506	2.00811
R21	2.04852	-0.00045	0.00762	-0.03747	-0.02985	2.01866
R22	1.81494	0.00121	-0.00023	0.00210	0.00187	1.81681
A1	1.87928	0.00013	-0.00238	0.01050	0.00840	1.88769
A2	2.27777	-0.00048	0.00149	-0.00780	-0.00639	2.27138
A3	2.12551	0.00040	0.00106	-0.00362	-0.00264	2.12287
A4	1.86773	0.00062	0.00153	-0.00652	-0.00489	1.86284
A5	2.27859	-0.00070	0.00126	-0.00712	-0.00595	2.27264
A6	2.13680	0.00010	-0.00278	0.01376	0.01090	2.14770
A7	1.88804	-0.00024	0.00309	-0.01204	-0.00905	1.87899
A8	2.20523	0.00268	-0.00951	0.05106	0.04131	2.24654
A9	2.14922	-0.00165	0.00450	-0.02342	-0.01969	2.12953
A10	1.89174	-0.00244	-0.00477	0.01984	0.01546	1.90720
A11	2.18298	0.00164	0.00155	-0.00563	-0.00460	2.17839
A12	2.18752	0.00047	0.00464	-0.02274	-0.01840	2.16913
A13	1.88297	0.00254	0.00479	-0.01515	-0.01051	1.87246
A14	2.17971	-0.00453	-0.00442	0.01555	0.01037	2.19008
A15	2.20491	0.00280	-0.00050	0.00973	0.00850	2.21341
A16	1.92318	0.03788	0.01038	0.02842	0.03845	1.96163
A17	1.90841	-0.01216	-0.00987	0.04119	0.03109	1.93950
A18	1.87262	-0.01179	0.00083	-0.03570	-0.03442	1.83819
A19	1.90200	-0.00116	0.00840	-0.01548	-0.00837	1.89363
A20	1.97730	-0.01932	-0.00801	-0.02251	-0.03037	1.94693
A21	1.87895	0.00554	-0.00252	0.00609	0.00361	1.88256
A22	1.92584	-0.00759	-0.00583	0.00337	-0.00770	1.91814
A23	1.84917	0.05017	0.01217	0.11344	0.12388	1.97305
A24	1.85991	-0.01955	0.02592	-0.15717	-0.13027	1.72964

A25	1.92333	-0.01302	-0.01766	0.04120	0.02070	1.94403
A26	1.94768	0.00685	-0.01022	0.02168	0.00886	1.95654
A27	1.95436	-0.01488	-0.00409	-0.02422	-0.02127	1.93308
A28	2.58981	0.05974	0.00304	0.08756	0.09060	2.68042
A29	2.16017	0.00164	-0.00520	0.02787	0.02265	2.18281
A30	1.96221	-0.00135	0.01058	-0.05258	-0.04202	1.92019
A31	2.16072	-0.00029	-0.00535	0.02449	0.01911	2.17984
A32	2.10170	-0.00232	0.01136	-0.05898	-0.04763	2.05407
A33	2.15819	0.00010	-0.00463	0.02188	0.01723	2.17543
A34	2.02319	0.00222	-0.00670	0.03690	0.03020	2.05339
A35	1.88021	0.00376	0.00876	-0.03134	-0.02258	1.85763
D1	0.01881	-0.00265	-0.00885	0.00527	-0.00354	0.01528
D2	-3.13398	-0.00107	-0.00786	0.01814	0.01045	-3.12354
D3	3.12232	-0.00108	0.00352	-0.02297	-0.01947	3.10284
D4	-0.03048	0.00050	0.00451	-0.01010	-0.00549	-0.03597
D5	-0.11327	0.00372	0.01591	-0.01458	0.00111	-0.11216
D6	-3.07573	-0.00127	0.01652	-0.07269	-0.05605	-3.13177
D7	3.06239	0.00233	0.00484	0.01083	0.01555	3.07794
D8	0.09994	-0.00265	0.00546	-0.04728	-0.04161	0.05832
D9	0.08181	0.00033	-0.00118	0.00523	0.00412	0.08592
D10	2.92590	0.00272	-0.00646	0.05443	0.04875	2.97465
D11	-3.04970	-0.00108	-0.00208	-0.00621	-0.00850	-3.05820
D12	-0.20561	0.00131	-0.00737	0.04299	0.03613	-0.16947
D13	-0.15396	0.00234	0.01167	-0.01701	-0.00544	-0.15941
D14	-3.08622	0.00396	0.00377	0.02744	0.03101	-3.05521
D15	-3.00972	-0.00085	0.01985	-0.07970	-0.05898	-3.06871
D16	0.34121	0.00077	0.01194	-0.03526	-0.02253	0.31868
D17	0.39110	-0.00096	-0.00792	0.01239	0.00440	0.39550
D18	-2.73727	-0.00052	-0.01165	0.03008	0.01819	-2.71909
D19	-3.08956	0.00215	-0.01474	0.07298	0.05849	-3.03108
D20	0.06525	0.00259	-0.01848	0.09068	0.07227	0.13752
D21	0.16501	-0.00380	-0.01701	0.01950	0.00273	0.16774
D22	3.12417	0.00032	-0.01814	0.07938	0.06108	-3.09794
D23	3.09659	-0.00525	-0.00950	-0.02250	-0.03145	3.06513
D24	-0.22745	-0.00113	-0.01062	0.03738	0.02690	-0.20055
D25	1.30392	-0.01096	-0.04339	0.03459	-0.00929	1.29463
D26	-2.88914	0.00331	-0.03300	0.05874	0.02652	-2.86263
D27	-0.85610	-0.00296	-0.04053	0.06793	0.02746	-0.82864
D28	-1.62559	-0.01662	-0.04309	-0.03191	-0.07572	-1.70131
D29	0.46453	-0.00235	-0.03270	-0.00776	-0.03992	0.42461
D30	2.49757	-0.00862	-0.04022	0.00143	-0.03897	2.45860
D31	-1.07515	-0.00170	-0.02681	0.07834	0.05189	-1.02326
D32	1.00653	0.00806	-0.04405	0.19570	0.15416	1.16069
D33	3.09064	0.00639	-0.02694	0.14681	0.11684	-3.07571

D34	3.11403	-0.00913	-0.02662	0.02011	-0.00593	3.10810
D35	-1.08748	0.00063	-0.04387	0.13747	0.09635	-0.99113
D36	0.99664	-0.00104	-0.02675	0.08858	0.05902	1.05566
D37	1.02285	-0.00291	-0.02396	0.03761	0.01394	1.03680
D38	3.10453	0.00685	-0.04120	0.15497	0.11622	-3.06244
D39	-1.09454	0.00518	-0.02409	0.10609	0.07889	-1.01565
D40	-0.42783	-0.00765	-0.02277	-0.02526	-0.04977	-0.47761
D41	1.65549	0.00558	-0.03240	0.06693	0.03678	1.69227
D42	-2.44876	-0.00610	-0.05975	0.10829	0.04803	-2.40073
D43	3.02566	-0.01844	-0.01675	0.00213	-0.01551	3.01015
D44	0.92225	-0.00072	-0.01980	0.08525	0.06469	0.98694
D45	-1.24313	0.02239	0.01235	0.03294	0.04694	-1.19619
D46	-3.11821	0.00030	-0.00662	0.02798	0.02144	-3.09677
D47	0.00737	0.00054	-0.00208	0.01261	0.01060	0.01798
D48	0.00868	-0.00020	-0.00246	0.00774	0.00521	0.01389
D49	3.13426	0.00004	0.00208	-0.00763	-0.00563	3.12864

Item	Value	Threshold	Converged?
Maximum Force	0.059742	0.000450	NO
RMS Force	0.010490	0.000300	NO
Maximum Displacement	1.427368	0.001800	NO
RMS Displacement	0.238062	0.001200	NO

Predicted change in Energy=-1.570201D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.453672	-1.892900	-1.304917
2	6	0	-1.775376	-1.664710	-1.453793
3	7	0	-2.194909	-0.983617	-0.315711
4	6	0	-1.103766	-0.725050	0.431371
5	7	0	-0.060389	-1.375473	-0.075618
6	6	0	1.300732	-1.406586	0.463469
7	6	0	2.217434	-0.409302	-0.222369
8	1	0	0.234605	-2.415248	-1.942167
9	1	0	-2.435186	-1.925888	-2.253518
10	1	0	1.304189	-1.200115	1.534218
11	1	0	1.644168	-2.430821	0.319411
12	1	0	2.257895	-0.618391	-1.300477
13	1	0	1.939375	0.635243	-0.027130
14	35	0	0.130893	2.660272	0.580725
15	1	0	-1.120943	-0.274751	1.409320

16	6	0	-3.412117	-0.372287	-0.072430
17	6	0	-4.545448	-0.665805	-0.686118
18	1	0	-3.297533	0.386523	0.661324
19	1	0	-5.404851	-0.092716	-0.436686
20	1	0	-4.653720	-1.422726	-1.432083
21	8	0	3.429042	-0.735143	0.428346
22	1	0	4.119926	-0.237387	-0.018012

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.349494	0.000000			
3	N	2.199371	1.391088	0.000000		
4	C	2.191162	2.210851	1.347435	0.000000	
5	N	1.390532	2.219055	2.183432	1.329934	0.000000
6	C	2.538036	3.633863	3.606319	2.499427	1.464320
7	C	3.241571	4.362910	4.450542	3.399624	2.478608
8	H	1.073620	2.200418	3.255375	3.206507	2.156886
9	H	2.197118	1.069169	2.168111	3.228516	3.268924
10	H	3.410384	4.315991	3.963937	2.690763	2.117639
11	H	2.707164	3.927398	4.151662	3.236253	2.043360
12	H	2.996163	4.169600	4.575000	3.783046	2.729083
13	H	3.708224	4.596142	4.449302	3.364717	2.836262
14	Br	4.962735	5.145736	4.414848	3.606535	4.093240
15	H	3.229666	3.249259	2.152121	1.076777	2.131057
16	C	3.547349	2.501488	1.383656	2.388879	3.498639
17	C	4.316399	3.043096	2.400674	3.619042	4.581713
18	H	4.141185	3.316359	2.011879	2.470038	3.758565
19	H	5.339351	4.083964	3.333477	4.433137	5.508096
20	H	4.228195	2.888579	2.735846	4.069568	4.789668
21	O	4.406822	5.611819	5.678397	4.532820	3.583313
22	H	5.031366	6.233241	6.365738	5.265616	4.332850

		6	7	8	9	10
6	C	0.000000				
7	C	1.518319	0.000000			
8	H	2.817998	3.303504	0.000000		
9	H	4.648524	5.298346	2.732068	0.000000	
10	H	1.090480	2.131900	3.834816	5.371835	0.000000
11	H	1.089843	2.169954	2.664929	4.849335	1.762379
12	H	2.156135	1.098941	2.781037	4.964156	3.046876
13	H	2.194907	1.098412	3.984859	5.536513	2.491948
14	Br	4.233392	3.797485	5.668919	5.970809	4.145884
15	H	2.835524	3.718235	4.201393	4.227277	2.598685
16	C	4.854679	5.631669	4.579103	2.850476	5.050758

17	C	6.004010	6.783615	5.242815	2.915091	6.279620
18	H	4.939476	5.641729	5.206158	3.819318	4.945220
19	H	6.892125	7.631867	6.282045	3.934503	7.079690
20	H	6.248910	7.050049	5.014080	2.418640	6.659217
21	O	2.231989	1.413363	4.318161	6.557396	2.440113
22	H	3.089774	1.921143	4.851924	7.128675	3.356283

		11	12	13	14	15
11	H	0.000000				
12	H	2.507110	0.000000			
13	H	3.099675	1.815066	0.000000		
14	Br	5.317661	4.337359	2.782236	0.000000	
15	H	3.671836	4.344840	3.501003	3.296669	0.000000
16	C	5.473310	5.806695	5.445698	4.709135	2.730307
17	C	6.514424	6.831190	6.646797	5.876721	4.033735
18	H	5.698661	5.976729	5.287819	4.114674	2.394645
19	H	7.465058	7.729175	7.391571	6.265663	4.668270
20	H	6.614180	6.959504	7.048264	6.604150	4.676744
21	O	2.464339	2.091422	2.074735	4.736016	4.677246
22	H	3.324813	2.292823	2.348695	4.966618	5.431885

		16	17	18	19	20
16	C	0.000000				
17	C	1.321819	0.000000			
18	H	1.061752	2.116669	0.000000		
19	H	2.044953	1.062648	2.424064	0.000000	
20	H	2.119825	1.068231	3.081393	1.823169	0.000000
21	O	6.869054	8.052287	6.823432	8.899363	8.322560
22	H	7.533447	8.701644	7.474587	9.535072	8.965572

		21	22
21	O	0.000000	
22	H	0.961414	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.204684	-2.000419	-0.719494
2	6	0	-2.326591	-1.252410	-0.773725
3	7	0	-2.194007	-0.260904	0.192952

4	6	0	-0.960285	-0.369840	0.723653
5	7	0	-0.391485	-1.489563	0.286147
6	6	0	0.925227	-2.009358	0.660732
7	6	0	1.997472	-1.653734	-0.353721
8	1	0	-0.929625	-2.876840	-1.275272
9	1	0	-3.186768	-1.342769	-1.402259
10	1	0	1.233499	-1.632484	1.636478
11	1	0	0.795670	-3.088205	0.744761
12	1	0	1.725884	-2.053340	-1.340750
13	1	0	2.204199	-0.575988	-0.401011
14	35	0	1.518094	2.106802	-0.131318
15	1	0	-0.593031	0.214016	1.550506
16	6	0	-2.988684	0.851501	0.406375
17	6	0	-4.246178	0.972391	0.017404
18	1	0	-2.432117	1.605438	0.905503
19	1	0	-4.734918	1.896791	0.206713
20	1	0	-4.798899	0.215138	-0.494637
21	8	0	3.086836	-2.348047	0.219699
22	1	0	3.808896	-2.290976	-0.412511

Rotational constants (GHZ): 0.7105285 0.4963019 0.3081022

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 828.7660108736 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 4.69D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Initial guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.966487 -0.013635 0.011858 0.256078 Ang= -29.75 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.31647411 A.U. after 14 cycles
NFock= 14 Conv=0.48D-08 -V/T= 2.0016
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.006216762	-0.008423227	0.003675097
2	6	-0.000586708	-0.002063175	0.003024367
3	7	0.026623470	0.003635247	-0.013642802
4	6	0.000849815	-0.011440657	0.019896453
5	7	-0.008054992	0.009192214	-0.009126969
6	6	-0.009601516	0.000845705	-0.003085140
7	6	-0.000678991	-0.005481717	0.005609883
8	1	0.001374574	-0.000605759	-0.001394196
9	1	-0.003070011	0.000237715	-0.002805547
10	1	-0.005911733	0.000547933	-0.000879985
11	1	0.005382162	0.000906032	-0.000239050
12	1	0.000539115	0.002381825	-0.000198685
13	1	-0.006441770	-0.002917040	-0.002688715
14	35	-0.003883451	-0.010603008	-0.000433218
15	1	0.000780730	0.006287096	-0.002588547
16	6	-0.014046007	-0.000775072	-0.002377987
17	6	0.003657359	0.003301519	0.003358431
18	1	-0.005676115	0.012950419	0.010414886
19	1	-0.012411110	0.005872714	0.002435424
20	1	0.000316362	-0.007551762	-0.006698093
21	8	0.019752999	0.003196162	-0.007236088
22	1	0.004869055	0.000506836	0.004980482

Cartesian Forces: Max 0.026623470 RMS 0.007426648

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.052482729 RMS 0.010528099
Search for a local minimum.
Step number 3 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 3 2
DE= 1.52D-02 DEPred=-1.57D-02 R=-9.71D-01
Trust test=-9.71D-01 RLast= 4.41D-01 DXMaxT set to 1.50D-01
ITU= -1 0 0
Use linear search instead of GDIIS.
Energy rises -- skip Quadratic/GDIIS search.
Quartic linear search produced a step of -0.79215.
Iteration 1 RMS(Cart)= 0.16216851 RMS(Int)= 0.01174576
Iteration 2 RMS(Cart)= 0.03088221 RMS(Int)= 0.00039780
Iteration 3 RMS(Cart)= 0.00054016 RMS(Int)= 0.00018291
Iteration 4 RMS(Cart)= 0.00000021 RMS(Int)= 0.00018291

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55017	0.00602	0.00699	0.00000	0.00700	2.55718
R2	2.62773	-0.00270	-0.00590	0.00000	-0.00590	2.62182
R3	2.02885	0.00200	0.00274	0.00000	0.00274	2.03159
R4	2.62878	0.00520	-0.00856	0.00000	-0.00855	2.62022
R5	2.02044	0.00394	0.00635	0.00000	0.00635	2.02679
R6	2.54628	0.00229	0.00143	0.00000	0.00142	2.54770
R7	2.61473	0.03213	0.07075	0.00000	0.07075	2.68548
R8	2.51321	0.00459	0.01570	0.00000	0.01569	2.52890
R9	2.03481	0.00027	-0.00409	0.00000	-0.00409	2.03073
R10	2.76716	0.00244	0.00526	0.00000	0.00526	2.77242
R11	2.86921	0.00003	0.00319	0.00000	0.00319	2.87240
R12	2.06071	-0.00078	0.00100	0.00000	0.00100	2.06171
R13	2.05950	0.00088	0.00493	0.00000	0.00493	2.06443
R14	2.07670	-0.00024	0.00018	0.00000	0.00018	2.07688
R15	2.07570	-0.01080	-0.00543	0.00000	-0.00543	2.07027
R16	2.67087	0.01922	0.01182	0.00000	0.01182	2.68269
R17	5.25766	-0.00529	-0.01640	0.00000	-0.01640	5.24127
R18	2.49788	0.00729	0.00210	0.00000	0.00210	2.49997
R19	2.00642	0.01584	0.02795	0.00000	0.02795	2.03437
R20	2.00811	0.01378	0.02777	0.00000	0.02777	2.03588
R21	2.01866	0.00999	0.02365	0.00000	0.02365	2.04231

R22	1.81681	0.00145	-0.00148	0.00000	-0.00148	1.81533
A1	1.88769	-0.00466	-0.00666	0.00000	-0.00667	1.88101
A2	2.27138	0.00254	0.00506	0.00000	0.00508	2.27646
A3	2.12287	0.00226	0.00209	0.00000	0.00211	2.12498
A4	1.86284	0.00274	0.00388	0.00000	0.00387	1.86671
A5	2.27264	-0.00029	0.00472	0.00000	0.00473	2.27737
A6	2.14770	-0.00245	-0.00863	0.00000	-0.00862	2.13908
A7	1.87899	-0.00104	0.00717	0.00000	0.00720	1.88619
A8	2.24654	-0.00242	-0.03272	0.00000	-0.03269	2.21385
A9	2.12953	0.00408	0.01560	0.00000	0.01573	2.14526
A10	1.90720	-0.00249	-0.01225	0.00000	-0.01229	1.89491
A11	2.17839	0.00169	0.00364	0.00000	0.00372	2.18211
A12	2.16913	0.00271	0.01457	0.00000	0.01462	2.18375
A13	1.87246	0.00652	0.00833	0.00000	0.00838	1.88083
A14	2.19008	0.00666	-0.00822	0.00000	-0.00810	2.18198
A15	2.21341	-0.01342	-0.00673	0.00000	-0.00663	2.20678
A16	1.96163	-0.02027	-0.03046	0.00000	-0.03040	1.93123
A17	1.93950	-0.00273	-0.02463	0.00000	-0.02456	1.91494
A18	1.83819	0.01515	0.02727	0.00000	0.02719	1.86538
A19	1.89363	0.00570	0.00663	0.00000	0.00683	1.90046
A20	1.94693	0.00477	0.02406	0.00000	0.02403	1.97096
A21	1.88256	-0.00196	-0.00286	0.00000	-0.00287	1.87969
A22	1.91814	0.00917	0.00610	0.00000	0.00692	1.92506
A23	1.97305	-0.04683	-0.09813	0.00000	-0.09788	1.87517
A24	1.72964	0.02984	0.10319	0.00000	0.10316	1.83280
A25	1.94403	0.00881	-0.01640	0.00000	-0.01591	1.92812
A26	1.95654	-0.01014	-0.00702	0.00000	-0.00655	1.94998
A27	1.93308	0.00980	0.01685	0.00000	0.01595	1.94904
A28	2.68042	-0.05248	-0.07177	0.00000	-0.07177	2.60864
A29	2.18281	-0.00195	-0.01794	0.00000	-0.01793	2.16488
A30	1.92019	0.00858	0.03329	0.00000	0.03329	1.95348
A31	2.17984	-0.00663	-0.01514	0.00000	-0.01514	2.16470
A32	2.05407	0.00369	0.03773	0.00000	0.03773	2.09180
A33	2.17543	-0.00326	-0.01365	0.00000	-0.01365	2.16178
A34	2.05339	-0.00040	-0.02392	0.00000	-0.02392	2.02947
A35	1.85763	0.01126	0.01789	0.00000	0.01789	1.87552
D1	0.01528	0.00012	0.00280	0.00000	0.00279	0.01807
D2	-3.12354	-0.00200	-0.00827	0.00000	-0.00830	-3.13184
D3	3.10284	0.00310	0.01542	0.00000	0.01542	3.11826
D4	-0.03597	0.00098	0.00435	0.00000	0.00433	-0.03164
D5	-0.11216	0.00315	-0.00088	0.00000	-0.00086	-0.11302
D6	-3.13177	0.00618	0.04440	0.00000	0.04437	-3.08740
D7	3.07794	0.00044	-0.01232	0.00000	-0.01231	3.06563
D8	0.05832	0.00347	0.03296	0.00000	0.03292	0.09125

D9	0.08592	-0.00348	-0.00326	0.00000	-0.00326	0.08266
D10	2.97465	-0.00005	-0.03862	0.00000	-0.03875	2.93590
D11	-3.05820	-0.00155	0.00673	0.00000	0.00677	-3.05143
D12	-0.16947	0.00189	-0.02862	0.00000	-0.02872	-0.19819
D13	-0.15941	0.00620	0.00431	0.00000	0.00434	-0.15506
D14	-3.05521	-0.00217	-0.02456	0.00000	-0.02453	-3.07974
D15	-3.06871	0.00412	0.04672	0.00000	0.04658	-3.02213
D16	0.31868	-0.00425	0.01785	0.00000	0.01771	0.33639
D17	0.39550	-0.00129	-0.00349	0.00000	-0.00348	0.39203
D18	-2.71909	-0.00152	-0.01441	0.00000	-0.01436	-2.73345
D19	-3.03108	0.00175	-0.04633	0.00000	-0.04638	-3.07745
D20	0.13752	0.00152	-0.05725	0.00000	-0.05726	0.08026
D21	0.16774	-0.00524	-0.00216	0.00000	-0.00220	0.16554
D22	-3.09794	-0.00649	-0.04838	0.00000	-0.04836	3.13688
D23	3.06513	0.00291	0.02491	0.00000	0.02483	3.08996
D24	-0.20055	0.00166	-0.02131	0.00000	-0.02134	-0.22188
D25	1.29463	0.00719	0.00736	0.00000	0.00742	1.30205
D26	-2.86263	-0.00182	-0.02100	0.00000	-0.02112	-2.88375
D27	-0.82864	0.00312	-0.02175	0.00000	-0.02176	-0.85041
D28	-1.70131	0.00905	0.05998	0.00000	0.06009	-1.64123
D29	0.42461	0.00005	0.03162	0.00000	0.03155	0.45616
D30	2.45860	0.00499	0.03087	0.00000	0.03090	2.48950
D31	-1.02326	-0.00271	-0.04110	0.00000	-0.04115	-1.06441
D32	1.16069	-0.01875	-0.12212	0.00000	-0.12251	1.03818
D33	-3.07571	-0.00937	-0.09255	0.00000	-0.09214	3.11534
D34	3.10810	0.01030	0.00469	0.00000	0.00464	3.11275
D35	-0.99113	-0.00574	-0.07632	0.00000	-0.07671	-1.06784
D36	1.05566	0.00364	-0.04676	0.00000	-0.04635	1.00931
D37	1.03680	0.00625	-0.01104	0.00000	-0.01106	1.02573
D38	-3.06244	-0.00979	-0.09206	0.00000	-0.09242	3.12833
D39	-1.01565	-0.00041	-0.06249	0.00000	-0.06205	-1.07770
D40	-0.47761	0.01119	0.03943	0.00000	0.03975	-0.43785
D41	1.69227	-0.00553	-0.02913	0.00000	-0.02947	1.66280
D42	-2.40073	-0.00486	-0.03805	0.00000	-0.03804	-2.43877
D43	3.01015	0.02047	0.01229	0.00000	0.01249	3.02264
D44	0.98694	-0.00200	-0.05125	0.00000	-0.05118	0.93576
D45	-1.19619	-0.01345	-0.03718	0.00000	-0.03746	-1.23365
D46	-3.09677	-0.00089	-0.01698	0.00000	-0.01700	-3.11377
D47	0.01798	-0.00006	-0.00840	0.00000	-0.00842	0.00956
D48	0.01389	-0.00039	-0.00413	0.00000	-0.00411	0.00978
D49	3.12864	0.00045	0.00446	0.00000	0.00447	3.13311

Item	Value	Threshold	Converged?
Maximum Force	0.052483	0.000450	NO
RMS Force	0.010528	0.000300	NO

Maximum Displacement 1.106578 0.001800 NO
RMS Displacement 0.188413 0.001200 NO
Predicted change in Energy=-7.631934D-03
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.438921	-1.941638	-1.253477
2	6	0	-1.755275	-1.660406	-1.392292
3	7	0	-2.141452	-0.962573	-0.258073
4	6	0	-1.042870	-0.742446	0.491770
5	7	0	-0.025333	-1.438891	-0.028286
6	6	0	1.351649	-1.478408	0.476444
7	6	0	2.214251	-0.450996	-0.238232
8	1	0	0.230488	-2.481602	-1.898541
9	1	0	-2.435462	-1.887362	-2.189888
10	1	0	1.358053	-1.262428	1.545844
11	1	0	1.709439	-2.501836	0.342176
12	1	0	2.247898	-0.664734	-1.315759
13	1	0	1.770188	0.533908	-0.056626
14	35	0	-0.454682	2.077339	0.543707
15	1	0	-1.039505	-0.270565	1.457228
16	6	0	-3.362619	-0.262466	-0.062870
17	6	0	-4.473416	-0.508668	-0.737893
18	1	0	-3.271504	0.502889	0.688707
19	1	0	-5.355424	0.081629	-0.552746
20	1	0	-4.559743	-1.272804	-1.497270
21	8	0	3.496131	-0.566609	0.360714
22	1	0	4.098460	-0.008211	-0.137485

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.353200	0.000000			
3	N	2.201820	1.386563	0.000000		
4	C	2.201977	2.213563	1.348185	0.000000	
5	N	1.387409	2.214109	2.181201	1.338235	0.000000
6	C	2.532459	3.630189	3.606571	2.505114	1.467104
7	C	3.208124	4.307165	4.385688	3.350625	2.456777
8	H	1.075070	2.207692	3.259552	3.218647	2.156512
9	H	2.205899	1.072531	2.161848	3.231321	3.268390

10	H	3.395091	4.299284	3.948489	2.673179	2.103042
11	H	2.734114	3.964925	4.190345	3.270021	2.067977
12	H	2.975459	4.125847	4.524798	3.755310	2.724791
13	H	3.527172	4.362099	4.192966	3.137374	2.667702
14	Br	4.402532	4.405720	3.567787	2.880946	3.588229
15	H	3.240542	3.250193	2.153003	1.074614	2.144827
16	C	3.575637	2.511007	1.421093	2.432949	3.538736
17	C	4.312352	3.023744	2.423698	3.651762	4.599380
18	H	4.215604	3.362938	2.078699	2.560557	3.849962
19	H	5.362522	4.086636	3.392168	4.513118	5.567487
20	H	4.181860	2.833072	2.734956	4.075041	4.769316
21	O	4.470006	5.643287	5.685247	4.544296	3.648686
22	H	5.056817	6.210515	6.313624	5.231475	4.366284

		6	7	8	9	10
6	C	0.000000				
7	C	1.520006	0.000000			
8	H	2.811397	3.288663	0.000000		
9	H	4.649600	5.243276	2.746869	0.000000	
10	H	1.091011	2.138790	3.823817	5.360690	0.000000
11	H	1.092450	2.190354	2.684869	4.895828	1.763072
12	H	2.162712	1.099037	2.776794	4.918616	3.055788
13	H	2.123383	1.095541	3.854429	5.301023	2.442251
14	Br	3.988820	3.758605	5.217084	5.207195	3.929927
15	H	2.852795	3.673428	4.214588	4.226605	2.596138
16	C	4.898336	5.582811	4.604853	2.832687	5.086515
17	C	6.028796	6.706555	5.231279	2.856981	6.307903
18	H	5.034295	5.644698	5.278729	3.833873	5.028302
19	H	6.962598	7.594906	6.291560	3.883727	7.161100
20	H	6.235574	6.938844	4.956665	2.317320	6.654395
21	O	2.333147	1.419619	4.408612	6.590429	2.541668
22	H	3.175430	1.938156	4.917335	7.101810	3.452026

		11	12	13	14	15
11	H	0.000000				
12	H	2.532515	0.000000			
13	H	3.062429	1.802878	0.000000		
14	Br	5.068814	4.275572	2.773558	0.000000	
15	H	3.711954	4.318778	3.291399	2.586347	0.000000
16	C	5.559192	5.762764	5.194224	3.781364	2.776261
17	C	6.585359	6.747914	6.366606	4.947742	4.082523
18	H	5.827370	5.987071	5.096581	3.230232	2.484084
19	H	7.575451	7.677874	7.157167	5.403919	4.774013
20	H	6.648062	6.837154	6.738523	5.678078	4.703788
21	O	2.633955	2.092434	2.089064	4.757402	4.675680
22	H	3.486497	2.289963	2.391920	5.054171	5.386151

		16	17	18	19	20
16	C	0.000000				
17	C	1.322929	0.000000			
18	H	1.076540	2.122035	0.000000		
19	H	2.080781	1.077343	2.461989	0.000000	
20	H	2.124004	1.080745	3.096957	1.832954	0.000000
21	O	6.878545	8.045121	6.859467	8.922144	8.297465
22	H	7.465783	8.607438	7.433719	9.463426	8.855094

		21	22
21	O	0.000000	
22	H	0.960630	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.159870	-2.228327	-0.589419
2	6	0	-1.476367	-1.922235	-0.654937
3	7	0	-1.696933	-0.890716	0.244994
4	6	0	-0.506043	-0.521255	0.757715
5	7	0	0.419719	-1.403794	0.364061
6	6	0	1.849054	-1.372706	0.693347
7	6	0	2.635449	-0.665700	-0.398506
8	1	0	0.408207	-2.978649	-1.109114
9	1	0	-2.258787	-2.338374	-1.259065
10	1	0	1.998323	-0.843131	1.635459
11	1	0	2.163075	-2.408545	0.841255
12	1	0	2.524888	-1.198070	-1.353619
13	1	0	2.241127	0.353174	-0.479840
14	35	0	0.148132	2.139556	-0.132224
15	1	0	-0.367359	0.220278	1.523019
16	6	0	-2.866403	-0.090798	0.354415
17	6	0	-4.060343	-0.461593	-0.078205
18	1	0	-2.661625	0.859471	0.817011
19	1	0	-4.897382	0.210038	0.016375
20	1	0	-4.261353	-1.413363	-0.549095
21	8	0	3.980922	-0.672530	0.054235
22	1	0	4.526516	-0.329790	-0.658273

```
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.8309317           0.5704488           0.3581423
 Standard basis: 6-311++G(d,p) (5D, 7F)
 There are     358 symmetry adapted cartesian basis functions of A      symmetry.
 There are     345 symmetry adapted basis functions of A      symmetry.
    345 basis functions,      553 primitive gaussians,      358 cartesian basis functions
     55 alpha electrons              55 beta electrons
          nuclear repulsion energy              868.7387654095 Hartrees.
 NAtoms=       22 NActive=       22 NUniq=       22 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      345 RedAO= T EigKep=    4.47D-06    NBF=      345
 NBsUse=      345 1.00D-06 EigRej= -1.00D+00 NBFU=      345
 Lowest energy guess from the checkpoint file:    "."
 B after Tr=          0.000000        0.000000        0.000000
             Rot=        0.999383      -0.004311        0.001878        0.034803 Ang=    -4.03 deg.
 B after Tr=          0.000000        0.000000        0.000000
             Rot=        0.974859        0.009602      -0.009482      -0.222412 Ang=    25.75 deg.
 Keep R1 ints in memory in canonical form, NReq=1804729152.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                    energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3032.33382694          A.U. after      11 cycles
                  NFock= 11    Conv=0.76D-08         -V/T= 2.0016
 Calling FoFJK, ICntrl=            2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center         Atomic                          Forces (Hartrees/Bohr)
 Number         Number                       X                   Y                   Z
 -------------------------------------------------------------------
        1              6              -0.000978352     -0.007050554     -0.001244571
        2              6               0.003552661     -0.004010145     -0.003028040
        3              7              -0.001738667      0.012899455     -0.005957812
        4              6               0.000150609     -0.005494620      0.017370340
        5              7              -0.000886793      0.005084265     -0.003096607
        6              6              -0.003930771     -0.002866560      0.000140473
        7              6              -0.001285169      0.000516343      0.003135344
        8              1               0.000262886     -0.000523121     -0.000627161
        9              1              -0.000558252      0.000222296     -0.001191681
```

10	1	-0.003282344	0.000250993	-0.000652336
11	1	0.002913445	0.001409621	-0.000708141
12	1	0.000043477	0.001048236	0.000688229
13	1	0.000788960	0.000998800	-0.004104612
14	35	-0.000929253	-0.000122125	-0.001196135
15	1	-0.000296412	-0.000956655	-0.001164297
16	6	0.003293892	-0.005140920	0.002308576
17	6	-0.003342712	-0.000950826	-0.002472737
18	1	-0.000170675	0.004087046	0.002064329
19	1	-0.001588550	0.002188906	0.001488331
20	1	0.000865089	-0.001671923	-0.000719649
21	8	0.004629747	-0.001448601	-0.003392305
22	1	0.002487187	0.001530088	0.002360463

Cartesian Forces: Max 0.017370340 RMS 0.003677530

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.007858193 RMS 0.002436486

Search for a local minimum.

Step number 4 out of a maximum of 116

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 3 2 4

ITU= 0 -1 0 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00247	0.00361	0.00760	0.01085	0.01282
Eigenvalues ---	0.01587	0.01800	0.01861	0.02045	0.02138
Eigenvalues ---	0.02195	0.02409	0.02445	0.02491	0.03067
Eigenvalues ---	0.03071	0.04496	0.05304	0.05344	0.06121
Eigenvalues ---	0.08420	0.09162	0.12703	0.13411	0.15437
Eigenvalues ---	0.15696	0.15981	0.15999	0.16000	0.16000
Eigenvalues ---	0.16032	0.18214	0.21748	0.22643	0.22733
Eigenvalues ---	0.23044	0.23558	0.24376	0.28844	0.30999
Eigenvalues ---	0.33847	0.33875	0.33875	0.33891	0.34150
Eigenvalues ---	0.34531	0.34647	0.35541	0.36286	0.36307
Eigenvalues ---	0.37221	0.40971	0.42963	0.45509	0.49162
Eigenvalues ---	0.53320	0.53813	0.55470	0.60489	2.11778

RFO step: Lambda=-6.87859457D-03 EMin= 2.46980176D-03

Quartic linear search produced a step of -0.09097.

Iteration 1 RMS(Cart)= 0.13708153 RMS(Int)= 0.00703075

Iteration 2 RMS(Cart)= 0.01038504 RMS(Int)= 0.00051016

Iteration 3 RMS(Cart)= 0.00005402 RMS(Int)= 0.00050968

Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00050968

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55718	0.00041	0.00017	-0.00104	-0.00061	2.55657
R2	2.62182	0.00326	-0.00014	0.00795	0.00748	2.62931
R3	2.03159	0.00080	0.00007	0.00145	0.00152	2.03311
R4	2.62022	0.00786	-0.00021	0.01627	0.01654	2.63677
R5	2.02679	0.00120	0.00015	0.00168	0.00183	2.02862
R6	2.54770	0.00349	0.00004	0.00557	0.00563	2.55333
R7	2.68548	0.00045	0.00169	-0.01371	-0.01202	2.67346
R8	2.52890	0.00232	0.00038	0.00096	0.00088	2.52977
R9	2.03073	-0.00147	-0.00010	-0.00279	-0.00288	2.02784
R10	2.77242	0.00003	0.00013	-0.00098	-0.00086	2.77157
R11	2.87240	0.00613	0.00008	0.01885	0.01893	2.89132
R12	2.06171	-0.00062	0.00002	-0.00183	-0.00181	2.05990
R13	2.06443	-0.00027	0.00012	-0.00177	-0.00165	2.06278
R14	2.07688	-0.00088	0.00000	-0.00241	-0.00241	2.07447
R15	2.07027	-0.00003	-0.00013	0.00124	0.00111	2.07139
R16	2.68269	0.00598	0.00028	0.01089	0.01117	2.69386
R17	5.24127	0.00042	-0.00039	0.00753	0.00713	5.24840
R18	2.49997	0.00436	0.00005	0.00621	0.00626	2.50624
R19	2.03437	0.00433	0.00067	0.00585	0.00652	2.04088
R20	2.03588	0.00276	0.00066	0.00164	0.00231	2.03819
R21	2.04231	0.00161	0.00056	-0.00058	-0.00002	2.04230
R22	1.81533	0.00122	-0.00004	0.00236	0.00232	1.81765
A1	1.88101	-0.00185	-0.00016	-0.00352	-0.00540	1.87561
A2	2.27646	0.00072	0.00012	0.00113	0.00140	2.27786
A3	2.12498	0.00121	0.00005	0.00443	0.00462	2.12960
A4	1.86671	0.00093	0.00009	0.00371	0.00325	1.86996
A5	2.27737	-0.00055	0.00011	-0.00359	-0.00322	2.27415
A6	2.13908	-0.00038	-0.00021	-0.00020	-0.00016	2.13892
A7	1.88619	-0.00017	0.00017	0.00527	0.00351	1.88970
A8	2.21385	0.00242	-0.00078	0.02101	0.01955	2.23340
A9	2.14526	-0.00157	0.00036	-0.00338	-0.00390	2.14136
A10	1.89491	-0.00226	-0.00029	0.00033	-0.00287	1.89204
A11	2.18211	0.00138	0.00008	0.01035	0.00995	2.19206
A12	2.18375	0.00143	0.00034	0.00795	0.00775	2.19149
A13	1.88083	0.00410	0.00019	0.01744	0.01567	1.89650
A14	2.18198	0.00268	-0.00021	0.01066	0.01137	2.19335
A15	2.20678	-0.00666	-0.00017	-0.02406	-0.02342	2.18336
A16	1.93123	0.00436	-0.00073	0.02431	0.02352	1.95475
A17	1.91494	-0.00566	-0.00059	-0.04442	-0.04481	1.87013
A18	1.86538	0.00286	0.00066	0.03177	0.03262	1.89800

A19	1.90046	0.00191	0.00014	0.00368	0.00394	1.90441
A20	1.97096	-0.00491	0.00058	-0.02497	-0.02487	1.94609
A21	1.87969	0.00118	-0.00007	0.00790	0.00809	1.88778
A22	1.92506	0.00041	0.00007	-0.00680	-0.00659	1.91847
A23	1.87517	0.00162	-0.00237	0.03238	0.02977	1.90494
A24	1.83280	0.00021	0.00247	-0.00861	-0.00674	1.82607
A25	1.92812	-0.00311	-0.00044	-0.03859	-0.03878	1.88934
A26	1.94998	-0.00081	-0.00021	-0.00553	-0.00563	1.94435
A27	1.94904	0.00198	0.00048	0.03035	0.03055	1.97959
A28	2.60864	-0.00304	-0.00171	0.00493	0.00322	2.61186
A29	2.16488	0.00098	-0.00043	0.00752	0.00708	2.17196
A30	1.95348	0.00041	0.00079	-0.00334	-0.00257	1.95092
A31	2.16470	-0.00139	-0.00036	-0.00436	-0.00475	2.15995
A32	2.09180	-0.00111	0.00090	-0.01322	-0.01233	2.07947
A33	2.16178	-0.00061	-0.00033	-0.00077	-0.00111	2.16067
A34	2.02947	0.00173	-0.00057	0.01410	0.01352	2.04300
A35	1.87552	0.00523	0.00043	0.02571	0.02614	1.90166
D1	0.01807	-0.00119	0.00007	-0.03027	-0.02982	-0.01175
D2	-3.13184	-0.00160	-0.00019	-0.04014	-0.04003	3.11131
D3	3.11826	0.00110	0.00037	0.02744	0.02792	-3.13700
D4	-0.03164	0.00070	0.00011	0.01757	0.01771	-0.01394
D5	-0.11302	0.00318	-0.00002	0.09846	0.09868	-0.01433
D6	-3.08740	0.00311	0.00106	0.07630	0.07697	-3.01043
D7	3.06563	0.00113	-0.00029	0.04688	0.04698	3.11261
D8	0.09125	0.00106	0.00079	0.02471	0.02527	0.11651
D9	0.08266	-0.00143	-0.00008	-0.04884	-0.04911	0.03356
D10	2.93590	0.00074	-0.00091	0.03489	0.03434	2.97024
D11	-3.05143	-0.00107	0.00016	-0.03991	-0.03984	-3.09127
D12	-0.19819	0.00110	-0.00067	0.04382	0.04361	-0.15458
D13	-0.15506	0.00387	0.00010	0.11259	0.11230	-0.04276
D14	-3.07974	0.00112	-0.00059	0.02301	0.02184	-3.05789
D15	-3.02213	0.00101	0.00113	0.02803	0.02956	-2.99257
D16	0.33639	-0.00174	0.00044	-0.06154	-0.06090	0.27549
D17	0.39203	-0.00076	-0.00008	-0.00455	-0.00459	0.38744
D18	-2.73345	-0.00039	-0.00035	0.00749	0.00720	-2.72624
D19	-3.07745	0.00205	-0.00110	0.09281	0.09165	-2.98580
D20	0.08026	0.00242	-0.00137	0.10485	0.10344	0.18370
D21	0.16554	-0.00417	-0.00005	-0.12976	-0.13003	0.03551
D22	3.13688	-0.00293	-0.00116	-0.10285	-0.10424	3.03264
D23	3.08996	-0.00142	0.00060	-0.03971	-0.03926	3.05070
D24	-0.22188	-0.00019	-0.00051	-0.01280	-0.01347	-0.23536
D25	1.30205	-0.00123	0.00017	0.01854	0.01895	1.32100
D26	-2.88375	0.00025	-0.00049	0.00989	0.00937	-2.87438
D27	-0.85041	0.00029	-0.00052	0.01375	0.01273	-0.83768

D28	-1.64123	-0.00256	0.00142	-0.01254	-0.01068	-1.65190
D29	0.45616	-0.00108	0.00076	-0.02119	-0.02026	0.43590
D30	2.48950	-0.00104	0.00073	-0.01733	-0.01690	2.47260
D31	-1.06441	-0.00256	-0.00098	-0.12124	-0.12206	-1.18648
D32	1.03818	-0.00510	-0.00288	-0.15219	-0.15500	0.88319
D33	3.11534	-0.00194	-0.00225	-0.10599	-0.10810	3.00724
D34	3.11275	0.00050	0.00012	-0.08378	-0.08363	3.02912
D35	-1.06784	-0.00204	-0.00179	-0.11474	-0.11656	-1.18441
D36	1.00931	0.00113	-0.00115	-0.06854	-0.06966	0.93965
D37	1.02573	0.00084	-0.00026	-0.08040	-0.08077	0.94496
D38	3.12833	-0.00170	-0.00216	-0.11136	-0.11370	3.01463
D39	-1.07770	0.00146	-0.00153	-0.06516	-0.06680	-1.14450
D40	-0.43785	-0.00033	0.00091	-0.04144	-0.04001	-0.47787
D41	1.66280	-0.00064	-0.00066	-0.05222	-0.05290	1.60990
D42	-2.43877	-0.00256	-0.00091	-0.06596	-0.06737	-2.50613
D43	3.02264	0.00025	0.00027	0.03163	0.03188	3.05453
D44	0.93576	0.00007	-0.00123	0.04801	0.04674	0.98251
D45	-1.23365	0.00327	-0.00086	0.08000	0.07920	-1.15444
D46	-3.11377	0.00013	-0.00040	0.00600	0.00559	-3.10818
D47	0.00956	0.00049	-0.00020	0.01379	0.01359	0.02315
D48	0.00978	-0.00026	-0.00010	-0.00745	-0.00754	0.00224
D49	3.13311	0.00010	0.00010	0.00035	0.00046	3.13357

Item	Value	Threshold	Converged?
Maximum Force	0.007858	0.000450	NO
RMS Force	0.002436	0.000300	NO
Maximum Displacement	0.949743	0.001800	NO
RMS Displacement	0.140931	0.001200	NO

Predicted change in Energy=-4.023874D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.450770	-1.986224	-1.274752
2	6	0	-1.751259	-1.640763	-1.414988
3	7	0	-2.122031	-0.956061	-0.257136
4	6	0	-1.037900	-0.859593	0.543491
5	7	0	-0.020662	-1.502383	-0.043162
6	6	0	1.362029	-1.516666	0.445738
7	6	0	2.216930	-0.437183	-0.221214
8	1	0	0.207038	-2.517063	-1.940335
9	1	0	-2.429583	-1.806266	-2.230396

10	1	0	1.325377	-1.330370	1.519128
11	1	0	1.779890	-2.512578	0.287327
12	1	0	2.358131	-0.675215	-1.283517
13	1	0	1.698580	0.526100	-0.151204
14	35	0	-0.668941	1.965349	0.041125
15	1	0	-1.028201	-0.449400	1.535037
16	6	0	-3.316506	-0.237405	-0.015826
17	6	0	-4.452739	-0.428741	-0.672550
18	1	0	-3.186174	0.509942	0.752851
19	1	0	-5.304804	0.190087	-0.439447
20	1	0	-4.581829	-1.171591	-1.446824
21	8	0	3.453325	-0.468189	0.487660
22	1	0	4.070451	0.137334	0.066148

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.352879	0.000000			
3	N	2.211310	1.395317	0.000000		
4	C	2.218113	2.225926	1.351166	0.000000	
5	N	1.391369	2.212695	2.181744	1.338698	0.000000
6	C	2.542993	3.629086	3.598192	2.490173	1.466650
7	C	3.259769	4.315116	4.370024	3.370033	2.484587
8	H	1.075873	2.208805	3.270237	3.235192	2.163489
9	H	2.204845	1.073501	2.170528	3.244598	3.267910
10	H	3.374998	4.262754	3.896132	2.599726	2.069338
11	H	2.773623	4.015838	4.236057	3.276876	2.090862
12	H	3.099798	4.223346	4.604800	3.860697	2.807373
13	H	3.491968	4.265423	4.099402	3.145007	2.661242
14	Br	4.170618	4.036796	3.276441	2.892888	3.528815
15	H	3.254254	3.262638	2.159874	1.073088	2.148167
16	C	3.585485	2.525285	1.414732	2.427344	3.530369
17	C	4.336376	3.052574	2.425455	3.650413	4.603492
18	H	4.221901	3.374024	2.074039	2.556274	3.834522
19	H	5.384766	4.114775	3.387762	4.502718	5.562702
20	H	4.214129	2.869366	2.740878	4.076534	4.783715
21	O	4.544500	5.664158	5.646002	4.508594	3.663320
22	H	5.171939	6.264799	6.296576	5.226564	4.408835

		6	7	8	9	10
6	C	0.000000				
7	C	1.530021	0.000000			
8	H	2.833398	3.364661	0.000000		
9	H	4.649934	5.244167	2.746113	0.000000	
10	H	1.090053	2.149754	3.824501	5.327770	0.000000

11	H	1.091578	2.181028	2.726969	4.955549	1.766786
12	H	2.165775	1.097764	2.907062	5.009796	3.057880
13	H	2.154646	1.096130	3.832300	5.177325	2.525029
14	Br	4.051293	3.764204	4.978508	4.741809	4.125962
15	H	2.835283	3.689911	4.228387	4.240689	2.513104
16	C	4.872190	5.540849	4.616919	2.855220	5.009763
17	C	6.020438	6.684928	5.261358	2.901314	6.245239
18	H	4.988748	5.571300	5.284875	3.851885	4.932344
19	H	6.938532	7.550999	6.321529	3.931898	7.078637
20	H	6.247425	6.947273	4.998709	2.376754	6.611896
21	O	2.339782	1.425530	4.542182	6.617166	2.517031
22	H	3.196147	1.961680	5.098799	7.162551	3.435220

		11	12	13	14	15
11	H	0.000000				
12	H	2.485521	0.000000			
13	H	3.071235	1.777723	0.000000		
14	Br	5.109718	4.229707	2.777334	0.000000	
15	H	3.701197	4.411631	3.351171	2.862141	0.000000
16	C	5.589415	5.830971	5.074677	3.444556	2.772446
17	C	6.641491	6.842659	6.246779	4.534107	4.074472
18	H	5.832163	6.024177	4.967736	2.993531	2.487769
19	H	7.617446	7.757691	7.017363	4.987358	4.753616
20	H	6.728818	6.959605	6.633575	5.231164	4.694819
21	O	2.649536	2.092696	2.115629	4.807762	4.602329
22	H	3.509647	2.326773	2.413329	5.079774	5.338366

		16	17	18	19	20
16	C	0.000000				
17	C	1.326244	0.000000			
18	H	1.079990	2.125342	0.000000		
19	H	2.077387	1.078564	2.452035	0.000000	
20	H	2.126383	1.080737	3.100641	1.841648	0.000000
21	O	6.792449	7.990838	6.716399	8.831630	8.294619
22	H	7.396910	8.573849	7.298562	9.389027	8.880559

		21	22
21	O	0.000000	
22	H	0.961860	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.104940	-2.120537	-0.766652
2	6	0	-1.224092	-1.870075	-0.801640
3	7	0	-1.506468	-0.999977	0.251974
4	6	0	-0.346945	-0.703965	0.879296
5	7	0	0.638735	-1.395375	0.294060
6	6	0	2.066034	-1.251873	0.599491
7	6	0	2.760569	-0.276027	-0.352512
8	1	0	0.717525	-2.734054	-1.403708
9	1	0	-1.978357	-2.217126	-1.482114
10	1	0	2.140049	-0.870581	1.617997
11	1	0	2.531867	-2.238648	0.570904
12	1	0	2.795060	-0.701005	-1.364089
13	1	0	2.187291	0.657419	-0.391669
14	35	0	-0.237677	1.992054	-0.163940
15	1	0	-0.252150	-0.116013	1.771957
16	6	0	-2.712810	-0.307046	0.508980
17	6	0	-3.900745	-0.671804	0.045638
18	1	0	-2.547808	0.575954	1.108532
19	1	0	-4.761728	-0.061942	0.269412
20	1	0	-4.065476	-1.551376	-0.560338
21	8	0	4.069376	-0.114916	0.188971
22	1	0	4.589842	0.430230	-0.408612

Rotational constants (GHZ): 0.9129079 0.5695641 0.3778747
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 358 symmetry adapted cartesian basis functions of A symmetry.
There are 345 symmetry adapted basis functions of A symmetry.
345 basis functions, 553 primitive gaussians, 358 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 879.8689953383 Hartrees.
NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 345 RedAO= T EigKep= 4.96D-06 NBF= 345
NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345
Initial guess from the checkpoint file: "."
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.998046 -0.012969 -0.004033 -0.060996 Ang= -7.17 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Keep R1 ints in memory in canonical form, NReq=1804729152.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3032.33444160 A.U. after 13 cycles

NFock= 13 Conv=0.83D-08 -V/T= 2.0016

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000338154	0.003121825	0.000594201
2	6	-0.000007281	0.001684511	0.003652557
3	7	0.001579213	-0.006290076	-0.001519027
4	6	0.000501047	0.005528684	-0.007723666
5	7	0.000313686	-0.006531442	0.000262046
6	6	-0.002551150	0.000830209	0.002097219
7	6	-0.001789327	-0.000930656	-0.000275386
8	1	0.000230318	0.000262005	0.000117789
9	1	-0.000842160	0.000514548	-0.000177230
10	1	0.001431936	0.000069066	0.000421313
11	1	0.000043414	0.000187563	-0.000124092
12	1	0.000633403	-0.000575460	-0.000226717
13	1	0.001754140	0.000188593	0.001405981
14	35	0.001996304	0.001170781	0.001831441
15	1	0.000118561	0.001264010	-0.000392401
16	6	-0.002173379	-0.002720810	0.001614990
17	6	-0.000299435	-0.000550815	0.000638693
18	1	-0.000401754	0.002186391	-0.000327447

19	1	-0.001322158	0.001252561	0.000359470
20	1	0.000450233	-0.001132885	-0.001182229
21	8	0.000717823	-0.000601495	-0.001985546
22	1	-0.000721588	0.001072893	0.000938041

Cartesian Forces: Max 0.007723666 RMS 0.002036999

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.010781175 RMS 0.002659719
Search for a local minimum.
Step number 5 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 1 2 4 5
DE= -6.15D-04 DEPred=-4.02D-03 R= 1.53D-01
Trust test= 1.53D-01 RLast= 4.77D-01 DXMaxT set to 1.50D-01
ITU= 0 0 -1 0 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00243	0.00454	0.00676	0.00876	0.01246
Eigenvalues ---	0.01572	0.01682	0.01861	0.02038	0.02147
Eigenvalues ---	0.02212	0.02377	0.02409	0.03066	0.03070
Eigenvalues ---	0.03651	0.04588	0.05426	0.05959	0.06619
Eigenvalues ---	0.08640	0.09245	0.13473	0.14160	0.15694
Eigenvalues ---	0.15805	0.15996	0.15997	0.15999	0.16051
Eigenvalues ---	0.16244	0.20644	0.21662	0.22512	0.22838
Eigenvalues ---	0.23495	0.24271	0.25542	0.28950	0.33407
Eigenvalues ---	0.33849	0.33875	0.33898	0.34101	0.34312
Eigenvalues ---	0.34645	0.34733	0.35994	0.36306	0.36446
Eigenvalues ---	0.37231	0.41077	0.42984	0.45941	0.48987
Eigenvalues ---	0.53437	0.54089	0.55452	0.60519	1.50594

RFO step: Lambda=-2.79127729D-03 EMin= 2.43333505D-03
Quartic linear search produced a step of -0.44437.
Iteration 1 RMS(Cart)= 0.15444011 RMS(Int)= 0.00837367
Iteration 2 RMS(Cart)= 0.01062094 RMS(Int)= 0.00025160
Iteration 3 RMS(Cart)= 0.00004433 RMS(Int)= 0.00025030
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00025030

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55657	-0.00049	0.00027	-0.00092	-0.00083	2.55574
R2	2.62931	-0.00143	-0.00333	0.00608	0.00275	2.63206
R3	2.03311	-0.00006	-0.00067	0.00161	0.00094	2.03404

R4	2.63677	-0.00502	-0.00735	0.01274	0.00528	2.64204
R5	2.02862	0.00058	-0.00081	0.00303	0.00221	2.03084
R6	2.55333	0.00086	-0.00250	0.00637	0.00398	2.55732
R7	2.67346	0.00286	0.00534	-0.00866	-0.00331	2.67014
R8	2.52977	0.00131	-0.00039	0.00202	0.00181	2.53159
R9	2.02784	0.00013	0.00128	-0.00251	-0.00123	2.02661
R10	2.77157	0.00276	0.00038	0.00304	0.00342	2.77499
R11	2.89132	0.00098	-0.00841	0.01883	0.01042	2.90174
R12	2.05990	0.00038	0.00080	-0.00147	-0.00067	2.05924
R13	2.06278	-0.00014	0.00073	-0.00214	-0.00140	2.06138
R14	2.07447	0.00043	0.00107	-0.00191	-0.00084	2.07363
R15	2.07139	-0.00037	-0.00050	-0.00247	-0.00297	2.06842
R16	2.69386	-0.00055	-0.00496	0.01230	0.00733	2.70120
R17	5.24840	-0.00097	-0.00317	-0.02507	-0.02824	5.22016
R18	2.50624	0.00115	-0.00278	0.00815	0.00537	2.51160
R19	2.04088	0.00123	-0.00290	0.00967	0.00678	2.04766
R20	2.03819	0.00184	-0.00102	0.00579	0.00477	2.04296
R21	2.04230	0.00157	0.00001	0.00262	0.00263	2.04493
R22	1.81765	-0.00019	-0.00103	0.00246	0.00143	1.81908
A1	1.87561	0.00166	0.00240	-0.00529	-0.00213	1.87348
A2	2.27786	-0.00049	-0.00062	0.00192	0.00122	2.27908
A3	2.12960	-0.00112	-0.00205	0.00314	0.00100	2.13061
A4	1.86996	0.00067	-0.00145	0.00319	0.00221	1.87218
A5	2.27415	0.00047	0.00143	-0.00053	0.00067	2.27481
A6	2.13892	-0.00112	0.00007	-0.00266	-0.00282	2.13611
A7	1.88970	-0.00059	-0.00156	0.00002	-0.00111	1.88859
A8	2.23340	-0.00231	-0.00869	0.01800	0.00863	2.24202
A9	2.14136	0.00289	0.00173	0.00249	0.00355	2.14491
A10	1.89204	0.00111	0.00128	-0.00486	-0.00200	1.89004
A11	2.19206	-0.00107	-0.00442	0.00456	0.00019	2.19225
A12	2.19149	-0.00044	-0.00344	0.00488	0.00154	2.19303
A13	1.89650	-0.00301	-0.00696	0.00952	0.00330	1.89981
A14	2.19335	-0.00390	-0.00505	0.00908	0.00343	2.19677
A15	2.18336	0.00700	0.01041	-0.01247	-0.00264	2.18072
A16	1.95475	0.00864	-0.01045	0.03319	0.02279	1.97754
A17	1.87013	0.00171	0.01991	-0.02512	-0.00529	1.86484
A18	1.89800	-0.00613	-0.01450	0.01692	0.00245	1.90045
A19	1.90441	-0.00377	-0.00175	-0.00316	-0.00502	1.89939
A20	1.94609	-0.00159	0.01105	-0.02896	-0.01776	1.92833
A21	1.88778	0.00107	-0.00360	0.00648	0.00267	1.89045
A22	1.91847	-0.00145	0.00293	0.00138	0.00423	1.92271
A23	1.90494	0.00498	-0.01323	0.01882	0.00570	1.91064
A24	1.82607	0.00027	0.00299	-0.00392	-0.00066	1.82540
A25	1.88934	0.00193	0.01723	-0.01658	0.00052	1.88986

A26	1.94435	-0.00010	0.00250	-0.01062	-0.00816	1.93619
A27	1.97959	-0.00555	-0.01358	0.01229	-0.00118	1.97841
A28	2.61186	0.01078	-0.00143	0.00105	-0.00038	2.61149
A29	2.17196	-0.00118	-0.00314	0.00512	0.00191	2.17387
A30	1.95092	0.00162	0.00114	0.00203	0.00311	1.95402
A31	2.15995	-0.00045	0.00211	-0.00787	-0.00583	2.15412
A32	2.07947	0.00023	0.00548	-0.01394	-0.00846	2.07102
A33	2.16067	-0.00075	0.00049	-0.00388	-0.00338	2.15729
A34	2.04300	0.00051	-0.00601	0.01784	0.01184	2.05483
A35	1.90166	-0.00025	-0.01162	0.02900	0.01739	1.91905
D1	-0.01175	0.00090	0.01325	-0.00944	0.00361	-0.00815
D2	3.11131	0.00194	0.01779	-0.00966	0.00802	3.11933
D3	-3.13700	-0.00173	-0.01241	0.00699	-0.00552	3.14066
D4	-0.01394	-0.00070	-0.00787	0.00677	-0.00110	-0.01504
D5	-0.01433	-0.00324	-0.04385	0.04432	0.00036	-0.01397
D6	-3.01043	-0.00457	-0.03420	0.00106	-0.03304	-3.04347
D7	3.11261	-0.00087	-0.02088	0.02958	0.00855	3.12116
D8	0.11651	-0.00221	-0.01123	-0.01367	-0.02486	0.09165
D9	0.03356	0.00169	0.02182	-0.02827	-0.00634	0.02722
D10	2.97024	0.00202	-0.01526	0.08245	0.06712	3.03736
D11	-3.09127	0.00074	0.01771	-0.02809	-0.01037	-3.10164
D12	-0.15458	0.00107	-0.01938	0.08262	0.06309	-0.09149
D13	-0.04276	-0.00378	-0.04990	0.05647	0.00671	-0.03605
D14	-3.05789	-0.00038	-0.00971	0.01829	0.00877	-3.04913
D15	-2.99257	-0.00337	-0.01314	-0.04940	-0.06254	-3.05510
D16	0.27549	0.00002	0.02706	-0.08757	-0.06048	0.21501
D17	0.38744	0.00076	0.00204	0.04418	0.04605	0.43349
D18	-2.72624	0.00127	-0.00320	0.07208	0.06876	-2.65749
D19	-2.98580	0.00064	-0.04073	0.16947	0.12887	-2.85694
D20	0.18370	0.00116	-0.04596	0.19737	0.15158	0.33528
D21	0.03551	0.00431	0.05778	-0.06228	-0.00438	0.03113
D22	3.03264	0.00450	0.04632	-0.01711	0.02927	3.06191
D23	3.05070	0.00085	0.01745	-0.02414	-0.00656	3.04414
D24	-0.23536	0.00105	0.00599	0.02102	0.02709	-0.20827
D25	1.32100	0.00069	-0.00842	0.09595	0.08744	1.40844
D26	-2.87438	0.00221	-0.00416	0.09541	0.09124	-2.78314
D27	-0.83768	0.00122	-0.00566	0.09831	0.09281	-0.74487
D28	-1.65190	0.00015	0.00475	0.04364	0.04826	-1.60365
D29	0.43590	0.00167	0.00900	0.04310	0.05206	0.48796
D30	2.47260	0.00068	0.00751	0.04600	0.05363	2.52623
D31	-1.18648	0.00333	0.05424	0.06298	0.11718	-1.06930
D32	0.88319	0.00782	0.06888	0.05494	0.12382	1.00701
D33	3.00724	0.00402	0.04804	0.07701	0.12503	3.13227
D34	3.02912	-0.00165	0.03716	0.07583	0.11300	-3.14107

D35	-1.18441	0.00284	0.05180	0.06779	0.11964	-1.06477
D36	0.93965	-0.00096	0.03096	0.08987	0.12085	1.06050
D37	0.94496	0.00045	0.03589	0.08779	0.12365	1.06862
D38	3.01463	0.00494	0.05053	0.07975	0.13029	-3.13827
D39	-1.14450	0.00114	0.02969	0.10183	0.13150	-1.01300
D40	-0.47787	0.00098	0.01778	0.08436	0.10192	-0.37595
D41	1.60990	0.00324	0.02351	0.08715	0.11066	1.72056
D42	-2.50613	0.00072	0.02994	0.06956	0.09972	-2.40642
D43	3.05453	-0.00072	-0.01417	0.09194	0.07779	3.13231
D44	0.98251	0.00089	-0.02077	0.09805	0.07731	1.05981
D45	-1.15444	0.00253	-0.03519	0.11889	0.08366	-1.07079
D46	-3.10818	0.00044	-0.00248	0.01797	0.01546	-3.09272
D47	0.02315	0.00013	-0.00604	0.02148	0.01541	0.03856
D48	0.00224	-0.00010	0.00335	-0.01300	-0.00962	-0.00738
D49	3.13357	-0.00042	-0.00020	-0.00949	-0.00967	3.12390

Item	Value	Threshold	Converged?
Maximum Force	0.010781	0.000450	NO
RMS Force	0.002660	0.000300	NO
Maximum Displacement	0.930448	0.001800	NO
RMS Displacement	0.155001	0.001200	NO

Predicted change in Energy=-3.085261D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.473715	-2.025475	-1.282925
2	6	0	-1.770899	-1.678488	-1.444199
3	7	0	-2.134737	-0.906405	-0.336851
4	6	0	-1.048164	-0.768588	0.457956
5	7	0	-0.038379	-1.460226	-0.086707
6	6	0	1.337772	-1.483419	0.425195
7	6	0	2.239852	-0.414685	-0.208784
8	1	0	0.176723	-2.613305	-1.907391
9	1	0	-2.455834	-1.898797	-2.242477
10	1	0	1.278725	-1.302366	1.498126
11	1	0	1.756290	-2.478432	0.267987
12	1	0	2.314276	-0.576372	-1.291568
13	1	0	1.806798	0.576045	-0.038543
14	35	0	-0.389533	2.150752	0.533497
15	1	0	-1.034623	-0.296215	1.420659
16	6	0	-3.347274	-0.219025	-0.104968

17	6	0	-4.514127	-0.543048	-0.652622
18	1	0	-3.208289	0.642157	0.537826
19	1	0	-5.374703	0.077281	-0.444419
20	1	0	-4.652807	-1.393226	-1.307578
21	8	0	3.509459	-0.594316	0.422920
22	1	0	4.143540	0.039273	0.072018

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.352440	0.000000			
3	N	2.215032	1.398110	0.000000		
4	C	2.222706	2.229003	1.353274	0.000000	
5	N	1.392825	2.211798	2.182660	1.339659	0.000000
6	C	2.548133	3.632701	3.601663	2.490932	1.468459
7	C	3.333448	4.382873	4.404000	3.373549	2.509660
8	H	1.076370	2.209448	3.274592	3.240092	2.165815
9	H	2.205807	1.074672	2.172408	3.248268	3.268605
10	H	3.365736	4.254286	3.895593	2.604090	2.066731
11	H	2.753801	4.001569	4.239951	3.290078	2.093654
12	H	3.142113	4.233983	4.562250	3.795232	2.787091
13	H	3.676566	4.456311	4.221652	3.194582	2.748345
14	Br	4.554925	4.525763	3.626216	2.993667	3.680641
15	H	3.257963	3.264995	2.161347	1.072435	2.149320
16	C	3.592796	2.531508	1.412978	2.429982	3.534077
17	C	4.349689	3.072640	2.427599	3.646526	4.603672
18	H	4.231936	3.373411	2.077406	2.581225	3.854657
19	H	5.398552	4.131548	3.387712	4.499858	5.564912
20	H	4.226719	2.899213	2.742259	4.062110	4.773674
21	O	4.563310	5.704712	5.703647	4.561087	3.687366
22	H	5.236230	6.342729	6.362251	5.268337	4.445463

		6	7	8	9	10
6	C	0.000000				
7	C	1.535536	0.000000			
8	H	2.840006	3.460592	0.000000		
9	H	4.656228	5.328036	2.748302	0.000000	
10	H	1.089701	2.150648	3.811892	5.319283	0.000000
11	H	1.090836	2.172601	2.691745	4.937651	1.767609
12	H	2.173378	1.097317	3.016201	5.040535	3.062978
13	H	2.162506	1.094560	4.040011	5.399278	2.483676
14	Br	4.025234	3.747814	5.382826	5.326769	3.954443
15	H	2.833489	3.659414	4.232279	4.243427	2.523871
16	C	4.881539	5.591515	4.625999	2.860986	5.014321
17	C	6.024177	6.769764	5.278682	2.932961	6.225706

18	H	5.019704	5.599695	5.294849	3.840927	4.983637
19	H	6.946174	7.634069	6.340180	3.956980	7.067179
20	H	6.236800	7.047953	5.017243	2.440559	6.562264
21	O	2.346643	1.429411	4.540241	6.662637	2.575573
22	H	3.211801	1.977108	5.166224	7.257048	3.470007

		11	12	13	14	15
11	H	0.000000				
12	H	2.522180	0.000000			
13	H	3.070234	1.776421	0.000000		
14	Br	5.109245	4.251900	2.762391	0.000000	
15	H	3.725577	4.318541	3.311161	2.681575	0.000000
16	C	5.593781	5.795591	5.215459	3.843399	2.771615
17	C	6.626565	6.858313	6.448532	5.067120	4.057877
18	H	5.870088	5.943923	5.048532	3.197071	2.526808
19	H	7.608565	7.763075	7.210234	5.487032	4.738598
20	H	6.688543	7.014824	6.871316	5.841647	4.662399
21	O	2.578274	2.090036	2.117013	4.769671	4.661870
22	H	3.475084	2.363174	2.400148	5.021957	5.361414

		16	17	18	19	20
16	C	0.000000				
17	C	1.329083	0.000000			
18	H	1.083575	2.127696	0.000000		
19	H	2.076895	1.081087	2.444840	0.000000	
20	H	2.128247	1.082128	3.104019	1.851639	0.000000
21	O	6.887256	8.095514	6.831559	8.951628	8.381853
22	H	7.497356	8.707434	7.391200	9.532319	9.018374

		21	22
21	O	0.000000	
22	H	0.962614	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.307305	-2.313109	-0.589163
2	6	0	-1.591460	-1.901587	-0.692549
3	7	0	-1.747781	-0.809658	0.166501
4	6	0	-0.552939	-0.555216	0.748706

5	7	0	0.326439	-1.471148	0.321569
6	6	0	1.757634	-1.480569	0.650145
7	6	0	2.621835	-0.735984	-0.377776
8	1	0	0.211791	-3.117910	-1.080496
9	1	0	-2.394825	-2.275184	-1.300784
10	1	0	1.862667	-0.991318	1.618158
11	1	0	2.090028	-2.514637	0.750837
12	1	0	2.531739	-1.211174	-1.362754
13	1	0	2.276682	0.299220	-0.463127
14	35	0	0.280966	2.180779	-0.135022
15	1	0	-0.374670	0.172239	1.516266
16	6	0	-2.872253	0.031539	0.322895
17	6	0	-4.122241	-0.320586	0.040053
18	1	0	-2.592602	1.023995	0.656004
19	1	0	-4.906283	0.415196	0.152533
20	1	0	-4.402672	-1.306123	-0.307909
21	8	0	3.955570	-0.849081	0.123801
22	1	0	4.569559	-0.410223	-0.473733

Rotational constants (GHZ): 0.7972368 0.5644655 0.3484152

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 859.9492840306 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 5.75D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Initial guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.996403 0.010754 0.004424 0.083940 Ang= 9.72 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.33603367 A.U. after 15 cycles
NFock= 15 Conv=0.37D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000852608	0.003555659	0.002616768
2	6	-0.002689456	0.001377757	0.002081297
3	7	0.007827952	-0.003127271	-0.001352868
4	6	-0.000574742	-0.001308923	-0.004220473
5	7	0.001549958	-0.002957912	-0.002343865
6	6	0.000740808	0.002975528	0.003407691
7	6	-0.000305453	-0.001207704	-0.001369168
8	1	0.000202028	0.000728011	0.000128031
9	1	-0.000493166	0.000794301	0.000149543
10	1	0.001630398	-0.000474208	0.000682307
11	1	-0.000859143	-0.000494548	-0.000381516
12	1	-0.000111845	-0.001302904	-0.000732684
13	1	0.001202062	0.000376415	0.001786125
14	35	-0.001868510	-0.002937484	-0.000149450
15	1	0.000393078	0.002613278	-0.000383260
16	6	-0.004943846	0.001556154	-0.000388597
17	6	0.002108324	0.001078239	0.001441676
18	1	0.000383572	0.000475094	0.000161620
19	1	-0.000550105	-0.000412245	-0.000438528
20	1	-0.000081014	-0.000699954	-0.000192017
21	8	-0.001596832	-0.001707815	-0.000872331
22	1	-0.002816678	0.001100532	0.000369700

Cartesian Forces: Max 0.007827952 RMS 0.001952364

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.018106450 RMS 0.003333648
Search for a local minimum.
Step number 6 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 4 5 6
DE= -1.59D-03 DEPred=-3.09D-03 R= 5.16D-01
TightC=F SS= 1.41D+00 RLast= 5.38D-01 DXNew= 2.5227D-01 1.6153D+00
Trust test= 5.16D-01 RLast= 5.38D-01 DXMaxT set to 2.52D-01
ITU= 1 0 0 -1 0 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00246	0.00521	0.00645	0.01025	0.01293
Eigenvalues ---	0.01590	0.01685	0.01887	0.02041	0.02141
Eigenvalues ---	0.02220	0.02375	0.02409	0.03065	0.03071
Eigenvalues ---	0.03685	0.04522	0.05433	0.05938	0.06501
Eigenvalues ---	0.08664	0.09392	0.13589	0.14521	0.15712
Eigenvalues ---	0.15800	0.15994	0.15999	0.15999	0.16095
Eigenvalues ---	0.16567	0.20721	0.21962	0.22862	0.23043
Eigenvalues ---	0.23928	0.24654	0.25765	0.29499	0.33269
Eigenvalues ---	0.33850	0.33868	0.33888	0.34102	0.34295
Eigenvalues ---	0.34432	0.34656	0.36060	0.36306	0.36403
Eigenvalues ---	0.37235	0.42143	0.43152	0.45927	0.50093
Eigenvalues ---	0.53440	0.54257	0.55551	0.60618	1.88545

RFO step: Lambda=-1.18166332D-03 EMin= 2.46044615D-03
Quartic linear search produced a step of -0.27227.
Iteration 1 RMS(Cart)= 0.05609065 RMS(Int)= 0.00154371
Iteration 2 RMS(Cart)= 0.00212866 RMS(Int)= 0.00007977
Iteration 3 RMS(Cart)= 0.00000521 RMS(Int)= 0.00007970
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00007970

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55574	0.00128	0.00023	0.00051	0.00079	2.55653
R2	2.63206	-0.00334	-0.00075	-0.00264	-0.00337	2.62868
R3	2.03404	-0.00035	-0.00026	-0.00041	-0.00066	2.03338
R4	2.64204	-0.00412	-0.00144	-0.00519	-0.00661	2.63543
R5	2.03084	0.00004	-0.00060	0.00056	-0.00004	2.03079
R6	2.55732	-0.00371	-0.00108	-0.00191	-0.00303	2.55429
R7	2.67014	0.00370	0.00090	0.00378	0.00468	2.67483
R8	2.53159	-0.00171	-0.00049	-0.00074	-0.00128	2.53031
R9	2.02661	0.00081	0.00034	0.00064	0.00097	2.02758

R10	2.77499	-0.00274	-0.00093	-0.00159	-0.00252	2.77246
R11	2.90174	-0.00674	-0.00284	-0.00584	-0.00868	2.89307
R12	2.05924	0.00050	0.00018	0.00081	0.00099	2.06022
R13	2.06138	0.00017	0.00038	-0.00020	0.00018	2.06156
R14	2.07363	0.00091	0.00023	0.00135	0.00158	2.07521
R15	2.06842	-0.00179	0.00081	-0.00104	-0.00023	2.06819
R16	2.70120	-0.00408	-0.00200	-0.00443	-0.00642	2.69477
R17	5.22016	-0.00022	0.00769	-0.00005	0.00764	5.22780
R18	2.51160	-0.00162	-0.00146	-0.00003	-0.00149	2.51011
R19	2.04766	0.00052	-0.00184	0.00174	-0.00011	2.04755
R20	2.04296	0.00011	-0.00130	0.00121	-0.00009	2.04287
R21	2.04493	0.00068	-0.00072	0.00168	0.00096	2.04589
R22	1.81908	-0.00125	-0.00039	-0.00091	-0.00130	1.81778
A1	1.87348	0.00005	0.00058	0.00238	0.00277	1.87624
A2	2.27908	0.00031	-0.00033	0.00013	-0.00015	2.27893
A3	2.13061	-0.00036	-0.00027	-0.00240	-0.00263	2.12798
A4	1.87218	-0.00089	-0.00060	-0.00141	-0.00218	1.86999
A5	2.27481	0.00128	-0.00018	0.00419	0.00408	2.27890
A6	2.13611	-0.00041	0.00077	-0.00286	-0.00202	2.13409
A7	1.88859	0.00073	0.00030	0.00004	0.00032	1.88891
A8	2.24202	-0.00123	-0.00235	-0.00189	-0.00390	2.23812
A9	2.14491	0.00048	-0.00097	0.00390	0.00328	2.14820
A10	1.89004	0.00089	0.00054	0.00169	0.00187	1.89191
A11	2.19225	-0.00072	-0.00005	-0.00320	-0.00316	2.18909
A12	2.19303	-0.00006	-0.00042	-0.00103	-0.00138	2.19166
A13	1.89981	-0.00079	-0.00090	-0.00397	-0.00513	1.89468
A14	2.19677	0.00433	-0.00093	0.00317	0.00233	2.19910
A15	2.18072	-0.00373	0.00072	-0.00051	0.00031	2.18104
A16	1.97754	-0.01494	-0.00621	-0.00944	-0.01568	1.96186
A17	1.86484	0.00478	0.00144	0.01765	0.01913	1.88398
A18	1.90045	0.00474	-0.00067	-0.00759	-0.00834	1.89211
A19	1.89939	0.00189	0.00137	0.00092	0.00236	1.90175
A20	1.92833	0.00595	0.00484	-0.00043	0.00429	1.93262
A21	1.89045	-0.00211	-0.00073	-0.00016	-0.00084	1.88961
A22	1.92271	0.00234	-0.00115	0.00519	0.00405	1.92676
A23	1.91064	-0.01247	-0.00155	-0.00682	-0.00842	1.90221
A24	1.82540	0.00388	0.00018	-0.00305	-0.00293	1.82247
A25	1.88986	0.00292	-0.00014	0.01255	0.01245	1.90231
A26	1.93619	-0.00122	0.00222	0.00016	0.00240	1.93860
A27	1.97841	0.00427	0.00032	-0.00852	-0.00826	1.97016
A28	2.61149	-0.01811	0.00010	-0.00638	-0.00628	2.60521
A29	2.17387	-0.00149	-0.00052	-0.00353	-0.00403	2.16984
A30	1.95402	0.00044	-0.00085	0.00160	0.00078	1.95480
A31	2.15412	0.00105	0.00159	0.00162	0.00322	2.15735

A32	2.07102	0.00115	0.00230	0.00110	0.00340	2.07441
A33	2.15729	-0.00064	0.00092	-0.00288	-0.00196	2.15533
A34	2.05483	-0.00051	-0.00322	0.00180	-0.00142	2.05341
A35	1.91905	-0.00398	-0.00473	-0.01009	-0.01482	1.90423
D1	-0.00815	0.00091	-0.00098	0.01920	0.01829	0.01014
D2	3.11933	-0.00001	-0.00218	0.01295	0.01076	3.13010
D3	3.14066	0.00090	0.00150	0.00110	0.00266	-3.13987
D4	-0.01504	-0.00002	0.00030	-0.00515	-0.00487	-0.01991
D5	-0.01397	-0.00109	-0.00010	-0.03854	-0.03860	-0.05257
D6	-3.04347	0.00102	0.00900	-0.02609	-0.01707	-3.06054
D7	3.12116	-0.00108	-0.00233	-0.02231	-0.02461	3.09655
D8	0.09165	0.00104	0.00677	-0.00985	-0.00307	0.08858
D9	0.02722	-0.00040	0.00173	0.00634	0.00805	0.03526
D10	3.03736	-0.00052	-0.01827	0.02418	0.00586	3.04322
D11	-3.10164	0.00042	0.00282	0.01192	0.01474	-3.08690
D12	-0.09149	0.00029	-0.01718	0.02976	0.01256	-0.07893
D13	-0.03605	-0.00032	-0.00183	-0.03054	-0.03240	-0.06845
D14	-3.04913	-0.00125	-0.00239	-0.00989	-0.01229	-3.06142
D15	-3.05510	-0.00005	0.01703	-0.04666	-0.02971	-3.08481
D16	0.21501	-0.00098	0.01647	-0.02601	-0.00960	0.20540
D17	0.43349	0.00058	-0.01254	0.04578	0.03330	0.46679
D18	-2.65749	0.00047	-0.01872	0.05236	0.03367	-2.62382
D19	-2.85694	0.00043	-0.03509	0.06564	0.03052	-2.82642
D20	0.33528	0.00032	-0.04127	0.07221	0.03089	0.36616
D21	0.03113	0.00086	0.00119	0.04262	0.04376	0.07489
D22	3.06191	-0.00060	-0.00797	0.03060	0.02267	3.08458
D23	3.04414	0.00172	0.00179	0.02176	0.02345	3.06759
D24	-0.20827	0.00027	-0.00738	0.00974	0.00236	-0.20591
D25	1.40844	0.00143	-0.02381	-0.00813	-0.03188	1.37656
D26	-2.78314	-0.00192	-0.02484	-0.00079	-0.02566	-2.80880
D27	-0.74487	0.00059	-0.02527	0.00460	-0.02073	-0.76560
D28	-1.60365	0.00357	-0.01314	0.00641	-0.00665	-1.61030
D29	0.48796	0.00022	-0.01417	0.01375	-0.00043	0.48753
D30	2.52623	0.00274	-0.01460	0.01914	0.00450	2.53073
D31	-1.06930	-0.00005	-0.03191	0.00063	-0.03128	-1.10057
D32	1.00701	-0.00273	-0.03371	0.01498	-0.01876	0.98825
D33	3.13227	-0.00199	-0.03404	-0.00044	-0.03448	3.09779
D34	-3.14107	0.00200	-0.03077	-0.01624	-0.04701	3.09510
D35	-1.06477	-0.00069	-0.03257	-0.00190	-0.03450	-1.09926
D36	1.06050	0.00006	-0.03290	-0.01732	-0.05022	1.01028
D37	1.06862	-0.00013	-0.03367	-0.01636	-0.05001	1.01861
D38	-3.13827	-0.00281	-0.03547	-0.00202	-0.03749	3.10743
D39	-1.01300	-0.00207	-0.03580	-0.01744	-0.05321	-1.06622
D40	-0.37595	0.00042	-0.02775	-0.09200	-0.11971	-0.49566

D41	1.72056	-0.00232	-0.03013	-0.08218	-0.11231	1.60825
D42	-2.40642	0.00117	-0.02715	-0.07854	-0.10573	-2.51215
D43	3.13231	0.00590	-0.02118	0.06674	0.04554	-3.10533
D44	1.05981	0.00151	-0.02105	0.06228	0.04122	1.10104
D45	-1.07079	-0.00447	-0.02278	0.05190	0.02915	-1.04164
D46	-3.09272	-0.00007	-0.00421	0.00558	0.00138	-3.09134
D47	0.03856	0.00019	-0.00420	0.00755	0.00337	0.04192
D48	-0.00738	0.00003	0.00262	-0.00174	0.00087	-0.00651
D49	3.12390	0.00029	0.00263	0.00023	0.00285	3.12675

Item	Value	Threshold	Converged?
Maximum Force	0.018106	0.000450	NO
RMS Force	0.003334	0.000300	NO
Maximum Displacement	0.382509	0.001800	NO
RMS Displacement	0.055909	0.001200	NO

Predicted change in Energy=-7.700671D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.462262	-1.972185	-1.306572
2	6	0	-1.761927	-1.628779	-1.458763
3	7	0	-2.124644	-0.884703	-0.336388
4	6	0	-1.035096	-0.750808	0.452261
5	7	0	-0.032076	-1.452844	-0.089929
6	6	0	1.337534	-1.503877	0.433535
7	6	0	2.244045	-0.444983	-0.199530
8	1	0	0.190735	-2.541000	-1.945212
9	1	0	-2.448219	-1.828302	-2.261300
10	1	0	1.292412	-1.334160	1.509522
11	1	0	1.734975	-2.505196	0.261674
12	1	0	2.344245	-0.622575	-1.278585
13	1	0	1.801762	0.543437	-0.040764
14	35	0	-0.447789	2.110094	0.331082
15	1	0	-1.020806	-0.287101	1.419728
16	6	0	-3.345868	-0.213805	-0.087330
17	6	0	-4.514379	-0.566026	-0.611630
18	1	0	-3.209676	0.656111	0.544104
19	1	0	-5.385168	0.038062	-0.398441
20	1	0	-4.645762	-1.428174	-1.253146
21	8	0	3.495510	-0.605674	0.464942
22	1	0	4.112803	0.055610	0.137897

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.352856	0.000000			
3	N	2.210744	1.394611	0.000000		
4	C	2.216618	2.225114	1.351670	0.000000	
5	N	1.391040	2.212926	2.182285	1.338982	0.000000
6	C	2.546870	3.633600	3.600394	2.489345	1.467124
7	C	3.298785	4.362895	4.392895	3.357250	2.491691
8	H	1.076019	2.209450	3.269957	3.233470	2.162361
9	H	2.208220	1.074649	2.168033	3.243659	3.270101
10	H	3.378807	4.269251	3.909689	2.622097	2.080048
11	H	2.751607	3.994538	4.228515	3.284432	2.086514
12	H	3.114275	4.231496	4.574649	3.798976	2.783730
13	H	3.613367	4.407848	4.188513	3.156883	2.711184
14	Br	4.398536	4.348526	3.496593	2.923076	3.611730
15	H	3.253335	3.261146	2.158594	1.072949	2.148397
16	C	3.590770	2.528210	1.415457	2.432940	3.537858
17	C	4.345099	3.069702	2.426550	3.642996	4.598875
18	H	4.228620	3.365736	2.080064	2.591651	3.866113
19	H	5.394516	4.126805	3.389153	4.502126	5.565390
20	H	4.219061	2.898107	2.737122	4.050203	4.758127
21	O	4.546379	5.691048	5.683847	4.532948	3.670074
22	H	5.208614	6.316561	6.325732	5.220153	4.416714

		6	7	8	9	10
6	C	0.000000				
7	C	1.530944	0.000000			
8	H	2.837113	3.414202	0.000000		
9	H	4.658252	5.308653	2.751714	0.000000	
10	H	1.090224	2.148744	3.821694	5.334378	0.000000
11	H	1.090933	2.171714	2.693753	4.931804	1.767573
12	H	2.172905	1.098152	2.960127	5.038573	3.063698
13	H	2.152200	1.094438	3.966873	5.349603	2.487608
14	Br	4.032203	3.749124	5.217461	5.121828	4.034836
15	H	2.831058	3.647763	4.227377	4.238251	2.540743
16	C	4.885677	5.595815	4.623324	2.852809	5.031776
17	C	6.018041	6.772058	5.274189	2.929807	6.229617
18	H	5.035364	5.613240	5.289708	3.823927	5.016174
19	H	6.947265	7.647077	6.335200	3.947053	7.079081
20	H	6.216949	7.038906	5.010892	2.450647	6.550044
21	O	2.337651	1.426012	4.525026	6.652452	2.544696
22	H	3.197111	1.963851	5.144351	7.235487	3.430368

		11	12	13	14	15

11	H	0.000000				
12	H	2.507563	0.000000			
13	H	3.064326	1.784957	0.000000		
14	Br	5.105896	4.225395	2.766435	0.000000	
15	H	3.722280	4.326315	3.284771	2.694446	0.000000
16	C	5.584553	5.827827	5.203237	3.738240	2.771734
17	C	6.601323	6.891208	6.438201	4.958576	4.050835
18	H	5.875645	5.983584	5.046709	3.128493	2.539196
19	H	7.589489	7.807363	7.213549	5.404001	4.739106
20	H	6.645935	7.036322	6.850378	5.714201	4.646139
21	O	2.597881	2.089397	2.108312	4.789877	4.627117
22	H	3.496730	2.365196	2.368714	5.005719	5.302309

		16	17	18	19	20
16	C	0.000000				
17	C	1.328295	0.000000			
18	H	1.083519	2.128753	0.000000		
19	H	2.078214	1.081039	2.450131	0.000000	
20	H	2.126862	1.082638	3.104303	1.851240	0.000000
21	O	6.874810	8.082010	6.823334	8.945740	8.361138
22	H	7.466933	8.681963	7.358281	9.513118	8.991611

		21	22
21	O	0.000000	
22	H	0.961928	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.166785	-2.225387	-0.687560
2	6	0	-1.470198	-1.870775	-0.762273
3	7	0	-1.673685	-0.853996	0.170301
4	6	0	-0.489270	-0.578277	0.760345
5	7	0	0.424885	-1.439328	0.295817
6	6	0	1.849950	-1.421712	0.644144
7	6	0	2.681664	-0.597767	-0.342343
8	1	0	0.389725	-2.965381	-1.235760
9	1	0	-2.257537	-2.232197	-1.398152
10	1	0	1.947165	-0.986818	1.639134

11	1	0	2.207475	-2.451599	0.684688
12	1	0	2.638547	-1.043607	-1.344993
13	1	0	2.277799	0.418461	-0.386717
14	35	0	0.117963	2.131245	-0.152963
15	1	0	-0.343047	0.111109	1.569409
16	6	0	-2.842637	-0.086099	0.388027
17	6	0	-4.074161	-0.503311	0.116641
18	1	0	-2.613359	0.906610	0.756772
19	1	0	-4.901275	0.174709	0.274175
20	1	0	-4.299869	-1.491247	-0.264334
21	8	0	4.006321	-0.645512	0.183502
22	1	0	4.585325	-0.116281	-0.373253

Rotational constants (GHZ): 0.8327088 0.5656686 0.3577358

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 866.9915581269 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 5.78D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Initial guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999635 -0.003952 -0.000808 -0.026703 Ang= -3.10 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Keep R1 ints in memory in canonical form, NReq=1804729152.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.33697657 A.U. after 12 cycles
NFock= 12 Conv=0.10D-07 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000551368	-0.000422339	0.001557907
2	6	-0.001180889	0.001169086	0.000919902
3	7	0.004163561	-0.001878208	-0.000726863
4	6	-0.001304315	0.000156740	-0.000384187
5	7	0.000579513	-0.000562570	-0.001348226
6	6	-0.000051283	0.001370892	-0.000199083
7	6	-0.000546848	-0.000824448	0.000924304
8	1	0.000077973	0.000237678	-0.000041627
9	1	-0.000166752	0.000739705	-0.000041331
10	1	-0.000040300	-0.000227169	-0.000007123
11	1	-0.000185215	-0.000463995	0.000165350
12	1	-0.000531103	-0.000453399	-0.000036682
13	1	0.001004969	0.000716868	-0.000105822
14	35	-0.000910072	-0.001498806	0.000164876
15	1	-0.000009021	0.000621409	-0.000342807
16	6	-0.002568977	0.001082184	-0.000530561
17	6	0.001259037	0.000515743	0.000883435
18	1	0.000293422	0.000448896	0.000099235
19	1	-0.000481124	-0.000294305	-0.000272947
20	1	0.000022795	-0.000442421	-0.000115021
21	8	0.001001200	-0.000898494	-0.001384949
22	1	-0.000977941	0.000906952	0.000822221

Cartesian Forces: Max 0.004163561 RMS 0.000956424

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.009081717 RMS 0.001528894
Search for a local minimum.

Step number 7 out of a maximum of 116

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 5 6 7

DE= -9.43D-04 DEPred=-7.70D-04 R= 1.22D+00

TightC=F SS= 1.41D+00 RLast= 2.73D-01 DXNew= 4.2426D-01 8.1875D-01

Trust test= 1.22D+00 RLast= 2.73D-01 DXMaxT set to 4.24D-01

ITU= 1 1 0 0 -1 0 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00257	0.00495	0.00646	0.01019	0.01274
Eigenvalues ---	0.01557	0.01700	0.01871	0.02038	0.02142
Eigenvalues ---	0.02225	0.02405	0.02413	0.03064	0.03070
Eigenvalues ---	0.03742	0.04563	0.05435	0.06039	0.06978
Eigenvalues ---	0.08639	0.09286	0.13106	0.13876	0.15705
Eigenvalues ---	0.15734	0.15911	0.15997	0.15999	0.16127
Eigenvalues ---	0.16443	0.20581	0.21478	0.22779	0.22862
Eigenvalues ---	0.24104	0.24466	0.25675	0.29661	0.32922
Eigenvalues ---	0.33850	0.33874	0.33912	0.34093	0.34282
Eigenvalues ---	0.34385	0.34672	0.36024	0.36307	0.36384
Eigenvalues ---	0.37266	0.42467	0.42858	0.45642	0.49311
Eigenvalues ---	0.53502	0.54324	0.55555	0.60518	1.54373

RFO step: Lambda=-7.11525141D-04 EMin= 2.56865625D-03

Quartic linear search produced a step of 0.37345.

Iteration 1 RMS(Cart)= 0.04549366 RMS(Int)= 0.00156869

Iteration 2 RMS(Cart)= 0.00205183 RMS(Int)= 0.00003504

Iteration 3 RMS(Cart)= 0.00000433 RMS(Int)= 0.00003490

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00003490

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55653	0.00061	0.00029	0.00091	0.00122	2.55775
R2	2.62868	-0.00129	-0.00126	-0.00164	-0.00289	2.62579
R3	2.03338	-0.00005	-0.00025	0.00006	-0.00019	2.03319
R4	2.63543	-0.00188	-0.00247	-0.00447	-0.00694	2.62850
R5	2.03079	0.00000	-0.00002	0.00041	0.00039	2.03119
R6	2.55429	-0.00182	-0.00113	-0.00246	-0.00361	2.55067
R7	2.67483	0.00190	0.00175	0.00615	0.00790	2.68273
R8	2.53031	0.00036	-0.00048	0.00245	0.00196	2.53227
R9	2.02758	-0.00004	0.00036	-0.00133	-0.00096	2.02662
R10	2.77246	-0.00100	-0.00094	-0.00217	-0.00311	2.76935
R11	2.89307	-0.00211	-0.00324	-0.00056	-0.00380	2.88927
R12	2.06022	-0.00004	0.00037	-0.00032	0.00005	2.06027
R13	2.06156	0.00033	0.00007	0.00114	0.00121	2.06277
R14	2.07521	0.00007	0.00059	-0.00018	0.00041	2.07561
R15	2.06819	-0.00073	-0.00009	0.00089	0.00080	2.06899

R16	2.69477	-0.00025	-0.00240	0.00075	-0.00165	2.69313
R17	5.22780	-0.00008	0.00285	0.01506	0.01792	5.24572
R18	2.51011	-0.00084	-0.00056	-0.00070	-0.00126	2.50886
R19	2.04755	0.00045	-0.00004	0.00298	0.00294	2.05049
R20	2.04287	0.00017	-0.00003	0.00165	0.00162	2.04449
R21	2.04589	0.00042	0.00036	0.00230	0.00266	2.04854
R22	1.81778	-0.00027	-0.00048	-0.00033	-0.00081	1.81697
A1	1.87624	-0.00039	0.00103	-0.00079	0.00014	1.87638
A2	2.27893	0.00026	-0.00006	0.00078	0.00065	2.27958
A3	2.12798	0.00013	-0.00098	0.00021	-0.00084	2.12714
A4	1.86999	-0.00009	-0.00082	-0.00017	-0.00104	1.86895
A5	2.27890	0.00052	0.00153	0.00417	0.00569	2.28459
A6	2.13409	-0.00044	-0.00075	-0.00415	-0.00491	2.12918
A7	1.88891	0.00070	0.00012	0.00297	0.00301	1.89192
A8	2.23812	-0.00116	-0.00146	-0.00597	-0.00740	2.23073
A9	2.14820	0.00043	0.00123	0.00372	0.00499	2.15319
A10	1.89191	-0.00022	0.00070	-0.00240	-0.00181	1.89010
A11	2.18909	-0.00003	-0.00118	0.00048	-0.00068	2.18842
A12	2.19166	0.00034	-0.00051	0.00295	0.00245	2.19411
A13	1.89468	0.00001	-0.00191	0.00116	-0.00088	1.89379
A14	2.19910	0.00102	0.00087	-0.00085	-0.00003	2.19908
A15	2.18104	-0.00111	0.00012	-0.00143	-0.00135	2.17968
A16	1.96186	-0.00605	-0.00586	-0.00714	-0.01302	1.94884
A17	1.88398	0.00156	0.00714	0.00257	0.00977	1.89375
A18	1.89211	0.00193	-0.00311	-0.00249	-0.00565	1.88646
A19	1.90175	0.00093	0.00088	0.00536	0.00629	1.90805
A20	1.93262	0.00267	0.00160	0.00241	0.00388	1.93650
A21	1.88961	-0.00092	-0.00032	-0.00053	-0.00085	1.88876
A22	1.92676	0.00054	0.00151	-0.00535	-0.00384	1.92292
A23	1.90221	-0.00602	-0.00314	-0.00030	-0.00346	1.89876
A24	1.82247	0.00322	-0.00110	0.01172	0.01060	1.83307
A25	1.90231	0.00140	0.00465	-0.00276	0.00189	1.90419
A26	1.93860	-0.00088	0.00090	-0.00141	-0.00050	1.93810
A27	1.97016	0.00161	-0.00308	-0.00159	-0.00469	1.96546
A28	2.60521	-0.00908	-0.00234	-0.00954	-0.01188	2.59332
A29	2.16984	-0.00131	-0.00150	-0.00791	-0.00941	2.16043
A30	1.95480	0.00044	0.00029	0.00263	0.00291	1.95771
A31	2.15735	0.00088	0.00120	0.00543	0.00663	2.16398
A32	2.07441	0.00090	0.00127	0.00630	0.00756	2.08197
A33	2.15533	-0.00056	-0.00073	-0.00523	-0.00597	2.14936
A34	2.05341	-0.00034	-0.00053	-0.00102	-0.00156	2.05186
A35	1.90423	-0.00095	-0.00553	-0.00386	-0.00940	1.89483
D1	0.01014	-0.00006	0.00683	-0.01742	-0.01056	-0.00042
D2	3.13010	-0.00046	0.00402	-0.02554	-0.02156	3.10854

D3	-3.13987	0.00046	0.00099	0.01093	0.01196	-3.12790
D4	-0.01991	0.00006	-0.00182	0.00281	0.00096	-0.01895
D5	-0.05257	0.00017	-0.01442	0.01871	0.00431	-0.04827
D6	-3.06054	0.00094	-0.00638	0.02772	0.02134	-3.03920
D7	3.09655	-0.00030	-0.00919	-0.00666	-0.01584	3.08071
D8	0.08858	0.00048	-0.00115	0.00234	0.00120	0.08978
D9	0.03526	-0.00001	0.00300	0.01031	0.01332	0.04858
D10	3.04322	-0.00011	0.00219	0.01686	0.01903	3.06225
D11	-3.08690	0.00033	0.00551	0.01749	0.02297	-3.06393
D12	-0.07893	0.00023	0.00469	0.02404	0.02868	-0.05026
D13	-0.06845	0.00012	-0.01210	0.00143	-0.01069	-0.07914
D14	-3.06142	-0.00052	-0.00459	-0.00601	-0.01061	-3.07203
D15	-3.08481	0.00036	-0.01109	-0.00380	-0.01494	-3.09975
D16	0.20540	-0.00029	-0.00359	-0.01124	-0.01486	0.19054
D17	0.46679	0.00053	0.01244	0.07956	0.09200	0.55879
D18	-2.62382	0.00040	0.01258	0.07619	0.08877	-2.53504
D19	-2.82642	0.00042	0.01140	0.08677	0.09816	-2.72826
D20	0.36616	0.00029	0.01154	0.08340	0.09493	0.46109
D21	0.07489	-0.00018	0.01634	-0.01236	0.00395	0.07884
D22	3.08458	-0.00074	0.00847	-0.02120	-0.01272	3.07186
D23	3.06759	0.00043	0.00876	-0.00517	0.00354	3.07113
D24	-0.20591	-0.00013	0.00088	-0.01401	-0.01313	-0.21904
D25	1.37656	0.00104	-0.01191	-0.00001	-0.01184	1.36472
D26	-2.80880	-0.00048	-0.00958	0.00399	-0.00560	-2.81440
D27	-0.76560	0.00030	-0.00774	0.00342	-0.00438	-0.76998
D28	-1.61030	0.00182	-0.00248	0.01023	0.00781	-1.60249
D29	0.48753	0.00030	-0.00016	0.01422	0.01405	0.50158
D30	2.53073	0.00108	0.00168	0.01365	0.01528	2.54600
D31	-1.10057	0.00027	-0.01168	0.03856	0.02687	-1.07370
D32	0.98825	-0.00144	-0.00701	0.03173	0.02472	1.01297
D33	3.09779	-0.00081	-0.01288	0.03621	0.02334	3.12113
D34	3.09510	0.00150	-0.01756	0.03624	0.01869	3.11379
D35	-1.09926	-0.00021	-0.01288	0.02941	0.01654	-1.08272
D36	1.01028	0.00042	-0.01875	0.03390	0.01516	1.02544
D37	1.01861	0.00044	-0.01868	0.03210	0.01341	1.03202
D38	3.10743	-0.00127	-0.01400	0.02527	0.01126	3.11869
D39	-1.06622	-0.00063	-0.01987	0.02976	0.00988	-1.05634
D40	-0.49566	0.00132	-0.04471	0.00704	-0.03765	-0.53332
D41	1.60825	-0.00081	-0.04194	-0.00132	-0.04327	1.56498
D42	-2.51215	0.00021	-0.03949	-0.00629	-0.04579	-2.55794
D43	-3.10533	0.00299	0.01701	0.09292	0.10993	-2.99540
D44	1.10104	0.00092	0.01539	0.09315	0.10854	1.20957
D45	-1.04164	-0.00142	0.01088	0.09897	0.10986	-0.93178
D46	-3.09134	-0.00010	0.00052	-0.00273	-0.00222	-3.09355

D47	0.04192	0.00009	0.00126	0.00491	0.00617	0.04809
D48	-0.00651	0.00002	0.00032	0.00088	0.00121	-0.00531
D49	3.12675	0.00020	0.00106	0.00853	0.00959	3.13634

Item	Value	Threshold	Converged?
Maximum Force	0.009082	0.000450	NO
RMS Force	0.001529	0.000300	NO
Maximum Displacement	0.204274	0.001800	NO
RMS Displacement	0.045457	0.001200	NO

Predicted change in Energy=-4.231577D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.457019	-1.967232	-1.308023
2	6	0	-1.747019	-1.594170	-1.477421
3	7	0	-2.109992	-0.857177	-0.355009
4	6	0	-1.029465	-0.739844	0.445328
5	7	0	-0.032061	-1.459698	-0.086320
6	6	0	1.332869	-1.520238	0.443701
7	6	0	2.234870	-0.465840	-0.198388
8	1	0	0.197578	-2.534413	-1.946309
9	1	0	-2.425873	-1.759304	-2.294250
10	1	0	1.293608	-1.354040	1.520492
11	1	0	1.720583	-2.525294	0.267432
12	1	0	2.307123	-0.637518	-1.280846
13	1	0	1.802050	0.524018	-0.020705
14	35	0	-0.460434	2.086927	0.359010
15	1	0	-1.020046	-0.275324	1.411898
16	6	0	-3.335358	-0.181143	-0.116627
17	6	0	-4.508869	-0.594654	-0.579750
18	1	0	-3.194373	0.735690	0.446335
19	1	0	-5.391934	0.001413	-0.391601
20	1	0	-4.633433	-1.511208	-1.145049
21	8	0	3.502491	-0.630757	0.431665
22	1	0	4.075052	0.092925	0.161591

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.353504	0.000000			
3	N	2.207437	1.390941	0.000000		

4	C	2.215494	2.222998	1.349757	0.000000	
5	N	1.389509	2.212313	2.180143	1.340021	0.000000
6	C	2.544020	3.630687	3.595954	2.487899	1.465477
7	C	3.275932	4.331801	4.365261	3.338463	2.477759
8	H	1.075918	2.210288	3.266533	3.232033	2.160394
9	H	2.211846	1.074858	2.162005	3.239527	3.270329
10	H	3.382483	4.276747	3.917764	2.632467	2.085763
11	H	2.745076	3.991963	4.224140	3.283633	2.081441
12	H	3.067467	4.170119	4.518444	3.758054	2.752209
13	H	3.600959	4.382309	4.162155	3.135604	2.702480
14	Br	4.383516	4.310250	3.449437	2.884768	3.600052
15	H	3.252310	3.258222	2.156037	1.072439	2.150236
16	C	3.590874	2.524129	1.419637	2.438254	3.542230
17	C	4.339567	3.071263	2.423641	3.630167	4.586239
18	H	4.228081	3.350212	2.086926	2.619929	3.886344
19	H	5.391547	4.124354	3.392589	4.503448	5.563837
20	H	4.204397	2.906671	2.723907	4.014086	4.721884
21	O	4.526632	5.668345	5.671869	4.533290	3.667221
22	H	5.190730	6.279265	6.278881	5.179779	4.397780

		6	7	8	9	10
6	C	0.000000				
7	C	1.528934	0.000000			
8	H	2.833652	3.388920	0.000000		
9	H	4.656357	5.271452	2.757599	0.000000	
10	H	1.090249	2.151609	3.822731	5.343316	0.000000
11	H	1.091573	2.173208	2.687057	4.933766	1.767570
12	H	2.168508	1.098367	2.913972	4.968565	3.064002
13	H	2.148204	1.094861	3.954273	5.315815	2.482116
14	Br	4.029237	3.753928	5.206175	5.069145	4.033108
15	H	2.832565	3.636454	4.226540	4.232502	2.555077
16	C	4.888711	5.578099	4.622473	2.838978	5.048087
17	C	6.002505	6.755742	5.270748	2.938501	6.217429
18	H	5.058176	5.597859	5.284283	3.785022	5.065843
19	H	6.945224	7.643547	6.331680	3.939253	7.084478
20	H	6.174218	7.011601	5.002762	2.501107	6.500741
21	O	2.344905	1.425141	4.494565	6.621912	2.566680
22	H	3.193970	1.956546	5.136239	7.191935	3.417126

		11	12	13	14	15
11	H	0.000000				
12	H	2.510954	0.000000			
13	H	3.063978	1.786678	0.000000		
14	Br	5.102726	4.215578	2.775915	0.000000	
15	H	3.726019	4.295592	3.264280	2.646124	0.000000
16	C	5.586152	5.779384	5.186465	3.692637	2.775956

17	C	6.576562	6.852089	6.433635	4.945905	4.029953
18	H	5.901086	5.927505	5.022667	3.050884	2.584987
19	H	7.576706	7.776534	7.222472	5.406708	4.737362
20	H	6.587639	6.996648	6.842641	5.711628	4.595862
21	O	2.606039	2.088455	2.104671	4.805815	4.641178
22	H	3.522754	2.395777	2.320692	4.958392	5.259173

		16	17	18	19	20
16	C	0.000000				
17	C	1.327630	0.000000			
18	H	1.085074	2.133206	0.000000		
19	H	2.082893	1.081897	2.463853	0.000000	
20	H	2.124081	1.084043	3.106758	1.852304	0.000000
21	O	6.874516	8.075033	6.834866	8.954787	8.333935
22	H	7.420694	8.643266	7.303340	9.483577	8.950880

		21	22
21	O	0.000000	
22	H	0.961499	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.128926	-2.225287	-0.674082
2	6	0	-1.429863	-1.866483	-0.777983
3	7	0	-1.648316	-0.849710	0.145687
4	6	0	-0.475545	-0.563360	0.749389
5	7	0	0.446705	-1.430300	0.309473
6	6	0	1.867505	-1.395800	0.666907
7	6	0	2.681801	-0.577046	-0.335192
8	1	0	0.439866	-2.961365	-1.214697
9	1	0	-2.206254	-2.216735	-1.433621
10	1	0	1.964246	-0.952399	1.658209
11	1	0	2.229587	-2.424385	0.716319
12	1	0	2.617073	-1.028323	-1.334476
13	1	0	2.275145	0.438761	-0.373764
14	35	0	0.079040	2.121582	-0.148058
15	1	0	-0.344293	0.137318	1.550606
16	6	0	-2.833667	-0.094129	0.344214

17	6	0	-4.056306	-0.574803	0.152618
18	1	0	-2.622583	0.932806	0.623915
19	1	0	-4.908436	0.079013	0.282616
20	1	0	-4.251393	-1.602631	-0.131386
21	8	0	4.018632	-0.613785	0.157314
22	1	0	4.552859	-0.005627	-0.361557

Rotational constants (GHZ): 0.8401314 0.5685336 0.3599859

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 869.6255049893 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 6.43D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Initial guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999978 0.000610 -0.000104 -0.006623 Ang= 0.76 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Keep R1 ints in memory in canonical form, NReq=1804729152.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3032.33748976 A.U. after 12 cycles

NFock= 12 Conv=0.19D-08 -V/T= 2.0016

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000918844	-0.000041539	-0.000763147
2	6	-0.000570680	-0.000629756	-0.000040235
3	7	0.000432980	0.000292568	0.000258175
4	6	-0.001159789	-0.000582813	0.000853954
5	7	-0.000979750	0.000378026	0.000431660
6	6	0.000555038	-0.000206234	-0.000966633
7	6	-0.000099414	-0.000101037	0.001277103
8	1	-0.000005461	-0.000024092	-0.000049122
9	1	-0.000001481	-0.000003309	0.000090342
10	1	-0.000699046	-0.000001259	-0.000197557
11	1	0.000401634	-0.000010207	0.000367276
12	1	-0.000421689	-0.000052347	0.000015891
13	1	0.000800587	0.000354565	-0.000728417
14	35	-0.000099007	0.000444143	-0.000132168
15	1	-0.000072323	-0.000267240	0.000222937
16	6	-0.000870367	0.001271153	-0.000296886
17	6	0.000250392	-0.000458550	0.000118280
18	1	0.000602922	-0.000293261	-0.000011002
19	1	0.000240194	-0.000222763	-0.000261232
20	1	0.000066375	0.000229796	0.000204709
21	8	0.000726508	-0.000773954	-0.001382638
22	1	-0.000016467	0.000698111	0.000988708

Cartesian Forces: Max 0.001382638 RMS 0.000547333

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.002120129 RMS 0.000511049

Search for a local minimum.

Step number 8 out of a maximum of 116

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 6 7 8

DE= -5.13D-04 DEPred=-4.23D-04 R= 1.21D+00

TightC=F SS= 1.41D+00 RLast= 2.94D-01 DXNew= 7.1352D-01 8.8124D-01

Trust test= 1.21D+00 RLast= 2.94D-01 DXMaxT set to 7.14D-01

ITU= 1 1 1 0 0 -1 0 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00195	0.00400	0.00628	0.00967	0.01224
Eigenvalues ---	0.01527	0.01725	0.01871	0.02036	0.02187
Eigenvalues ---	0.02303	0.02414	0.02445	0.03062	0.03076
Eigenvalues ---	0.03789	0.04694	0.05439	0.06005	0.07029
Eigenvalues ---	0.08638	0.09177	0.13613	0.13844	0.15709
Eigenvalues ---	0.15737	0.15846	0.15993	0.16001	0.16181
Eigenvalues ---	0.16728	0.20719	0.21233	0.22858	0.22976
Eigenvalues ---	0.24210	0.24785	0.25782	0.30068	0.33147
Eigenvalues ---	0.33849	0.33873	0.33915	0.34088	0.34278
Eigenvalues ---	0.34397	0.34680	0.36134	0.36309	0.36427
Eigenvalues ---	0.37272	0.42769	0.43025	0.46010	0.49719
Eigenvalues ---	0.53483	0.54481	0.55705	0.60479	1.89455

RFO step: Lambda=-3.87995707D-04 EMin= 1.94616772D-03

Quartic linear search produced a step of 0.34328.

Iteration 1 RMS(Cart)= 0.04493128 RMS(Int)= 0.00219587

Iteration 2 RMS(Cart)= 0.00266642 RMS(Int)= 0.00003069

Iteration 3 RMS(Cart)= 0.00001199 RMS(Int)= 0.00002959

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00002959

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55775	0.00035	0.00042	0.00121	0.00163	2.55938
R2	2.62579	0.00037	-0.00099	0.00008	-0.00092	2.62488
R3	2.03319	0.00004	-0.00007	0.00005	-0.00002	2.03317
R4	2.62850	0.00044	-0.00238	0.00005	-0.00233	2.62617
R5	2.03119	-0.00007	0.00014	0.00018	0.00032	2.03151
R6	2.55067	-0.00037	-0.00124	-0.00183	-0.00307	2.54760
R7	2.68273	-0.00005	0.00271	0.00036	0.00308	2.68580
R8	2.53227	0.00051	0.00067	0.00056	0.00124	2.53351
R9	2.02662	0.00009	-0.00033	0.00053	0.00020	2.02681
R10	2.76935	0.00076	-0.00107	0.00145	0.00038	2.76973
R11	2.88927	0.00094	-0.00130	0.00093	-0.00037	2.88889
R12	2.06027	-0.00017	0.00002	-0.00042	-0.00041	2.05986
R13	2.06277	0.00009	0.00042	0.00007	0.00048	2.06326
R14	2.07561	-0.00003	0.00014	0.00035	0.00048	2.07610
R15	2.06899	0.00031	0.00027	-0.00047	-0.00020	2.06879
R16	2.69313	0.00046	-0.00056	0.00036	-0.00020	2.69292
R17	5.24572	0.00032	0.00615	0.01333	0.01948	5.26520
R18	2.50886	-0.00037	-0.00043	-0.00024	-0.00067	2.50819
R19	2.05049	-0.00018	0.00101	0.00079	0.00180	2.05229
R20	2.04449	-0.00037	0.00056	-0.00066	-0.00011	2.04438
R21	2.04854	-0.00030	0.00091	-0.00039	0.00052	2.04907

R22	1.81697	0.00025	-0.00028	0.00034	0.00006	1.81703
A1	1.87638	-0.00036	0.00005	-0.00121	-0.00120	1.87518
A2	2.27958	0.00014	0.00022	0.00090	0.00110	2.28068
A3	2.12714	0.00022	-0.00029	0.00042	0.00011	2.12724
A4	1.86895	0.00003	-0.00036	0.00010	-0.00038	1.86858
A5	2.28459	0.00002	0.00195	0.00170	0.00355	2.28814
A6	2.12918	-0.00006	-0.00168	-0.00242	-0.00420	2.12499
A7	1.89192	0.00030	0.00103	0.00143	0.00242	1.89434
A8	2.23073	-0.00027	-0.00254	-0.00065	-0.00323	2.22749
A9	2.15319	-0.00002	0.00171	0.00086	0.00254	2.15573
A10	1.89010	-0.00024	-0.00062	-0.00035	-0.00101	1.88909
A11	2.18842	0.00015	-0.00023	0.00074	0.00048	2.18890
A12	2.19411	0.00012	0.00084	0.00162	0.00243	2.19654
A13	1.89379	0.00031	-0.00030	0.00089	0.00054	1.89433
A14	2.19908	-0.00072	-0.00001	0.00031	0.00026	2.19933
A15	2.17968	0.00043	-0.00047	-0.00219	-0.00269	2.17699
A16	1.94884	0.00212	-0.00447	0.00255	-0.00193	1.94691
A17	1.89375	-0.00119	0.00336	-0.00566	-0.00229	1.89146
A18	1.88646	-0.00029	-0.00194	0.00524	0.00330	1.88976
A19	1.90805	0.00010	0.00216	0.00131	0.00347	1.91152
A20	1.93650	-0.00103	0.00133	-0.00304	-0.00173	1.93477
A21	1.88876	0.00023	-0.00029	-0.00055	-0.00084	1.88792
A22	1.92292	-0.00046	-0.00132	-0.00102	-0.00235	1.92057
A23	1.89876	0.00203	-0.00119	0.00231	0.00112	1.89987
A24	1.83307	-0.00046	0.00364	0.00045	0.00409	1.83717
A25	1.90419	-0.00074	0.00065	-0.00396	-0.00332	1.90087
A26	1.93810	0.00024	-0.00017	-0.00007	-0.00023	1.93786
A27	1.96546	-0.00054	-0.00161	0.00251	0.00089	1.96635
A28	2.59332	0.00152	-0.00408	-0.00665	-0.01073	2.58259
A29	2.16043	-0.00081	-0.00323	-0.00572	-0.00895	2.15148
A30	1.95771	-0.00026	0.00100	-0.00230	-0.00130	1.95641
A31	2.16398	0.00107	0.00228	0.00805	0.01033	2.17431
A32	2.08197	0.00023	0.00259	0.00108	0.00367	2.08564
A33	2.14936	-0.00016	-0.00205	-0.00292	-0.00498	2.14438
A34	2.05186	-0.00007	-0.00053	0.00185	0.00131	2.05317
A35	1.89483	0.00049	-0.00323	0.00094	-0.00229	1.89254
D1	-0.00042	0.00022	-0.00362	0.02322	0.01957	0.01915
D2	3.10854	-0.00005	-0.00740	0.00064	-0.00686	3.10167
D3	-3.12790	0.00015	0.00411	0.01469	0.01882	-3.10908
D4	-0.01895	-0.00012	0.00033	-0.00788	-0.00761	-0.02656
D5	-0.04827	0.00006	0.00148	-0.01362	-0.01214	-0.06040
D6	-3.03920	-0.00013	0.00732	-0.00643	0.00092	-3.03829
D7	3.08071	0.00012	-0.00544	-0.00599	-0.01146	3.06926
D8	0.08978	-0.00007	0.00041	0.00119	0.00160	0.09137

D9	0.04858	-0.00041	0.00457	-0.02477	-0.02020	0.02838
D10	3.06225	-0.00036	0.00653	-0.01049	-0.00397	3.05828
D11	-3.06393	-0.00017	0.00788	-0.00474	0.00306	-3.06087
D12	-0.05026	-0.00012	0.00984	0.00954	0.01929	-0.03097
D13	-0.07914	0.00046	-0.00367	0.01645	0.01278	-0.06636
D14	-3.07203	0.00024	-0.00364	0.00222	-0.00139	-3.07342
D15	-3.09975	0.00044	-0.00513	0.00308	-0.00212	-3.10188
D16	0.19054	0.00022	-0.00510	-0.01115	-0.01629	0.17425
D17	0.55879	0.00015	0.03158	0.04938	0.08096	0.63975
D18	-2.53504	0.00005	0.03047	0.04848	0.07895	-2.45609
D19	-2.72826	0.00022	0.03370	0.06564	0.09933	-2.62893
D20	0.46109	0.00013	0.03259	0.06473	0.09733	0.55842
D21	0.07884	-0.00032	0.00136	-0.00194	-0.00057	0.07827
D22	3.07186	-0.00025	-0.00437	-0.00876	-0.01311	3.05875
D23	3.07113	-0.00009	0.00121	0.01226	0.01346	3.08459
D24	-0.21904	-0.00003	-0.00451	0.00543	0.00093	-0.21811
D25	1.36472	-0.00045	-0.00407	0.00083	-0.00322	1.36149
D26	-2.81440	0.00021	-0.00192	0.00031	-0.00161	-2.81601
D27	-0.76998	-0.00032	-0.00150	-0.00054	-0.00205	-0.77203
D28	-1.60249	-0.00064	0.00268	0.00885	0.01154	-1.59095
D29	0.50158	0.00002	0.00482	0.00833	0.01315	0.51473
D30	2.54600	-0.00051	0.00524	0.00748	0.01271	2.55872
D31	-1.07370	-0.00013	0.00922	0.02297	0.03219	-1.04151
D32	1.01297	-0.00006	0.00849	0.01893	0.02742	1.04039
D33	3.12113	0.00009	0.00801	0.02332	0.03133	-3.13072
D34	3.11379	-0.00006	0.00642	0.02756	0.03398	-3.13541
D35	-1.08272	0.00001	0.00568	0.02352	0.02921	-1.05351
D36	1.02544	0.00016	0.00520	0.02791	0.03312	1.05856
D37	1.03202	0.00023	0.00460	0.02929	0.03389	1.06590
D38	3.11869	0.00030	0.00387	0.02525	0.02911	-3.13538
D39	-1.05634	0.00046	0.00339	0.02964	0.03303	-1.02331
D40	-0.53332	-0.00013	-0.01293	-0.07833	-0.09126	-0.62458
D41	1.56498	0.00008	-0.01485	-0.08056	-0.09541	1.46957
D42	-2.55794	-0.00053	-0.01572	-0.08180	-0.09752	-2.65546
D43	-2.99540	-0.00020	0.03774	0.09756	0.13530	-2.86011
D44	1.20957	0.00050	0.03726	0.09854	0.13580	1.34537
D45	-0.93178	0.00168	0.03771	0.10194	0.13965	-0.79213
D46	-3.09355	0.00009	-0.00076	0.00550	0.00473	-3.08882
D47	0.04809	0.00002	0.00212	0.00447	0.00658	0.05468
D48	-0.00531	0.00015	0.00041	0.00617	0.00659	0.00128
D49	3.13634	0.00008	0.00329	0.00514	0.00844	-3.13841

Item	Value	Threshold	Converged?
Maximum Force	0.002120	0.000450	NO
RMS Force	0.000511	0.000300	NO

Maximum Displacement 0.238354 0.001800 NO
RMS Displacement 0.045284 0.001200 NO
Predicted change in Energy=-2.269431D-04
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.454913	-1.960432	-1.324505
2	6	0	-1.744790	-1.583668	-1.493545
3	7	0	-2.101880	-0.839000	-0.375848
4	6	0	-1.028896	-0.740725	0.434402
5	7	0	-0.034997	-1.467905	-0.095490
6	6	0	1.327956	-1.534401	0.439437
7	6	0	2.230941	-0.474091	-0.190955
8	1	0	0.201806	-2.520868	-1.966542
9	1	0	-2.422321	-1.731382	-2.315016
10	1	0	1.281905	-1.379459	1.517418
11	1	0	1.719222	-2.537070	0.255989
12	1	0	2.278404	-0.618580	-1.279001
13	1	0	1.812929	0.515991	0.017609
14	35	0	-0.454629	2.102918	0.338369
15	1	0	-1.019855	-0.273768	1.399914
16	6	0	-3.325425	-0.153918	-0.144337
17	6	0	-4.505479	-0.618622	-0.535726
18	1	0	-3.171279	0.803802	0.343994
19	1	0	-5.393675	-0.023334	-0.371045
20	1	0	-4.627811	-1.581590	-1.018918
21	8	0	3.510029	-0.667139	0.406862
22	1	0	4.043108	0.116361	0.244089

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.354366	0.000000			
3	N	2.206821	1.389709	0.000000		
4	C	2.216053	2.222619	1.348131	0.000000	
5	N	1.389025	2.211640	2.178561	1.340675	0.000000
6	C	2.543937	3.630512	3.593334	2.486905	1.465677
7	C	3.272302	4.328319	4.352090	3.329970	2.476138
8	H	1.075909	2.211630	3.265878	3.232346	2.160010
9	H	2.214558	1.075027	2.158565	3.237643	3.270326

10	H	3.380916	4.274164	3.914914	2.630723	2.084113
11	H	2.749062	3.996151	4.228887	3.287984	2.084211
12	H	3.045268	4.142887	4.477852	3.726781	2.733839
13	H	3.616220	4.398809	4.161314	3.135127	2.713571
14	Br	4.390440	4.314087	3.446509	2.902639	3.621479
15	H	3.253684	3.257833	2.154901	1.072542	2.152242
16	C	3.591117	2.522489	1.421265	2.439944	3.543425
17	C	4.339321	3.077359	2.418970	3.611467	4.571684
18	H	4.219422	3.333381	2.088201	2.642640	3.897443
19	H	5.390065	4.124198	3.391349	4.496076	5.556811
20	H	4.201188	2.921829	2.710223	3.971320	4.686105
21	O	4.515640	5.662570	5.668835	4.539604	3.668896
22	H	5.196706	6.277678	6.249633	5.147430	4.388184

		6	7	8	9	10
6	C	0.000000				
7	C	1.528736	0.000000			
8	H	2.833737	3.385173	0.000000		
9	H	4.657294	5.267378	2.762384	0.000000	
10	H	1.090033	2.153811	3.821963	5.341600	0.000000
11	H	1.091828	2.171981	2.691181	4.940808	1.767064
12	H	2.166819	1.098623	2.898908	4.940492	3.064622
13	H	2.148777	1.094758	3.969267	5.331901	2.474701
14	Br	4.051903	3.759448	5.207967	5.061040	4.066037
15	H	2.832654	3.624731	4.227877	4.229924	2.556259
16	C	4.888811	5.565778	4.622147	2.831225	5.048848
17	C	5.984861	6.746786	5.274876	2.956968	6.187737
18	H	5.071431	5.577021	5.269697	3.749457	5.096508
19	H	6.936896	7.640052	6.331880	3.940228	7.068857
20	H	6.131899	6.996754	5.010533	2.562518	6.434174
21	O	2.348328	1.425033	4.473667	6.613169	2.589454
22	H	3.183587	1.954954	5.157273	7.194786	3.388671

		11	12	13	14	15
11	H	0.000000				
12	H	2.519818	0.000000			
13	H	3.063787	1.784689	0.000000		
14	Br	5.124638	4.182333	2.786225	0.000000	
15	H	3.732780	4.263097	3.249485	2.663643	0.000000
16	C	5.593580	5.736398	5.184369	3.683447	2.777540
17	C	6.561567	6.824480	6.443276	4.957843	4.001900
18	H	5.923358	5.861427	5.003168	3.011298	2.627689
19	H	7.570030	7.748516	7.237201	5.423873	4.725391
20	H	6.543941	6.977882	6.852545	5.730033	4.536353
21	O	2.593530	2.088395	2.105104	4.836985	4.654110
22	H	3.527221	2.444202	2.276993	4.917819	5.207853

		16	17	18	19	20
16	C	0.000000				
17	C	1.327277	0.000000			
18	H	1.086027	2.139460	0.000000		
19	H	2.084733	1.081841	2.476788	0.000000	
20	H	2.121167	1.084319	3.109519	1.853227	0.000000
21	O	6.876819	8.070886	6.841600	8.960780	8.312251
22	H	7.383712	8.615489	7.247754	9.457843	8.925417

		21	22
21	O	0.000000	
22	H	0.961531	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.115273	-2.219134	-0.696202
2	6	0	-1.418303	-1.864507	-0.799446
3	7	0	-1.639068	-0.849640	0.123916
4	6	0	-0.474906	-0.575512	0.746041
5	7	0	0.450208	-1.439800	0.304928
6	6	0	1.869103	-1.402916	0.670420
7	6	0	2.681286	-0.563135	-0.315563
8	1	0	0.460446	-2.942142	-1.247008
9	1	0	-2.191138	-2.199635	-1.467352
10	1	0	1.955500	-0.976250	1.669751
11	1	0	2.240529	-2.429042	0.705039
12	1	0	2.594988	-0.982312	-1.327401
13	1	0	2.286490	0.457950	-0.319636
14	35	0	0.066706	2.132931	-0.146317
15	1	0	-0.349516	0.122470	1.550680
16	6	0	-2.828638	-0.096344	0.317472
17	6	0	-4.045261	-0.614642	0.204079
18	1	0	-2.620954	0.950049	0.520909
19	1	0	-4.909777	0.026006	0.316163
20	1	0	-4.220710	-1.665624	0.003079
21	8	0	4.025447	-0.630267	0.152885
22	1	0	4.529842	0.071302	-0.268930

```
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.8327476           0.5695747           0.3592507
 Standard basis: 6-311++G(d,p) (5D, 7F)
 There are     358 symmetry adapted cartesian basis functions of A      symmetry.
 There are     345 symmetry adapted basis functions of A      symmetry.
    345 basis functions,      553 primitive gaussians,      358 cartesian basis functions
     55 alpha electrons              55 beta electrons
          nuclear repulsion energy             868.9658615625 Hartrees.
 NAtoms=       22 NActive=       22 NUniq=       22 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      345 RedAO= T EigKep=    6.78D-06    NBF=      345
 NBsUse=      345 1.00D-06 EigRej= -1.00D+00 NBFU=      345
 Initial guess from the checkpoint file:    "."
 B after Tr=          0.000000        0.000000        0.000000
             Rot=        0.999996      -0.001655        0.000043      -0.002076 Ang=    -0.30 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn=                5 AccDes=
0.00D+00
 Harris functional with IExCor=    402 and IRadAn=             5 diagonalized for initial guess.
 HarFok:    IExCor=    402 AccDes= 0.00D+00 IRadAn=                5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=    3500011 ScaDFX=    1.000000    1.000000    1.000000    1.000000
 FoFCou: FMM=F IPFlag=                  0 FMFlag=           100000 FMFlg1=                  0
             NFxFlg=                    0 DoJE=T BraDBF=F KetDBF=T FulRan=T
             wScrn=      0.000000  ICntrl=             500  IOpCl=      0  I1Cent=        200000004  NGrid=
0
             NMat0=         1 NMatS0=            1 NMatT0=         0 NMatD0=         1 NMtDS0=         0
NMtDT0=        0
 Petite list used in FoFCou.
 Keep R1 ints in memory in canonical form, NReq=1804729152.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                    energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3032.33774609          A.U. after      12 cycles
                  NFock= 12    Conv=0.18D-08         -V/T= 2.0016
 Calling FoFJK, ICntrl=             2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 ---------------------------------------------------------------------
 Center          Atomic                             Forces (Hartrees/Bohr)
 Number          Number                       X                      Y                      Z
```

1	6	0.000059925	-0.001127489	-0.000242224
2	6	0.000504110	0.001123260	-0.001227749
3	7	-0.000681720	-0.001482293	0.001658867
4	6	-0.000369572	-0.000447125	-0.000199485
5	7	-0.000736891	0.001548551	0.000463800
6	6	0.000512220	-0.000239875	-0.000705952
7	6	-0.000134185	-0.000106510	0.000993450
8	1	-0.000164375	-0.000394291	0.000136610
9	1	0.000131902	-0.000239401	0.000060448
10	1	-0.000471879	-0.000012505	-0.000052404
11	1	0.000070815	0.000054612	0.000193253
12	1	-0.000144408	0.000106786	0.000195621
13	1	0.000663310	0.000245481	-0.000780549
14	35	-0.000002817	0.000128436	0.000072789
15	1	0.000087086	-0.000128395	0.000215746
16	6	-0.000766699	0.001377670	-0.000401903
17	6	0.000166537	-0.000326657	-0.000019016
18	1	0.000415446	-0.000490531	0.000027206
19	1	0.000175612	-0.000142677	-0.000111184
20	1	-0.000029278	0.000405613	0.000076367
21	8	0.000544005	-0.000081393	-0.001168838
22	1	0.000170856	0.000228735	0.000815146

Cartesian Forces: Max 0.001658867 RMS 0.000587830

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.001740974 RMS 0.000392176
Search for a local minimum.
Step number 9 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 8 9
DE= -2.56D-04 DEPred=-2.27D-04 R= 1.13D+00
TightC=F SS= 1.41D+00 RLast= 3.59D-01 DXNew= 1.2000D+00 1.0757D+00
Trust test= 1.13D+00 RLast= 3.59D-01 DXMaxT set to 1.08D+00
ITU= 1 1 1 1 0 0 -1 0 0
Eigenvalues --- 0.00157 0.00390 0.00593 0.00905 0.01222
Eigenvalues --- 0.01514 0.01737 0.01895 0.02049 0.02196
Eigenvalues --- 0.02384 0.02416 0.02961 0.03071 0.03131

Eigenvalues --- 0.03846 0.04690 0.05434 0.05980 0.06930
Eigenvalues --- 0.08640 0.09155 0.13609 0.13839 0.15725
Eigenvalues --- 0.15782 0.15802 0.15977 0.16001 0.16116
Eigenvalues --- 0.16620 0.20694 0.21353 0.22863 0.22941
Eigenvalues --- 0.24226 0.24733 0.25709 0.29924 0.33136
Eigenvalues --- 0.33867 0.33873 0.33916 0.34083 0.34233
Eigenvalues --- 0.34457 0.34682 0.36113 0.36308 0.36420
Eigenvalues --- 0.37269 0.42706 0.43005 0.45889 0.49806
Eigenvalues --- 0.53463 0.54435 0.55652 0.60467 1.86169
En-DIIS/RFO-DIIS IScMMF= 0 using points: 9 8
RFO step: Lambda=-4.09921387D-05.
DidBck=F Rises=F RFO-DIIS coefs: 1.21517 -0.21517
Iteration 1 RMS(Cart)= 0.02513475 RMS(Int)= 0.00137371
Iteration 2 RMS(Cart)= 0.00147399 RMS(Int)= 0.00002654
Iteration 3 RMS(Cart)= 0.00000791 RMS(Int)= 0.00002595
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00002595

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55938	0.00006	0.00035	0.00119	0.00151	2.56089
R2	2.62488	0.00055	-0.00020	-0.00002	-0.00025	2.62463
R3	2.03317	0.00002	0.00000	-0.00006	-0.00006	2.03311
R4	2.62617	0.00079	-0.00050	-0.00002	-0.00050	2.62567
R5	2.03151	-0.00010	0.00007	-0.00013	-0.00006	2.03144
R6	2.54760	0.00005	-0.00066	-0.00177	-0.00239	2.54521
R7	2.68580	0.00034	0.00066	0.00456	0.00522	2.69102
R8	2.53351	-0.00007	0.00027	-0.00027	0.00000	2.53351
R9	2.02681	0.00014	0.00004	0.00082	0.00086	2.02767
R10	2.76973	0.00093	0.00008	0.00222	0.00230	2.77203
R11	2.88889	0.00101	-0.00008	0.00096	0.00088	2.88978
R12	2.05986	-0.00003	-0.00009	0.00006	-0.00003	2.05983
R13	2.06326	-0.00006	0.00010	0.00001	0.00011	2.06337
R14	2.07610	-0.00021	0.00010	-0.00011	-0.00001	2.07609
R15	2.06879	-0.00004	-0.00004	-0.00070	-0.00074	2.06805
R16	2.69292	0.00046	-0.00004	-0.00041	-0.00045	2.69247
R17	5.26520	0.00009	0.00419	0.01191	0.01610	5.28130
R18	2.50819	-0.00023	-0.00014	-0.00103	-0.00117	2.50702
R19	2.05229	-0.00037	0.00039	-0.00024	0.00015	2.05244
R20	2.04438	-0.00024	-0.00002	-0.00052	-0.00055	2.04384
R21	2.04907	-0.00038	0.00011	-0.00062	-0.00051	2.04856
R22	1.81703	0.00016	0.00001	-0.00004	-0.00003	1.81700
A1	1.87518	-0.00014	-0.00026	-0.00056	-0.00089	1.87429
A2	2.28068	0.00001	0.00024	0.00028	0.00052	2.28121
A3	2.12724	0.00013	0.00002	0.00015	0.00018	2.12742
A4	1.86858	0.00002	-0.00008	0.00022	0.00011	1.86869

A5	2.28814	-0.00020	0.00076	0.00063	0.00137	2.28951
A6	2.12499	0.00020	-0.00090	-0.00028	-0.00120	2.12378
A7	1.89434	-0.00011	0.00052	-0.00018	0.00027	1.89461
A8	2.22749	0.00015	-0.00070	-0.00248	-0.00330	2.22419
A9	2.15573	-0.00009	0.00055	-0.00030	0.00011	2.15584
A10	1.88909	0.00011	-0.00022	0.00091	0.00066	1.88976
A11	2.18890	0.00011	0.00010	0.00108	0.00110	2.18999
A12	2.19654	-0.00020	0.00052	0.00009	0.00053	2.19707
A13	1.89433	0.00015	0.00012	0.00048	0.00056	1.89490
A14	2.19933	-0.00078	0.00006	-0.00100	-0.00093	2.19840
A15	2.17699	0.00068	-0.00058	0.00096	0.00039	2.17738
A16	1.94691	0.00174	-0.00041	0.00063	0.00021	1.94712
A17	1.89146	-0.00077	-0.00049	-0.00309	-0.00358	1.88788
A18	1.88976	-0.00053	0.00071	0.00078	0.00149	1.89125
A19	1.91152	-0.00014	0.00075	0.00236	0.00311	1.91463
A20	1.93477	-0.00056	-0.00037	0.00047	0.00009	1.93486
A21	1.88792	0.00020	-0.00018	-0.00132	-0.00150	1.88642
A22	1.92057	-0.00021	-0.00050	-0.00042	-0.00093	1.91965
A23	1.89987	0.00099	0.00024	-0.00014	0.00009	1.89996
A24	1.83717	0.00001	0.00088	0.00458	0.00545	1.84262
A25	1.90087	-0.00035	-0.00071	-0.00367	-0.00439	1.89649
A26	1.93786	-0.00001	-0.00005	-0.00102	-0.00107	1.93680
A27	1.96635	-0.00038	0.00019	0.00094	0.00112	1.96747
A28	2.58259	0.00057	-0.00231	-0.00856	-0.01086	2.57173
A29	2.15148	-0.00003	-0.00193	-0.00394	-0.00587	2.14561
A30	1.95641	-0.00048	-0.00028	-0.00352	-0.00380	1.95261
A31	2.17431	0.00052	0.00222	0.00765	0.00987	2.18418
A32	2.08564	0.00002	0.00079	0.00273	0.00352	2.08916
A33	2.14438	0.00007	-0.00107	-0.00160	-0.00267	2.14171
A34	2.05317	-0.00010	0.00028	-0.00113	-0.00085	2.05232
A35	1.89254	0.00078	-0.00049	0.00121	0.00072	1.89326
D1	0.01915	-0.00060	0.00421	-0.02184	-0.01763	0.00152
D2	3.10167	-0.00017	-0.00148	-0.01037	-0.01185	3.08982
D3	-3.10908	-0.00037	0.00405	-0.01022	-0.00617	-3.11525
D4	-0.02656	0.00006	-0.00164	0.00125	-0.00039	-0.02695
D5	-0.06040	0.00062	-0.00261	0.02120	0.01858	-0.04182
D6	-3.03829	0.00023	0.00020	0.01821	0.01841	-3.01988
D7	3.06926	0.00041	-0.00247	0.01083	0.00836	3.07761
D8	0.09137	0.00002	0.00034	0.00783	0.00818	0.09955
D9	0.02838	0.00037	-0.00435	0.01507	0.01073	0.03911
D10	3.05828	-0.00010	-0.00085	-0.01425	-0.01508	3.04320
D11	-3.06087	0.00000	0.00066	0.00487	0.00551	-3.05536
D12	-0.03097	-0.00047	0.00415	-0.02445	-0.02029	-0.05126
D13	-0.06636	0.00001	0.00275	-0.00194	0.00081	-0.06555

D14	-3.07342	-0.00015	-0.00030	-0.01795	-0.01827	-3.09169
D15	-3.10188	0.00044	-0.00046	0.02608	0.02565	-3.07623
D16	0.17425	0.00027	-0.00351	0.01006	0.00657	0.18082
D17	0.63975	0.00016	0.01742	0.03115	0.04854	0.68829
D18	-2.45609	0.00009	0.01699	0.02640	0.04339	-2.41270
D19	-2.62893	-0.00037	0.02137	-0.00224	0.01913	-2.60979
D20	0.55842	-0.00045	0.02094	-0.00699	0.01398	0.57239
D21	0.07827	-0.00038	-0.00012	-0.01170	-0.01183	0.06644
D22	3.05875	-0.00017	-0.00282	-0.00899	-0.01181	3.04695
D23	3.08459	-0.00018	0.00290	0.00450	0.00740	3.09199
D24	-0.21811	0.00003	0.00020	0.00722	0.00742	-0.21069
D25	1.36149	0.00001	-0.00069	0.00715	0.00645	1.36794
D26	-2.81601	0.00042	-0.00035	0.00844	0.00809	-2.80792
D27	-0.77203	-0.00004	-0.00044	0.00563	0.00519	-0.76684
D28	-1.59095	-0.00036	0.00248	0.00377	0.00626	-1.58469
D29	0.51473	0.00005	0.00283	0.00507	0.00790	0.52264
D30	2.55872	-0.00041	0.00274	0.00226	0.00500	2.56371
D31	-1.04151	0.00007	0.00693	0.03265	0.03958	-1.00193
D32	1.04039	0.00012	0.00590	0.02784	0.03373	1.07413
D33	-3.13072	0.00019	0.00674	0.03144	0.03818	-3.09254
D34	-3.13541	0.00001	0.00731	0.03455	0.04186	-3.09355
D35	-1.05351	0.00006	0.00628	0.02974	0.03602	-1.01749
D36	1.05856	0.00013	0.00713	0.03334	0.04047	1.09903
D37	1.06590	0.00019	0.00729	0.03439	0.04168	1.10758
D38	-3.13538	0.00024	0.00626	0.02958	0.03584	-3.09955
D39	-1.02331	0.00031	0.00711	0.03318	0.04029	-0.98302
D40	-0.62458	0.00013	-0.01964	-0.03730	-0.05693	-0.68151
D41	1.46957	0.00025	-0.02053	-0.04006	-0.06059	1.40898
D42	-2.65546	-0.00029	-0.02098	-0.04340	-0.06438	-2.71984
D43	-2.86011	0.00000	0.02911	0.08912	0.11823	-2.74188
D44	1.34537	0.00025	0.02922	0.08745	0.11667	1.46204
D45	-0.79213	0.00100	0.03005	0.09230	0.12236	-0.66977
D46	-3.08882	0.00001	0.00102	0.00084	0.00184	-3.08698
D47	0.05468	-0.00010	0.00142	-0.00211	-0.00070	0.05397
D48	0.00128	0.00007	0.00142	0.00584	0.00726	0.00854
D49	-3.13841	-0.00005	0.00182	0.00289	0.00472	-3.13369

Item	Value	Threshold	Converged?
Maximum Force	0.001741	0.000450	NO
RMS Force	0.000392	0.000300	NO
Maximum Displacement	0.101618	0.001800	NO
RMS Displacement	0.025032	0.001200	NO

Predicted change in Energy=-1.385477D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.456828	-1.980825	-1.318977
2	6	0	-1.742840	-1.591432	-1.495103
3	7	0	-2.101808	-0.851249	-0.375362
4	6	0	-1.031461	-0.756082	0.436642
5	7	0	-0.035594	-1.480104	-0.093879
6	6	0	1.331068	-1.537007	0.436003
7	6	0	2.223966	-0.468730	-0.196438
8	1	0	0.198551	-2.546918	-1.957358
9	1	0	-2.418005	-1.731022	-2.319892
10	1	0	1.284071	-1.385282	1.514384
11	1	0	1.730190	-2.536433	0.251421
12	1	0	2.235435	-0.587326	-1.288576
13	1	0	1.818698	0.518915	0.044293
14	35	0	-0.452271	2.114288	0.373066
15	1	0	-1.019315	-0.278992	1.397661
16	6	0	-3.318267	-0.143167	-0.159258
17	6	0	-4.501933	-0.612408	-0.531769
18	1	0	-3.146478	0.825134	0.301727
19	1	0	-5.387392	-0.008321	-0.387562
20	1	0	-4.629044	-1.589905	-0.982889
21	8	0	3.521395	-0.680240	0.353089
22	1	0	4.018214	0.140228	0.285930

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.355165	0.000000			
3	N	2.207331	1.389442	0.000000		
4	C	2.216392	2.221600	1.346866	0.000000	
5	N	1.388893	2.211449	2.178057	1.340676	0.000000
6	C	2.544307	3.630570	3.593496	2.488250	1.466894
7	C	3.276153	4.322330	4.346338	3.328839	2.477702
8	H	1.075878	2.212607	3.266444	3.232840	2.159970
9	H	2.215953	1.074993	2.157586	3.235968	3.270164
10	H	3.378363	4.273370	3.914142	2.630420	2.082551
11	H	2.749163	4.000663	4.232837	3.290999	2.086398
12	H	3.031673	4.108229	4.440190	3.698305	2.716970
13	H	3.644890	4.416770	4.174186	3.146897	2.730122
14	Br	4.430912	4.346031	3.474986	2.928912	3.648467

15	H	3.254651	3.257925	2.154735	1.072996	2.152921
16	C	3.593016	2.522682	1.424027	2.441360	3.545083
17	C	4.342250	3.082060	2.417045	3.605917	4.570867
18	H	4.211212	3.322437	2.088072	2.644190	3.892072
19	H	5.391546	4.125003	3.392011	4.495841	5.558249
20	H	4.203946	2.931304	2.702152	3.956379	4.679976
21	O	4.507059	5.653163	5.672768	4.554254	3.673110
22	H	5.205824	6.273793	6.234983	5.130820	4.382134

		6	7	8	9	10
6	C	0.000000				
7	C	1.529203	0.000000			
8	H	2.833847	3.394408	0.000000		
9	H	4.657053	5.258357	2.764684	0.000000	
10	H	1.090017	2.156475	3.818474	5.341027	0.000000
11	H	1.091889	2.172507	2.687887	4.946499	1.766139
12	H	2.166551	1.098618	2.904508	4.901647	3.065683
13	H	2.148961	1.094366	4.003850	5.348012	2.464337
14	Br	4.064014	3.762786	5.251789	5.089454	4.069948
15	H	2.834023	3.618843	4.228811	4.229057	2.557946
16	C	4.890137	5.551911	4.623763	2.828444	5.052270
17	C	5.984594	6.735786	5.279127	2.965036	6.185622
18	H	5.064203	5.546523	5.259602	3.733295	5.097670
19	H	6.939225	7.627665	6.333363	3.939398	7.072611
20	H	6.126907	6.988511	5.017084	2.587699	6.422085
21	O	2.353393	1.424794	4.456898	6.597381	2.617501
22	H	3.171182	1.955208	5.181016	7.191439	3.363305

		11	12	13	14	15
11	H	0.000000				
12	H	2.534932	0.000000			
13	H	3.063640	1.781567	0.000000		
14	Br	5.138788	4.157347	2.794746	0.000000	
15	H	3.737604	4.231351	3.243852	2.664418	0.000000
16	C	5.602079	5.684737	5.183453	3.686923	2.779861
17	C	6.569217	6.779787	6.446868	4.965215	3.995310
18	H	5.923222	5.786976	4.981266	2.987601	2.635335
19	H	7.580212	7.697698	7.238246	5.425813	4.726561
20	H	6.546701	6.944039	6.861166	5.745006	4.518369
21	O	2.581512	2.087436	2.105352	4.857963	4.676556
22	H	3.521472	2.487310	2.244920	4.887713	5.175750

		16	17	18	19	20
16	C	0.000000				
17	C	1.326657	0.000000			
18	H	1.086105	2.144412	0.000000		
19	H	2.086045	1.081552	2.488265	0.000000	

20	H	2.118858	1.084051	3.111375	1.852273	0.000000
21	O	6.879819	8.072259	6.835884	8.964738	8.309151
22	H	7.355437	8.592323	7.197372	9.430858	8.909453

		21	22
21	O	0.000000	
22	H	0.961514	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.114573	-2.245067	-0.673563
2	6	0	-1.414837	-1.882583	-0.793538
3	7	0	-1.640636	-0.864162	0.124276
4	6	0	-0.480725	-0.586069	0.749833
5	7	0	0.448316	-1.450060	0.316459
6	6	0	1.869267	-1.400731	0.677354
7	6	0	2.672651	-0.560738	-0.316351
8	1	0	0.462476	-2.976366	-1.211827
9	1	0	-2.183728	-2.217170	-1.466194
10	1	0	1.951819	-0.968750	1.674707
11	1	0	2.249400	-2.423488	0.718448
12	1	0	2.552964	-0.963479	-1.331455
13	1	0	2.293266	0.465631	-0.299862
14	35	0	0.068703	2.149781	-0.139987
15	1	0	-0.355649	0.127141	1.541671
16	6	0	-2.826499	-0.092736	0.287008
17	6	0	-4.043531	-0.612641	0.194546
18	1	0	-2.606353	0.958058	0.451306
19	1	0	-4.908852	0.030928	0.276969
20	1	0	-4.218079	-1.670863	0.036853
21	8	0	4.028207	-0.653501	0.112484
22	1	0	4.508180	0.106971	-0.227835

Rotational constants (GHZ): 0.8213875 0.5708270 0.3571262
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 358 symmetry adapted cartesian basis functions of A symmetry.
There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 867.2952205396 Hartrees.
NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 345 RedAO= T EigKep= 7.03D-06 NBF= 345
NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345
Initial guess from the checkpoint file: "."
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 0.000247 -0.000018 0.000223 Ang= 0.04 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.33791557 A.U. after 12 cycles
NFock= 12 Conv=0.39D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000039257	0.000674115	-0.000841865
2	6	0.000550654	-0.000380686	-0.000621324
3	7	-0.000963987	0.000247337	0.000855797
4	6	0.000480875	-0.000534977	-0.000005708

5	7	-0.000801064	0.000480512	0.000748236
6	6	-0.000037057	-0.000457597	0.000139816
7	6	-0.000446333	0.000023297	0.000419203
8	1	-0.000076287	-0.000239123	0.000048221
9	1	0.000033187	-0.000582615	0.000124066
10	1	-0.000156649	-0.000009739	-0.000005410
11	1	-0.000012546	0.000131975	-0.000124151
12	1	0.000091551	-0.000001455	0.000292193
13	1	0.000533868	0.000332216	-0.000740366
14	35	-0.000091707	-0.000303073	0.000131042
15	1	0.000105921	0.000104406	-0.000033353
16	6	0.000375574	0.000467910	-0.000029971
17	6	-0.000069287	-0.000186165	-0.000256239
18	1	-0.000003190	-0.000166954	-0.000031257
19	1	0.000085851	0.000105758	0.000109267
20	1	-0.000055510	0.000205298	-0.000046340
21	8	0.000375663	0.000150640	-0.000658856
22	1	0.000119730	-0.000061079	0.000526997

Cartesian Forces: Max 0.000963987 RMS 0.000377407

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.001410687 RMS 0.000267354
Search for a local minimum.
Step number 10 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 9 10
DE= -1.69D-04 DEPred=-1.39D-04 R= 1.22D+00
TightC=F SS= 1.41D+00 RLast= 2.77D-01 DXNew= 1.8091D+00 8.2954D-01
Trust test= 1.22D+00 RLast= 2.77D-01 DXMaxT set to 1.08D+00
ITU= 1 1 1 1 1 0 0 -1 0 0

Eigenvalues ---	0.00171	0.00347	0.00535	0.00780	0.01225
Eigenvalues ---	0.01407	0.01678	0.01868	0.02057	0.02182
Eigenvalues ---	0.02369	0.02418	0.03060	0.03079	0.03359
Eigenvalues ---	0.04162	0.04722	0.05438	0.05949	0.06981
Eigenvalues ---	0.08655	0.09198	0.13656	0.13846	0.15724
Eigenvalues ---	0.15834	0.15932	0.15984	0.15992	0.16009
Eigenvalues ---	0.16505	0.20691	0.21401	0.22826	0.22895
Eigenvalues ---	0.24210	0.24607	0.25425	0.29578	0.33137

Eigenvalues --- 0.33848 0.33873 0.33900 0.34095 0.34236
Eigenvalues --- 0.34473 0.34683 0.35985 0.36309 0.36385
Eigenvalues --- 0.37273 0.42643 0.42909 0.45716 0.49611
Eigenvalues --- 0.53491 0.54476 0.55657 0.60475 1.90168
En-DIIS/RFO-DIIS IScMMF= 0 using points: 10 9 8
RFO step: Lambda=-2.32022419D-05.
DidBck=F Rises=F RFO-DIIS coefs: 1.26152 -0.25353 -0.00800
Iteration 1 RMS(Cart)= 0.02846359 RMS(Int)= 0.00073280
Iteration 2 RMS(Cart)= 0.00082604 RMS(Int)= 0.00002933
Iteration 3 RMS(Cart)= 0.00000180 RMS(Int)= 0.00002931
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00002931

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56089	-0.00035	0.00041	-0.00025	0.00013	2.56103
R2	2.62463	0.00043	-0.00007	0.00068	0.00058	2.62521
R3	2.03311	0.00005	-0.00002	0.00011	0.00009	2.03321
R4	2.62567	0.00100	-0.00015	0.00229	0.00215	2.62782
R5	2.03144	-0.00004	-0.00001	-0.00020	-0.00021	2.03123
R6	2.54521	0.00027	-0.00065	-0.00012	-0.00074	2.54447
R7	2.69102	-0.00013	0.00139	0.00168	0.00307	2.69409
R8	2.53351	-0.00052	0.00001	-0.00138	-0.00137	2.53214
R9	2.02767	0.00002	0.00023	0.00032	0.00055	2.02822
R10	2.77203	0.00033	0.00060	0.00159	0.00219	2.77422
R11	2.88978	0.00051	0.00023	0.00253	0.00276	2.89254
R12	2.05983	0.00000	-0.00001	0.00008	0.00007	2.05990
R13	2.06337	-0.00011	0.00003	-0.00031	-0.00028	2.06309
R14	2.07609	-0.00028	0.00000	-0.00090	-0.00090	2.07519
R15	2.06805	-0.00026	-0.00020	-0.00044	-0.00063	2.06742
R16	2.69247	0.00037	-0.00012	0.00022	0.00010	2.69257
R17	5.28130	-0.00007	0.00437	0.00544	0.00981	5.29112
R18	2.50702	0.00006	-0.00031	-0.00045	-0.00077	2.50625
R19	2.05244	-0.00017	0.00005	-0.00065	-0.00059	2.05185
R20	2.04384	0.00000	-0.00014	-0.00026	-0.00040	2.04343
R21	2.04856	-0.00015	-0.00013	-0.00064	-0.00077	2.04779
R22	1.81700	-0.00001	-0.00001	-0.00018	-0.00018	1.81681
A1	1.87429	0.00002	-0.00024	-0.00009	-0.00037	1.87392
A2	2.28121	-0.00005	0.00015	-0.00002	0.00011	2.28132
A3	2.12742	0.00003	0.00005	0.00041	0.00045	2.12787
A4	1.86869	-0.00007	0.00003	-0.00006	-0.00002	1.86867
A5	2.28951	-0.00025	0.00039	-0.00155	-0.00117	2.28834
A6	2.12378	0.00032	-0.00035	0.00168	0.00132	2.12511
A7	1.89461	-0.00024	0.00009	-0.00060	-0.00057	1.89404
A8	2.22419	0.00042	-0.00089	-0.00013	-0.00118	2.22301
A9	2.15584	-0.00019	0.00005	-0.00164	-0.00175	2.15409

A10	1.88976	0.00010	0.00017	0.00101	0.00115	1.89091
A11	2.18999	0.00001	0.00029	0.00083	0.00101	2.19100
A12	2.19707	-0.00009	0.00016	-0.00009	-0.00004	2.19702
A13	1.89490	0.00019	0.00015	0.00029	0.00044	1.89534
A14	2.19840	-0.00018	-0.00024	-0.00120	-0.00145	2.19695
A15	2.17738	-0.00002	0.00008	0.00039	0.00046	2.17784
A16	1.94712	0.00000	0.00004	0.00143	0.00147	1.94859
A17	1.88788	-0.00011	-0.00095	-0.00186	-0.00282	1.88506
A18	1.89125	0.00004	0.00042	-0.00082	-0.00040	1.89085
A19	1.91463	0.00002	0.00084	0.00278	0.00363	1.91825
A20	1.93486	0.00000	0.00001	-0.00181	-0.00180	1.93307
A21	1.88642	0.00006	-0.00040	0.00020	-0.00020	1.88622
A22	1.91965	0.00004	-0.00026	-0.00165	-0.00190	1.91774
A23	1.89996	-0.00042	0.00003	0.00503	0.00504	1.90500
A24	1.84262	0.00036	0.00146	0.00307	0.00452	1.84713
A25	1.89649	0.00002	-0.00117	-0.00453	-0.00570	1.89079
A26	1.93680	-0.00018	-0.00028	-0.00269	-0.00297	1.93382
A27	1.96747	0.00018	0.00030	0.00111	0.00138	1.96884
A28	2.57173	-0.00141	-0.00293	-0.00575	-0.00868	2.56305
A29	2.14561	0.00037	-0.00161	-0.00015	-0.00176	2.14385
A30	1.95261	-0.00020	-0.00100	-0.00244	-0.00345	1.94916
A31	2.18418	-0.00017	0.00266	0.00261	0.00527	2.18945
A32	2.08916	-0.00027	0.00095	-0.00037	0.00058	2.08973
A33	2.14171	0.00022	-0.00074	0.00083	0.00009	2.14180
A34	2.05232	0.00005	-0.00021	-0.00045	-0.00067	2.05165
A35	1.89326	0.00060	0.00017	0.00343	0.00360	1.89686
D1	0.00152	0.00024	-0.00445	0.00995	0.00550	0.00702
D2	3.08982	0.00025	-0.00315	0.01178	0.00863	3.09845
D3	-3.11525	-0.00006	-0.00146	-0.00453	-0.00600	-3.12125
D4	-0.02695	-0.00004	-0.00016	-0.00270	-0.00287	-0.02982
D5	-0.04182	-0.00013	0.00476	-0.00367	0.00109	-0.04073
D6	-3.01988	-0.00009	0.00482	-0.00033	0.00448	-3.01540
D7	3.07761	0.00013	0.00209	0.00926	0.01135	3.08896
D8	0.09955	0.00017	0.00215	0.01259	0.01474	0.11429
D9	0.03911	-0.00028	0.00264	-0.01286	-0.01021	0.02889
D10	3.04320	-0.00043	-0.00398	-0.03197	-0.03595	3.00726
D11	-3.05536	-0.00028	0.00147	-0.01436	-0.01290	-3.06825
D12	-0.05126	-0.00042	-0.00515	-0.03348	-0.03863	-0.08989
D13	-0.06555	0.00020	0.00031	0.01062	0.01093	-0.05461
D14	-3.09169	-0.00001	-0.00479	-0.00525	-0.01005	-3.10174
D15	-3.07623	0.00028	0.00669	0.02868	0.03538	-3.04085
D16	0.18082	0.00008	0.00159	0.01281	0.01439	0.19521
D17	0.68829	-0.00011	0.01334	-0.00724	0.00608	0.69438
D18	-2.41270	-0.00007	0.01198	-0.00770	0.00428	-2.40843

D19	-2.60979	-0.00027	0.00580	-0.02890	-0.02310	-2.63289
D20	0.57239	-0.00023	0.00443	-0.02935	-0.02490	0.54749
D21	0.06644	-0.00004	-0.00310	-0.00434	-0.00744	0.05900
D22	3.04695	-0.00010	-0.00319	-0.00781	-0.01101	3.03594
D23	3.09199	0.00018	0.00204	0.01168	0.01372	3.10572
D24	-0.21069	0.00012	0.00195	0.00822	0.01016	-0.20053
D25	1.36794	0.00011	0.00166	-0.00482	-0.00315	1.36479
D26	-2.80792	0.00006	0.00210	-0.00170	0.00040	-2.80752
D27	-0.76684	0.00009	0.00134	-0.00291	-0.00157	-0.76841
D28	-1.58469	0.00014	0.00173	-0.00092	0.00081	-1.58388
D29	0.52264	0.00009	0.00217	0.00219	0.00436	0.52700
D30	2.56371	0.00012	0.00141	0.00098	0.00239	2.56610
D31	-1.00193	0.00000	0.01061	0.00505	0.01566	-0.98627
D32	1.07413	-0.00020	0.00904	0.00160	0.01064	1.08476
D33	-3.09254	-0.00001	0.01024	0.00735	0.01760	-3.07494
D34	-3.09355	0.00013	0.01122	0.00463	0.01585	-3.07771
D35	-1.01749	-0.00007	0.00965	0.00118	0.01082	-1.00667
D36	1.09903	0.00012	0.01085	0.00693	0.01778	1.11681
D37	1.10758	0.00005	0.01117	0.00374	0.01491	1.12249
D38	-3.09955	-0.00015	0.00961	0.00029	0.00989	-3.08966
D39	-0.98302	0.00004	0.01080	0.00604	0.01685	-0.96618
D40	-0.68151	0.00035	-0.01562	0.05188	0.03627	-0.64524
D41	1.40898	0.00017	-0.01661	0.05017	0.03356	1.44254
D42	-2.71984	0.00007	-0.01762	0.04420	0.02658	-2.69326
D43	-2.74188	0.00035	0.03200	0.05757	0.08957	-2.65231
D44	1.46204	0.00019	0.03160	0.05915	0.09075	1.55279
D45	-0.66977	0.00017	0.03312	0.06622	0.09934	-0.57043
D46	-3.08698	-0.00004	0.00052	-0.00117	-0.00065	-3.08763
D47	0.05397	-0.00007	-0.00013	-0.00276	-0.00290	0.05108
D48	0.00854	-0.00007	0.00195	-0.00078	0.00118	0.00972
D49	-3.13369	-0.00011	0.00130	-0.00238	-0.00107	-3.13476

Item	Value	Threshold	Converged?
Maximum Force	0.001411	0.000450	NO
RMS Force	0.000267	0.000300	YES
Maximum Displacement	0.133603	0.001800	NO
RMS Displacement	0.028392	0.001200	NO

Predicted change in Energy=-9.097813D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.457289	-1.999667	-1.311125
2	6	0	-1.746933	-1.619980	-1.482358
3	7	0	-2.104174	-0.872868	-0.365255
4	6	0	-1.033015	-0.775846	0.444808
5	7	0	-0.034487	-1.492505	-0.088873
6	6	0	1.337539	-1.534277	0.431687
7	6	0	2.218148	-0.459695	-0.210757
8	1	0	0.196490	-2.570580	-1.946932
9	1	0	-2.425995	-1.773118	-2.301380
10	1	0	1.293524	-1.382136	1.510174
11	1	0	1.745011	-2.530049	0.246479
12	1	0	2.209690	-0.573837	-1.302920
13	1	0	1.816410	0.527739	0.035181
14	35	0	-0.468389	2.093754	0.443766
15	1	0	-1.015523	-0.286605	1.399943
16	6	0	-3.309107	-0.137616	-0.165188
17	6	0	-4.496895	-0.585248	-0.549545
18	1	0	-3.118573	0.827028	0.295355
19	1	0	-5.372299	0.035779	-0.418066
20	1	0	-4.637419	-1.560651	-1.000245
21	8	0	3.528059	-0.668291	0.309638
22	1	0	3.995577	0.171791	0.312768

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.355237	0.000000			
3	N	2.208297	1.390582	0.000000		
4	C	2.216416	2.221759	1.346476	0.000000	
5	N	1.389200	2.211453	2.178059	1.339953	0.000000
6	C	2.544679	3.631100	3.594158	2.488959	1.468054
7	C	3.277238	4.322627	4.344772	3.331633	2.481111
8	H	1.075927	2.212773	3.267566	3.233137	2.160551
9	H	2.215340	1.074882	2.159305	3.236741	3.270052
10	H	3.377339	4.272728	3.914197	2.629710	2.081525
11	H	2.749102	4.001347	4.235173	3.291503	2.087000
12	H	3.024208	4.096521	4.424710	3.689240	2.711861
13	H	3.656505	4.428661	4.182467	3.160119	2.742734
14	Br	4.453747	4.374523	3.482981	2.924621	3.651469
15	H	3.255165	3.258913	2.155177	1.073287	2.152487
16	C	3.593505	2.524426	1.425653	2.441317	3.544671
17	C	4.347298	3.082709	2.416982	3.608812	4.576944
18	H	4.201598	3.321071	2.086878	2.634596	3.878074
19	H	5.394249	4.125231	3.392502	4.498075	5.562038

20	H	4.214602	2.931017	2.700664	3.961796	4.692785
21	O	4.503602	5.651770	5.676212	4.564344	3.678297
22	H	5.213470	6.277687	6.225592	5.118807	4.378654

		6	7	8	9	10
6	C	0.000000				
7	C	1.530664	0.000000			
8	H	2.834387	3.399594	0.000000		
9	H	4.657348	5.259643	2.763875	0.000000	
10	H	1.090054	2.160424	3.816735	5.340003	0.000000
11	H	1.091741	2.172393	2.685258	4.945889	1.765919
12	H	2.166092	1.098143	2.907698	4.891296	3.066953
13	H	2.153705	1.094031	4.019016	5.362038	2.469137
14	Br	4.052670	3.763772	5.283324	5.130375	4.040220
15	H	2.833921	3.616759	4.229314	4.230714	2.558132
16	C	4.888583	5.536819	4.624191	2.831620	5.053700
17	C	5.992002	6.724755	5.284136	2.961180	6.197291
18	H	5.044927	5.512930	5.249880	3.739446	5.081613
19	H	6.943277	7.609426	6.335768	3.936964	7.082499
20	H	6.144205	6.988147	5.028206	2.574586	6.442838
21	O	2.358644	1.424848	4.450861	6.594605	2.635148
22	H	3.160692	1.957577	5.201913	7.200904	3.339096

		11	12	13	14	15
11	H	0.000000				
12	H	2.538371	0.000000			
13	H	3.065911	1.777259	0.000000		
14	Br	5.130070	4.164019	2.799938	0.000000	
15	H	3.739528	4.217816	3.247396	2.622926	0.000000
16	C	5.606899	5.651712	5.172405	3.663266	2.780712
17	C	6.586144	6.748776	6.437271	4.938884	4.001204
18	H	5.909891	5.736488	4.950892	2.941105	2.623569
19	H	7.594814	7.657752	7.219765	5.387611	4.731869
20	H	6.574912	6.924473	6.861880	5.728932	4.527938
21	O	2.578641	2.085033	2.106076	4.859885	4.688133
22	H	3.517013	2.521071	2.225426	4.861902	5.148126

		16	17	18	19	20
16	C	0.000000				
17	C	1.326252	0.000000			
18	H	1.085791	2.146660	0.000000		
19	H	2.085851	1.081339	2.492855	0.000000	
20	H	2.118198	1.083646	3.112312	1.851369	0.000000
21	O	6.874148	8.071243	6.812775	8.957770	8.317880
22	H	7.326840	8.569642	7.144283	9.397326	8.902471

		21	22
21	O	0.000000	

22 H 0.961416 0.000000

Stoichiometry C7H11BrN2O

Framework group C1[X(C7H11BrN2O)]

Deg. of freedom 60

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.103861	-2.272798	-0.633225
2	6	0	-1.407980	-1.924938	-0.755429
3	7	0	-1.637264	-0.881715	0.134981
4	6	0	-0.478790	-0.585236	0.753881
5	7	0	0.455929	-1.449394	0.335546
6	6	0	1.880162	-1.376038	0.683919
7	6	0	2.669252	-0.551763	-0.336297
8	1	0	0.475194	-3.017620	-1.150481
9	1	0	-2.177684	-2.287717	-1.412177
10	1	0	1.962546	-0.921903	1.671437
11	1	0	2.271603	-2.393343	0.745252
12	1	0	2.532815	-0.972047	-1.341615
13	1	0	2.290752	0.474706	-0.338140
14	35	0	0.056601	2.149833	-0.132777
15	1	0	-0.352859	0.155214	1.520576
16	6	0	-2.816513	-0.089524	0.254531
17	6	0	-4.037426	-0.597729	0.154311
18	1	0	-2.581358	0.961172	0.394816
19	1	0	-4.896571	0.057084	0.203140
20	1	0	-4.221667	-1.657203	0.020679
21	8	0	4.033249	-0.636729	0.066796
22	1	0	4.490486	0.157258	-0.224478

Rotational constants (GHZ): 0.8202195 0.5727689 0.3567439

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 867.4277501161 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 345 RedAO= T EigKep= 6.92D-06 NBF= 345
NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345
Initial guess from the checkpoint file: "."
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999995 0.002309 -0.000304 -0.001923 Ang= 0.35 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.33800221 A.U. after 12 cycles
NFock= 12 Conv=0.22D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000603255	0.000202041	-0.000330792
2	6	0.000895734	0.000184811	-0.000524094
3	7	-0.001356242	0.000411129	0.000122067
4	6	0.000701951	-0.000192070	0.000367674
5	7	0.000196614	-0.000065583	0.000202842
6	6	-0.000461795	-0.000177902	0.000510268
7	6	-0.000531523	0.000053755	-0.000088476
8	1	-0.000034781	-0.000130368	0.000034920
9	1	0.000025014	-0.000288516	0.000001397

10	1	0.000117414	0.000125852	-0.000066435
11	1	0.000043706	0.000091547	-0.000178306
12	1	0.000233488	-0.000257875	0.000012890
13	1	0.000253442	0.000120831	-0.000089980
14	35	0.000246317	0.000685233	-0.000035531
15	1	-0.000037603	-0.000117031	-0.000083292
16	6	0.000919718	-0.001005875	0.000311524
17	6	-0.000333374	0.000067677	-0.000277008
18	1	-0.000220544	0.000208968	0.000020599
19	1	-0.000005934	0.000245837	0.000114270
20	1	-0.000097357	-0.000092654	-0.000057965
21	8	0.000172065	0.000029386	-0.000206468
22	1	-0.000123056	-0.000099194	0.000239894

Cartesian Forces: Max 0.001356242 RMS 0.000361554

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.003558420 RMS 0.000633212
Search for a local minimum.
Step number 11 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 9 10 11
DE= -8.66D-05 DEPred=-9.10D-05 R= 9.52D-01
TightC=F SS= 1.41D+00 RLast= 1.96D-01 DXNew= 1.8091D+00 5.8942D-01
Trust test= 9.52D-01 RLast= 1.96D-01 DXMaxT set to 1.08D+00
ITU= 1 1 1 1 1 1 0 0 -1 0 0

Eigenvalues ---	0.00140	0.00337	0.00519	0.00710	0.01231
Eigenvalues ---	0.01602	0.01680	0.01880	0.02071	0.02172
Eigenvalues ---	0.02365	0.02442	0.03066	0.03081	0.03389
Eigenvalues ---	0.04181	0.04712	0.05442	0.05924	0.07180
Eigenvalues ---	0.08692	0.09339	0.13676	0.13860	0.15714
Eigenvalues ---	0.15814	0.15903	0.15987	0.16003	0.16337
Eigenvalues ---	0.16505	0.20691	0.21477	0.22792	0.22878
Eigenvalues ---	0.24138	0.24561	0.25617	0.29744	0.33133
Eigenvalues ---	0.33868	0.33875	0.33905	0.34114	0.34344
Eigenvalues ---	0.34563	0.34695	0.36131	0.36309	0.36407
Eigenvalues ---	0.37276	0.42576	0.42924	0.45674	0.49323
Eigenvalues ---	0.53540	0.54541	0.55749	0.60557	2.11977

En-DIIS/RFO-DIIS IScMMF= 0 using points: 11 10 9 8

RFO step: Lambda=-3.69876696D-05.

DidBck=F Rises=F RFO-DIIS coefs: 0.88555 0.36771 -0.29452 0.04127

Iteration 1 RMS(Cart)= 0.00807372 RMS(Int)= 0.00015701

Iteration 2 RMS(Cart)= 0.00015876 RMS(Int)= 0.00001786

Iteration 3 RMS(Cart)= 0.00000007 RMS(Int)= 0.00001786

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56103	-0.00054	0.00030	-0.00103	-0.00074	2.56028
R2	2.62521	0.00033	-0.00009	0.00064	0.00052	2.62573
R3	2.03321	0.00003	-0.00003	0.00013	0.00010	2.03331
R4	2.62782	0.00050	-0.00028	0.00217	0.00191	2.62973
R5	2.03123	0.00002	-0.00001	0.00002	0.00001	2.03125
R6	2.54447	0.00073	-0.00039	0.00094	0.00056	2.54504
R7	2.69409	-0.00053	0.00084	-0.00174	-0.00090	2.69320
R8	2.53214	-0.00024	0.00011	-0.00118	-0.00108	2.53106
R9	2.02822	-0.00013	0.00015	-0.00008	0.00006	2.02828
R10	2.77422	-0.00005	0.00032	-0.00009	0.00023	2.77445
R11	2.89254	0.00064	-0.00008	0.00108	0.00100	2.89354
R12	2.05990	-0.00006	0.00000	-0.00019	-0.00019	2.05971
R13	2.06309	-0.00004	0.00004	-0.00032	-0.00027	2.06282
R14	2.07519	0.00002	0.00008	-0.00036	-0.00028	2.07491
R15	2.06742	0.00053	-0.00011	-0.00017	-0.00028	2.06714
R16	2.69257	0.00005	-0.00012	0.00063	0.00052	2.69309
R17	5.29112	0.00019	0.00215	0.00148	0.00363	5.29475
R18	2.50625	0.00040	-0.00018	0.00062	0.00044	2.50669
R19	2.05185	0.00015	0.00003	0.00026	0.00029	2.05214
R20	2.04343	0.00015	-0.00009	0.00023	0.00014	2.04358
R21	2.04779	0.00013	-0.00006	0.00000	-0.00007	2.04773
R22	1.81681	-0.00013	0.00001	-0.00018	-0.00017	1.81664
A1	1.87392	0.00025	-0.00013	0.00015	0.00001	1.87393
A2	2.28132	-0.00014	0.00007	-0.00016	-0.00008	2.28124
A3	2.12787	-0.00011	-0.00001	0.00011	0.00011	2.12798
A4	1.86867	0.00004	0.00004	0.00015	0.00020	1.86887
A5	2.28834	-0.00018	0.00034	-0.00131	-0.00100	2.28734
A6	2.12511	0.00016	-0.00028	0.00155	0.00123	2.12634
A7	1.89404	-0.00027	0.00003	-0.00111	-0.00110	1.89294
A8	2.22301	0.00034	-0.00057	0.00223	0.00156	2.22457
A9	2.15409	-0.00007	0.00012	-0.00124	-0.00123	2.15286
A10	1.89091	0.00001	0.00008	0.00051	0.00059	1.89149
A11	2.19100	-0.00003	0.00014	-0.00010	-0.00001	2.19099
A12	2.19702	-0.00001	0.00004	-0.00008	-0.00009	2.19693
A13	1.89534	-0.00004	0.00007	0.00017	0.00022	1.89556
A14	2.19695	-0.00041	-0.00008	0.00054	0.00047	2.19742
A15	2.17784	0.00050	0.00016	-0.00053	-0.00037	2.17747

A16	1.94859	0.00220	-0.00004	0.00123	0.00120	1.94979
A17	1.88506	-0.00042	-0.00049	0.00020	-0.00028	1.88478
A18	1.89085	-0.00082	0.00029	-0.00005	0.00023	1.89108
A19	1.91825	-0.00028	0.00023	0.00021	0.00044	1.91869
A20	1.93307	-0.00111	0.00030	-0.00321	-0.00290	1.93016
A21	1.88622	0.00039	-0.00032	0.00172	0.00140	1.88761
A22	1.91774	-0.00038	0.00008	0.00060	0.00068	1.91842
A23	1.90500	0.00284	-0.00060	0.00231	0.00170	1.90671
A24	1.84713	-0.00120	0.00070	-0.00165	-0.00096	1.84617
A25	1.89079	-0.00046	-0.00032	0.00075	0.00043	1.89122
A26	1.93382	0.00032	0.00008	-0.00167	-0.00159	1.93223
A27	1.96884	-0.00106	0.00009	-0.00028	-0.00020	1.96865
A28	2.56305	0.00356	-0.00132	-0.00209	-0.00341	2.55964
A29	2.14385	0.00063	-0.00092	0.00284	0.00192	2.14577
A30	1.94916	-0.00004	-0.00051	-0.00061	-0.00112	1.94804
A31	2.18945	-0.00059	0.00147	-0.00239	-0.00093	2.18853
A32	2.08973	-0.00033	0.00067	-0.00287	-0.00219	2.08754
A33	2.14180	0.00024	-0.00048	0.00158	0.00110	2.14290
A34	2.05165	0.00009	-0.00019	0.00129	0.00110	2.05274
A35	1.89686	0.00004	-0.00014	0.00196	0.00183	1.89869
D1	0.00702	-0.00019	-0.00590	0.00134	-0.00456	0.00246
D2	3.09845	0.00020	-0.00371	0.01042	0.00671	3.10516
D3	-3.12125	-0.00032	-0.00165	-0.00715	-0.00881	-3.13006
D4	-0.02982	0.00007	0.00054	0.00193	0.00247	-0.02735
D5	-0.04073	0.00002	0.00508	-0.00228	0.00280	-0.03793
D6	-3.01540	-0.00031	0.00411	-0.00335	0.00076	-3.01464
D7	3.08896	0.00013	0.00129	0.00530	0.00659	3.09556
D8	0.11429	-0.00020	0.00032	0.00423	0.00455	0.11884
D9	0.02889	0.00028	0.00472	0.00001	0.00473	0.03362
D10	3.00726	0.00029	0.00046	-0.00097	-0.00050	3.00676
D11	-3.06825	-0.00006	0.00275	-0.00795	-0.00521	-3.07346
D12	-0.08989	-0.00004	-0.00151	-0.00892	-0.01044	-0.10032
D13	-0.05461	-0.00027	-0.00157	-0.00144	-0.00302	-0.05763
D14	-3.10174	0.00004	-0.00342	-0.00514	-0.00857	-3.11031
D15	-3.04085	-0.00033	0.00253	-0.00091	0.00163	-3.03921
D16	0.19521	-0.00002	0.00069	-0.00461	-0.00392	0.19129
D17	0.69438	-0.00014	0.00826	-0.01284	-0.00459	0.68979
D18	-2.40843	-0.00004	0.00724	-0.00851	-0.00128	-2.40970
D19	-2.63289	-0.00013	0.00339	-0.01387	-0.01047	-2.64337
D20	0.54749	-0.00004	0.00237	-0.00954	-0.00716	0.54033
D21	0.05900	0.00015	-0.00212	0.00231	0.00019	0.05920
D22	3.03594	0.00037	-0.00119	0.00350	0.00231	3.03825
D23	3.10572	-0.00016	-0.00025	0.00603	0.00578	3.11149
D24	-0.20053	0.00006	0.00068	0.00721	0.00789	-0.19264

D25	1.36479	-0.00065	0.00213	-0.00373	-0.00160	1.36319
D26	-2.80752	0.00008	0.00207	-0.00257	-0.00051	-2.80802
D27	-0.76841	-0.00012	0.00158	-0.00046	0.00111	-0.76730
D28	-1.58388	-0.00096	0.00102	-0.00505	-0.00403	-1.58791
D29	0.52700	-0.00023	0.00096	-0.00390	-0.00294	0.52406
D30	2.56610	-0.00043	0.00047	-0.00179	-0.00132	2.56478
D31	-0.98627	-0.00003	0.00690	-0.00291	0.00399	-0.98228
D32	1.08476	0.00089	0.00619	-0.00026	0.00594	1.09070
D33	-3.07494	0.00049	0.00636	-0.00029	0.00607	-3.06886
D34	-3.07771	-0.00073	0.00739	-0.00410	0.00328	-3.07442
D35	-1.00667	0.00019	0.00668	-0.00145	0.00523	-1.00144
D36	1.11681	-0.00022	0.00685	-0.00148	0.00537	1.12218
D37	1.12249	-0.00034	0.00745	-0.00435	0.00310	1.12559
D38	-3.08966	0.00058	0.00674	-0.00169	0.00505	-3.08461
D39	-0.96618	0.00018	0.00691	-0.00173	0.00518	-0.96099
D40	-0.64524	-0.00057	-0.01480	0.00343	-0.01138	-0.65662
D41	1.44254	0.00033	-0.01525	0.00592	-0.00932	1.43322
D42	-2.69326	-0.00029	-0.01532	0.00415	-0.01118	-2.70444
D43	-2.65231	-0.00089	0.01411	0.03040	0.04450	-2.60781
D44	1.55279	0.00010	0.01356	0.03155	0.04511	1.59791
D45	-0.57043	0.00121	0.01386	0.03200	0.04586	-0.52458
D46	-3.08763	0.00002	0.00035	0.00100	0.00134	-3.08629
D47	0.05108	0.00005	-0.00012	0.00206	0.00193	0.05301
D48	0.00972	-0.00007	0.00143	-0.00387	-0.00243	0.00729
D49	-3.13476	-0.00003	0.00097	-0.00281	-0.00184	-3.13660

Item	Value	Threshold	Converged?
Maximum Force	0.003558	0.000450	NO
RMS Force	0.000633	0.000300	NO
Maximum Displacement	0.055547	0.001800	NO
RMS Displacement	0.008102	0.001200	NO

Predicted change in Energy=-3.441641D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.457755	-2.000144	-1.312536
2	6	0	-1.747178	-1.620935	-1.483378
3	7	0	-2.106355	-0.877462	-0.363211
4	6	0	-1.033328	-0.778057	0.444584
5	7	0	-0.034332	-1.491814	-0.090670
6	6	0	1.338044	-1.531809	0.429445

7	6	0	2.219599	-0.458395	-0.214915
8	1	0	0.194716	-2.574410	-1.946758
9	1	0	-2.427532	-1.780048	-2.300193
10	1	0	1.294012	-1.378464	1.507656
11	1	0	1.747049	-2.526723	0.243862
12	1	0	2.208689	-0.571445	-1.307019
13	1	0	1.823080	0.530470	0.033077
14	35	0	-0.460683	2.103735	0.432693
15	1	0	-1.013537	-0.284748	1.397617
16	6	0	-3.310738	-0.143085	-0.160012
17	6	0	-4.499298	-0.584529	-0.549892
18	1	0	-3.118905	0.818902	0.305878
19	1	0	-5.371839	0.039841	-0.414639
20	1	0	-4.643053	-1.556227	-1.007440
21	8	0	3.530704	-0.672790	0.300844
22	1	0	3.988988	0.171258	0.342162

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.354842	0.000000			
3	N	2.208963	1.391594	0.000000		
4	C	2.216360	2.221949	1.346775	0.000000	
5	N	1.389476	2.211368	2.178299	1.339380	0.000000
6	C	2.545335	3.631174	3.594490	2.488328	1.468174
7	C	3.278717	4.323865	4.348734	3.334465	2.482659
8	H	1.075982	2.212417	3.268361	3.233186	2.160912
9	H	2.214482	1.074889	2.160952	3.237529	3.269935
10	H	3.377671	4.272460	3.913266	2.628141	2.081344
11	H	2.749695	4.001679	4.235248	3.290687	2.087167
12	H	3.025085	4.096512	4.427644	3.690729	2.712513
13	H	3.662908	4.435642	4.192825	3.168698	2.748623
14	Br	4.459558	4.381730	3.497033	2.938161	3.658368
15	H	3.255212	3.259410	2.155476	1.073321	2.151941
16	C	3.593952	2.525877	1.425179	2.440353	3.543827
17	C	4.349674	3.085401	2.418023	3.611009	4.579299
18	H	4.200953	3.322029	2.085806	2.630428	3.874436
19	H	5.395922	4.127777	3.392266	4.497766	5.562365
20	H	4.219818	2.935438	2.703810	3.967876	4.699460
21	O	4.502519	5.651413	5.679727	4.567508	3.678800
22	H	5.217906	6.280776	6.224996	5.112274	4.374958

		6	7	8	9	10
6	C	0.000000				
7	C	1.531194	0.000000			

8	H	2.835587	3.402492	0.000000		
9	H	4.657479	5.262222	2.762628	0.000000	
10	H	1.089952	2.161131	3.817292	5.339558	0.000000
11	H	1.091595	2.170659	2.685299	4.945389	1.766612
12	H	2.166940	1.097995	2.911567	4.893022	3.067623
13	H	2.155311	1.093884	4.026363	5.371252	2.469479
14	Br	4.056182	3.764016	5.289270	5.140129	4.044776
15	H	2.832394	3.617123	4.229335	4.231915	2.555994
16	C	4.887452	5.539590	4.625150	2.835503	5.050842
17	C	5.994248	6.728425	5.286268	2.963956	6.198894
18	H	5.040388	5.513832	5.250621	3.744883	5.074104
19	H	6.942989	7.610391	6.337841	3.941605	7.080987
20	H	6.151322	6.994950	5.032199	2.574848	6.450275
21	O	2.358434	1.425121	4.449348	6.594846	2.637644
22	H	3.152072	1.958963	5.212902	7.208423	3.320077

		11	12	13	14	15
11	H	0.000000				
12	H	2.538002	0.000000			
13	H	3.065394	1.777293	0.000000		
14	Br	5.133311	4.160376	2.801861	0.000000	
15	H	3.738775	4.216633	3.251607	2.634688	0.000000
16	C	5.605894	5.653600	5.181413	3.677270	2.779102
17	C	6.589311	6.750593	6.446359	4.950016	4.004147
18	H	5.905469	5.737401	4.957906	2.955170	2.615819
19	H	7.596015	7.657311	7.225512	5.394171	4.731218
20	H	6.583390	6.928630	6.873708	5.741213	4.535895
21	O	2.573274	2.084039	2.106066	4.863912	4.690802
22	H	3.509281	2.537887	2.217144	4.852034	5.132951

		16	17	18	19	20
16	C	0.000000				
17	C	1.326483	0.000000			
18	H	1.085943	2.146496	0.000000		
19	H	2.084810	1.081415	2.490339	0.000000	
20	H	2.119002	1.083611	3.112727	1.852019	0.000000
21	O	6.877376	8.075425	6.814872	8.959634	8.324805
22	H	7.323728	8.568430	7.137430	9.392289	8.906052

		21	22
21	O	0.000000	
22	H	0.961326	0.000000

Stoichiometry C7H11BrN2O

Framework group C1[X(C7H11BrN2O)]

Deg. of freedom 60

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.111447	-2.272002	-0.638181
2	6	0	-1.414266	-1.920674	-0.759957
3	7	0	-1.643347	-0.882812	0.138318
4	6	0	-0.483197	-0.590066	0.756503
5	7	0	0.449999	-1.452716	0.333515
6	6	0	1.874330	-1.382780	0.682692
7	6	0	2.667342	-0.558378	-0.335173
8	1	0	0.465145	-3.019090	-1.155036
9	1	0	-2.185193	-2.284059	-1.414945
10	1	0	1.956780	-0.931515	1.671406
11	1	0	2.264559	-2.400640	0.739814
12	1	0	2.528455	-0.973376	-1.342188
13	1	0	2.296905	0.470870	-0.332580
14	35	0	0.066787	2.155371	-0.133939
15	1	0	-0.354161	0.150403	1.522710
16	6	0	-2.819757	-0.088015	0.262790
17	6	0	-4.043324	-0.588281	0.152449
18	1	0	-2.580110	0.960451	0.412988
19	1	0	-4.897561	0.072745	0.205173
20	1	0	-4.234187	-1.645045	0.007421
21	8	0	4.031362	-0.655282	0.066112
22	1	0	4.486258	0.153406	-0.185365

Rotational constants (GHZ): 0.8166874 0.5720897 0.3559362

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 866.5752417039 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 6.91D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Initial guess from the checkpoint file: "."
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999999 -0.000381 0.000103 0.001656 Ang= -0.20 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.33804165 A.U. after 10 cycles
NFock= 10 Conv=0.53D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000261713	0.000332810	-0.000053236
2	6	0.000118837	-0.000111186	0.000194247
3	7	-0.000419959	0.000396227	-0.000440933
4	6	0.000375589	-0.000076505	0.000073387
5	7	0.000286205	-0.000331349	0.000097580
6	6	-0.000446036	0.000056503	0.000140759
7	6	-0.000349897	-0.000003553	0.000193384
8	1	0.000019565	0.000058126	-0.000013174
9	1	-0.000019355	-0.000088703	0.000011845
10	1	0.000163521	0.000071023	-0.000041119
11	1	-0.000034350	-0.000055163	-0.000049517
12	1	0.000190250	-0.000219751	0.000048307
13	1	0.000128214	0.000085704	-0.000152343
14	35	0.000067353	0.000089025	0.000065321
15	1	-0.000046066	0.000054837	-0.000056660

16	6	0.000710240	-0.000670113	0.000066432
17	6	-0.000041827	0.000259189	-0.000017387
18	1	-0.000369490	0.000145614	0.000006007
19	1	-0.000055921	0.000090341	0.000068106
20	1	-0.000081195	-0.000066013	-0.000084601
21	8	0.000261536	0.000045019	-0.000143248
22	1	-0.000195502	-0.000062082	0.000086842

Cartesian Forces: Max 0.000710240 RMS 0.000216034

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000608714 RMS 0.000150239

Search for a local minimum.

Step number 12 out of a maximum of 116

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 9 10 11 12

DE= -3.94D-05 DEPred=-3.44D-05 R= 1.15D+00

TightC=F SS= 1.41D+00 RLast= 8.70D-02 DXNew= 1.8091D+00 2.6094D-01

Trust test= 1.15D+00 RLast= 8.70D-02 DXMaxT set to 1.08D+00

ITU= 1 1 1 1 1 1 1 0 0 -1 0 0

Eigenvalues ---	0.00150	0.00290	0.00498	0.00703	0.01243
Eigenvalues ---	0.01596	0.01739	0.01915	0.02077	0.02160
Eigenvalues ---	0.02364	0.02419	0.03065	0.03074	0.03484
Eigenvalues ---	0.04340	0.04716	0.05434	0.05924	0.07036
Eigenvalues ---	0.08699	0.09259	0.13649	0.14126	0.15541
Eigenvalues ---	0.15755	0.15911	0.15993	0.16004	0.16285
Eigenvalues ---	0.16925	0.20775	0.21156	0.22781	0.22883
Eigenvalues ---	0.24100	0.24730	0.25597	0.29806	0.33129
Eigenvalues ---	0.33868	0.33878	0.33911	0.34113	0.34290
Eigenvalues ---	0.34511	0.34684	0.36132	0.36310	0.36419
Eigenvalues ---	0.37274	0.42648	0.43063	0.46099	0.49421
Eigenvalues ---	0.53477	0.54503	0.55690	0.60534	2.15401

En-DIIS/RFO-DIIS IScMMF= 0 using points: 12 11 10 9 8

RFO step: Lambda=-5.14502031D-06.

DidBck=F Rises=F RFO-DIIS coefs: 1.48383 -0.34244 -0.29336 0.15319 -0.00122

Iteration 1 RMS(Cart)= 0.00975941 RMS(Int)= 0.00008715

Iteration 2 RMS(Cart)= 0.00015077 RMS(Int)= 0.00000846

Iteration 3 RMS(Cart)= 0.00000002 RMS(Int)= 0.00000846

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56028	-0.00017	-0.00057	-0.00006	-0.00062	2.55966
R2	2.62573	0.00001	0.00037	-0.00003	0.00035	2.62608
R3	2.03331	-0.00001	0.00007	-0.00006	0.00001	2.03332
R4	2.62973	-0.00015	0.00130	-0.00057	0.00073	2.63046
R5	2.03125	0.00002	-0.00001	0.00002	0.00000	2.03125
R6	2.54504	0.00033	0.00053	0.00033	0.00085	2.54588
R7	2.69320	-0.00028	-0.00079	-0.00041	-0.00119	2.69201
R8	2.53106	-0.00008	-0.00072	-0.00005	-0.00076	2.53030
R9	2.02828	-0.00003	-0.00002	0.00012	0.00010	2.02838
R10	2.77445	-0.00017	0.00007	-0.00031	-0.00024	2.77421
R11	2.89354	0.00002	0.00074	-0.00025	0.00049	2.89403
R12	2.05971	-0.00004	-0.00008	-0.00019	-0.00027	2.05944
R13	2.06282	0.00004	-0.00019	0.00020	0.00002	2.06283
R14	2.07491	-0.00002	-0.00026	-0.00006	-0.00032	2.07459
R15	2.06714	0.00008	-0.00011	-0.00009	-0.00020	2.06694
R16	2.69309	0.00003	0.00033	0.00013	0.00047	2.69355
R17	5.29475	0.00002	0.00072	0.00175	0.00247	5.29722
R18	2.50669	0.00009	0.00028	-0.00004	0.00024	2.50693
R19	2.05214	0.00006	0.00004	0.00010	0.00014	2.05227
R20	2.04358	0.00010	0.00010	0.00012	0.00022	2.04379
R21	2.04773	0.00012	-0.00006	0.00022	0.00016	2.04788
R22	1.81664	-0.00013	-0.00010	-0.00023	-0.00033	1.81631
A1	1.87393	0.00017	0.00008	0.00046	0.00056	1.87449
A2	2.28124	-0.00007	-0.00010	-0.00013	-0.00026	2.28099
A3	2.12798	-0.00010	0.00009	-0.00034	-0.00028	2.12770
A4	1.86887	0.00002	0.00008	-0.00009	-0.00002	1.86884
A5	2.28734	-0.00003	-0.00086	0.00015	-0.00072	2.28662
A6	2.12634	0.00002	0.00096	0.00000	0.00095	2.12729
A7	1.89294	-0.00009	-0.00065	-0.00012	-0.00076	1.89218
A8	2.22457	0.00011	0.00109	0.00052	0.00164	2.22621
A9	2.15286	-0.00001	-0.00085	0.00016	-0.00066	2.15221
A10	1.89149	0.00004	0.00034	0.00031	0.00065	1.89215
A11	2.19099	-0.00009	-0.00003	-0.00054	-0.00055	2.19045
A12	2.19693	0.00004	-0.00013	0.00030	0.00020	2.19712
A13	1.89556	-0.00015	0.00009	-0.00059	-0.00049	1.89507
A14	2.19742	0.00002	0.00016	0.00045	0.00061	2.19803
A15	2.17747	0.00013	-0.00017	0.00014	-0.00004	2.17743
A16	1.94979	0.00030	0.00075	0.00007	0.00082	1.95061
A17	1.88478	0.00008	0.00000	0.00081	0.00081	1.88559
A18	1.89108	-0.00018	-0.00017	-0.00007	-0.00023	1.89085
A19	1.91869	-0.00013	0.00026	-0.00059	-0.00033	1.91836
A20	1.93016	-0.00014	-0.00168	-0.00024	-0.00192	1.92824

A21	1.88761	0.00007	0.00087	0.00005	0.00092	1.88854
A22	1.91842	-0.00016	0.00020	-0.00057	-0.00037	1.91805
A23	1.90671	0.00043	0.00153	0.00025	0.00178	1.90848
A24	1.84617	0.00003	-0.00065	0.00169	0.00104	1.84721
A25	1.89122	0.00006	0.00006	0.00125	0.00131	1.89253
A26	1.93223	-0.00005	-0.00103	-0.00172	-0.00275	1.92948
A27	1.96865	-0.00031	-0.00007	-0.00092	-0.00098	1.96766
A28	2.55964	0.00061	-0.00124	-0.00097	-0.00221	2.55743
A29	2.14577	0.00032	0.00156	0.00097	0.00253	2.14831
A30	1.94804	0.00025	-0.00046	0.00172	0.00126	1.94930
A31	2.18853	-0.00057	-0.00119	-0.00264	-0.00383	2.18470
A32	2.08754	-0.00011	-0.00151	-0.00022	-0.00173	2.08581
A33	2.14290	0.00012	0.00094	0.00052	0.00147	2.14436
A34	2.05274	-0.00002	0.00057	-0.00030	0.00027	2.05301
A35	1.89869	-0.00021	0.00128	-0.00153	-0.00025	1.89844
D1	0.00246	0.00008	0.00127	-0.00103	0.00024	0.00269
D2	3.10516	0.00012	0.00626	0.00079	0.00704	3.11220
D3	-3.13006	-0.00001	-0.00415	0.00036	-0.00379	-3.13384
D4	-0.02735	0.00002	0.00084	0.00218	0.00301	-0.02434
D5	-0.03793	-0.00013	-0.00133	0.00052	-0.00080	-0.03873
D6	-3.01464	-0.00015	-0.00180	0.00055	-0.00124	-3.01589
D7	3.09556	-0.00004	0.00351	-0.00072	0.00279	3.09835
D8	0.11884	-0.00007	0.00304	-0.00069	0.00235	0.12119
D9	0.03362	-0.00002	-0.00081	0.00119	0.00038	0.03400
D10	3.00676	0.00008	-0.00304	0.00480	0.00176	3.00852
D11	-3.07346	-0.00005	-0.00518	-0.00043	-0.00562	-3.07907
D12	-0.10032	0.00005	-0.00740	0.00318	-0.00424	-0.10456
D13	-0.05763	-0.00006	-0.00002	-0.00089	-0.00091	-0.05854
D14	-3.11031	0.00003	-0.00279	-0.00178	-0.00456	-3.11487
D15	-3.03921	-0.00017	0.00189	-0.00437	-0.00249	-3.04171
D16	0.19129	-0.00008	-0.00088	-0.00525	-0.00614	0.18515
D17	0.68979	-0.00012	-0.00864	-0.00720	-0.01584	0.67395
D18	-2.40970	-0.00010	-0.00651	-0.00835	-0.01486	-2.42456
D19	-2.64337	-0.00001	-0.01112	-0.00311	-0.01423	-2.65760
D20	0.54033	0.00001	-0.00899	-0.00426	-0.01326	0.52707
D21	0.05920	0.00011	0.00084	0.00022	0.00106	0.06026
D22	3.03825	0.00012	0.00134	0.00023	0.00157	3.03982
D23	3.11149	0.00001	0.00363	0.00106	0.00468	3.11618
D24	-0.19264	0.00002	0.00413	0.00107	0.00519	-0.18745
D25	1.36319	-0.00015	-0.00220	-0.00733	-0.00953	1.35366
D26	-2.80802	-0.00008	-0.00142	-0.00748	-0.00890	-2.81692
D27	-0.76730	-0.00005	-0.00047	-0.00702	-0.00750	-0.77480
D28	-1.58791	-0.00015	-0.00277	-0.00724	-0.01001	-1.59793
D29	0.52406	-0.00008	-0.00199	-0.00739	-0.00938	0.51468

D30	2.56478	-0.00005	-0.00105	-0.00693	-0.00798	2.55681
D31	-0.98228	0.00000	-0.00183	-0.00182	-0.00365	-0.98594
D32	1.09070	0.00024	-0.00072	-0.00048	-0.00120	1.08950
D33	-3.06886	0.00013	-0.00034	-0.00045	-0.00079	-3.06966
D34	-3.07442	-0.00020	-0.00249	-0.00249	-0.00498	-3.07941
D35	-1.00144	0.00004	-0.00138	-0.00115	-0.00253	-1.00397
D36	1.12218	-0.00008	-0.00100	-0.00112	-0.00212	1.12006
D37	1.12559	-0.00012	-0.00269	-0.00203	-0.00471	1.12088
D38	-3.08461	0.00013	-0.00157	-0.00069	-0.00226	-3.08687
D39	-0.96099	0.00001	-0.00119	-0.00066	-0.00185	-0.96284
D40	-0.65662	0.00006	0.00816	0.02140	0.02957	-0.62705
D41	1.43322	0.00016	0.00932	0.02160	0.03093	1.46415
D42	-2.70444	-0.00007	0.00801	0.01970	0.02771	-2.67672
D43	-2.60781	-0.00011	0.01639	0.01932	0.03571	-2.57210
D44	1.59791	0.00008	0.01709	0.01992	0.03701	1.63492
D45	-0.52458	0.00026	0.01781	0.02019	0.03800	-0.48658
D46	-3.08629	-0.00005	0.00028	-0.00187	-0.00158	-3.08787
D47	0.05301	-0.00002	0.00064	-0.00133	-0.00069	0.05232
D48	0.00729	-0.00005	-0.00210	-0.00043	-0.00254	0.00475
D49	-3.13660	-0.00002	-0.00175	0.00010	-0.00165	-3.13825

Item	Value	Threshold	Converged?
Maximum Force	0.000609	0.000450	NO
RMS Force	0.000150	0.000300	YES
Maximum Displacement	0.039413	0.001800	NO
RMS Displacement	0.009770	0.001200	NO

Predicted change in Energy=-1.438608D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.457534	-1.997269	-1.312421
2	6	0	-1.747650	-1.621172	-1.482319
3	7	0	-2.108112	-0.879052	-0.361188
4	6	0	-1.033849	-0.777663	0.445463
5	7	0	-0.034047	-1.489168	-0.090272
6	6	0	1.338228	-1.527544	0.429873
7	6	0	2.222929	-0.461550	-0.223054
8	1	0	0.194858	-2.572192	-1.946139
9	1	0	-2.429172	-1.786524	-2.296922
10	1	0	1.295545	-1.365796	1.506767
11	1	0	1.745716	-2.524244	0.250596

12	1	0	2.214804	-0.586130	-1.313758
13	1	0	1.829659	0.531021	0.014626
14	35	0	-0.452981	2.101668	0.439327
15	1	0	-1.013447	-0.281425	1.397023
16	6	0	-3.313704	-0.148994	-0.154061
17	6	0	-4.501317	-0.583116	-0.555317
18	1	0	-3.126467	0.807181	0.325628
19	1	0	-5.372839	0.041184	-0.412474
20	1	0	-4.645909	-1.547365	-1.028296
21	8	0	3.533819	-0.673335	0.295006
22	1	0	3.981819	0.174606	0.359065

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.354516	0.000000			
3	N	2.208996	1.391981	0.000000		
4	C	2.215792	2.222018	1.347222	0.000000	
5	N	1.389660	2.211708	2.178849	1.338975	0.000000
6	C	2.545779	3.631513	3.594938	2.487833	1.468047
7	C	3.275673	4.323883	4.353310	3.339677	2.483460
8	H	1.075988	2.211991	3.268404	3.232618	2.160921
9	H	2.213823	1.074891	2.161863	3.238117	3.270221
10	H	3.379329	4.273276	3.912934	2.626469	2.081723
11	H	2.752279	4.002767	4.234729	3.288540	2.086895
12	H	3.022037	4.098874	4.436305	3.699364	2.714725
13	H	3.658491	4.435078	4.199475	3.177728	2.750558
14	Br	4.457570	4.385024	3.502139	2.937345	3.653777
15	H	3.254880	3.259538	2.155633	1.073375	2.151723
16	C	3.593831	2.526678	1.424548	2.439753	3.543485
17	C	4.350312	3.085381	2.419234	3.614242	4.581888
18	H	4.203730	3.326666	2.086179	2.627764	3.874178
19	H	5.396797	4.129163	3.392330	4.498155	5.563136
20	H	4.222040	2.934534	2.707783	3.976354	4.706649
21	O	4.501947	5.652539	5.683687	4.571336	3.680176
22	H	5.217160	6.280313	6.222236	5.105997	4.370038

		6	7	8	9	10
6	C	0.000000				
7	C	1.531454	0.000000			
8	H	2.836198	3.396602	0.000000		
9	H	4.657873	5.262939	2.761495	0.000000	
10	H	1.089810	2.161015	3.819616	5.340279	0.000000
11	H	1.091603	2.169512	2.689444	4.946086	1.767094
12	H	2.166771	1.097825	2.902504	4.896333	3.067292

13	H	2.156763	1.093778	4.018346	5.371397	2.471777
14	Br	4.047184	3.764217	5.287260	5.148828	4.027416
15	H	2.831707	3.623703	4.228989	4.232591	2.553301
16	C	4.886905	5.545877	4.625304	2.838266	5.048180
17	C	5.996902	6.733547	5.286290	2.962290	6.202289
18	H	5.039376	5.525103	5.254739	3.753837	5.066666
19	H	6.943261	7.614743	6.338857	3.944215	7.080283
20	H	6.159265	7.000596	5.032467	2.565255	6.462227
21	O	2.359763	1.425368	4.447140	6.596555	2.637753
22	H	3.144980	1.958890	5.215356	7.211179	3.302443

		11	12	13	14	15
11	H	0.000000				
12	H	2.534469	0.000000			
13	H	3.065514	1.777911	0.000000		
14	Br	5.125325	4.173086	2.803168	0.000000	
15	H	3.735975	4.226439	3.264099	2.628772	0.000000
16	C	5.603864	5.665720	5.190863	3.687997	2.777514
17	C	6.591123	6.758811	6.453480	4.958469	4.008477
18	H	5.902728	5.758306	4.973547	2.972566	2.607260
19	H	7.595716	7.666692	7.231758	5.401496	4.731031
20	H	6.591110	6.933603	6.880433	5.748914	4.547478
21	O	2.573936	2.082193	2.105528	4.859635	4.695281
22	H	3.506524	2.549391	2.208498	4.836059	5.122304

		16	17	18	19	20
16	C	0.000000				
17	C	1.326610	0.000000			
18	H	1.086016	2.144576	0.000000		
19	H	2.083982	1.081529	2.485504	0.000000	
20	H	2.120024	1.083694	3.112187	1.852337	0.000000
21	O	6.882235	8.080508	6.822923	8.963237	8.332047
22	H	7.320701	8.565853	7.136456	9.387369	8.906607

		21	22
21	O	0.000000	
22	H	0.961151	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.120950	-2.270130	-0.634935
2	6	0	-1.423046	-1.917398	-0.756744
3	7	0	-1.650497	-0.877588	0.140291
4	6	0	-0.488771	-0.585728	0.756909
5	7	0	0.442581	-1.450543	0.335562
6	6	0	1.866761	-1.383007	0.685296
7	6	0	2.665494	-0.573378	-0.340316
8	1	0	0.453511	-3.020889	-1.148848
9	1	0	-2.195556	-2.285078	-1.407461
10	1	0	1.951108	-0.921998	1.669187
11	1	0	2.252748	-2.401918	0.751870
12	1	0	2.528971	-1.001078	-1.342141
13	1	0	2.300532	0.457651	-0.351741
14	35	0	0.080039	2.154693	-0.134462
15	1	0	-0.357421	0.158520	1.519127
16	6	0	-2.825042	-0.081521	0.267005
17	6	0	-4.050623	-0.574148	0.143864
18	1	0	-2.584896	0.964966	0.430180
19	1	0	-4.900758	0.091930	0.201436
20	1	0	-4.247610	-1.627807	-0.015483
21	8	0	4.028910	-0.670757	0.063773
22	1	0	4.479198	0.146269	-0.167575

Rotational constants (GHZ): 0.8172623 0.5713390 0.3557519

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 866.4421146724 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 6.84D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Initial guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999998 0.000437 0.000157 0.002115 Ang= 0.25 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.33807180 A.U. after 11 cycles
NFock= 11 Conv=0.22D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000028937	0.000024788	0.000054720
2	6	-0.000229770	-0.000174578	0.000389431
3	7	0.000078115	0.000372528	-0.000502134
4	6	-0.000023411	0.000127124	0.000193540
5	7	0.000151796	-0.000282838	-0.000079606
6	6	-0.000225629	0.000102146	-0.000101826
7	6	-0.000094031	-0.000041958	0.000169642
8	1	0.000028339	0.000107881	-0.000055386
9	1	0.000009271	0.000090577	-0.000031494
10	1	0.000045410	0.000051645	-0.000003068
11	1	-0.000057074	-0.000102589	0.000081436
12	1	0.000088778	-0.000098142	-0.000002806
13	1	-0.000046256	-0.000015653	-0.000147003
14	35	0.000056816	0.000093275	0.000052993
15	1	-0.000062210	-0.000046661	-0.000016774
16	6	0.000480023	-0.000371582	0.000058120
17	6	0.000003487	0.000201765	0.000074216
18	1	-0.000226085	-0.000028710	-0.000044927
19	1	-0.000030665	-0.000010456	-0.000032985
20	1	-0.000045467	0.000003392	-0.000035550

```
      21        8             0.000165763     -0.000006106     -0.000086345
      22        1            -0.000096136      0.000004154      0.000065805
 ---------------------------------------------------------------------
 Cartesian Forces:  Max        0.000502134 RMS        0.000153230

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 Internal  Forces:  Max        0.000574193 RMS        0.000100427
 Search for a local minimum.
 Step number   13 out of a maximum of   116
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swapping is turned off.
 Update second derivatives using D2CorX and points      9     10     11     12     13
 DE= -3.02D-05 DEPred=-1.44D-05 R= 2.10D+00
 TightC=F SS=   1.41D+00  RLast= 9.19D-02 DXNew= 1.8091D+00 2.7562D-01
 Trust test= 2.10D+00 RLast= 9.19D-02 DXMaxT set to 1.08D+00
 ITU=   1   1   1   1   1   1   1   1   0   0 -1   0   0
      Eigenvalues ---      0.00106     0.00200     0.00488     0.00755     0.01247
      Eigenvalues ---      0.01480     0.01706     0.01897     0.02075     0.02301
      Eigenvalues ---      0.02393     0.02481     0.03063     0.03088     0.03562
      Eigenvalues ---      0.04269     0.04737     0.05440     0.05918     0.07127
      Eigenvalues ---      0.08712     0.09406     0.13655     0.14269     0.14953
      Eigenvalues ---      0.15806     0.15916     0.15996     0.16010     0.16157
      Eigenvalues ---      0.16622     0.20475     0.21903     0.22873     0.22999
      Eigenvalues ---      0.24158     0.24749     0.25700     0.29748     0.33204
      Eigenvalues ---      0.33865     0.33876     0.33928     0.34122     0.34247
      Eigenvalues ---      0.34497     0.34681     0.36101     0.36311     0.36429
      Eigenvalues ---      0.37280     0.42637     0.43548     0.45928     0.50587
      Eigenvalues ---      0.53590     0.54613     0.55719     0.60581     2.14579
 En-DIIS/RFO-DIIS IScMMF=        0 using points:     13     12     11     10      9
 RFO step:  Lambda=-2.91908910D-06.
 DidBck=F Rises=F RFO-DIIS coefs:      2.24503     -1.43396      0.13587      0.11586     -
0.06279
 Iteration  1 RMS(Cart)=  0.01540640 RMS(Int)=  0.00020664
 Iteration  2 RMS(Cart)=  0.00042899 RMS(Int)=  0.00000598
 Iteration  3 RMS(Cart)=  0.00000019 RMS(Int)=  0.00000598
 Variable          Old X      -DE/DX     Delta X     Delta X     Delta X          New X
                                         (Linear)    (Quad)      (Total)
      R1           2.55966     0.00001    -0.00054     0.00004    -0.00050     2.55916
      R2           2.62608    -0.00007     0.00029    -0.00002     0.00026     2.62633
      R3           2.03332    -0.00001    -0.00001     0.00004     0.00003     2.03335
```

R4	2.63046	-0.00029	0.00040	-0.00022	0.00019	2.63065
R5	2.03125	0.00000	0.00001	0.00001	0.00002	2.03127
R6	2.54588	0.00002	0.00084	-0.00033	0.00051	2.54639
R7	2.69201	-0.00028	-0.00115	-0.00097	-0.00212	2.68989
R8	2.53030	0.00009	-0.00067	0.00002	-0.00066	2.52964
R9	2.02838	-0.00004	0.00014	-0.00011	0.00003	2.02842
R10	2.77421	-0.00016	-0.00031	-0.00043	-0.00075	2.77346
R11	2.89403	0.00002	0.00033	0.00029	0.00062	2.89465
R12	2.05944	0.00000	-0.00030	0.00008	-0.00022	2.05922
R13	2.06283	0.00006	0.00009	0.00007	0.00016	2.06299
R14	2.07459	0.00002	-0.00030	0.00007	-0.00023	2.07436
R15	2.06694	0.00006	-0.00021	-0.00009	-0.00030	2.06664
R16	2.69355	0.00004	0.00045	0.00025	0.00070	2.69426
R17	5.29722	0.00003	0.00288	0.00213	0.00500	5.30222
R18	2.50693	0.00001	0.00018	0.00012	0.00030	2.50723
R19	2.05227	-0.00009	0.00016	-0.00055	-0.00039	2.05188
R20	2.04379	0.00001	0.00023	-0.00005	0.00018	2.04397
R21	2.04788	0.00003	0.00022	-0.00008	0.00014	2.04802
R22	1.81631	-0.00002	-0.00037	0.00004	-0.00033	1.81598
A1	1.87449	-0.00001	0.00066	-0.00048	0.00018	1.87466
A2	2.28099	0.00000	-0.00028	0.00006	-0.00021	2.28078
A3	2.12770	0.00001	-0.00038	0.00041	0.00004	2.12774
A4	1.86884	0.00003	-0.00006	-0.00001	-0.00007	1.86877
A5	2.28662	0.00001	-0.00056	-0.00011	-0.00068	2.28594
A6	2.12729	-0.00004	0.00080	0.00003	0.00082	2.12811
A7	1.89218	0.00009	-0.00069	0.00058	-0.00012	1.89206
A8	2.22621	-0.00004	0.00161	0.00037	0.00194	2.22815
A9	2.15221	-0.00003	-0.00048	-0.00020	-0.00072	2.15149
A10	1.89215	-0.00009	0.00068	-0.00067	0.00001	1.89216
A11	2.19045	0.00000	-0.00066	0.00022	-0.00046	2.18999
A12	2.19712	0.00008	0.00030	0.00050	0.00078	2.19790
A13	1.89507	-0.00002	-0.00065	0.00064	-0.00001	1.89506
A14	2.19803	-0.00001	0.00069	-0.00005	0.00064	2.19867
A15	2.17743	0.00003	0.00002	-0.00085	-0.00083	2.17660
A16	1.95061	0.00012	0.00073	-0.00048	0.00024	1.95085
A17	1.88559	0.00002	0.00099	-0.00066	0.00033	1.88592
A18	1.89085	-0.00010	-0.00022	0.00030	0.00008	1.89094
A19	1.91836	-0.00004	-0.00049	0.00013	-0.00037	1.91799
A20	1.92824	-0.00001	-0.00174	0.00071	-0.00103	1.92722
A21	1.88854	0.00000	0.00080	0.00000	0.00080	1.88933
A22	1.91805	-0.00008	-0.00055	0.00084	0.00029	1.91834
A23	1.90848	0.00022	0.00163	-0.00066	0.00097	1.90945
A24	1.84721	0.00007	0.00158	0.00053	0.00210	1.84932
A25	1.89253	0.00002	0.00158	0.00023	0.00180	1.89433

A26	1.92948	-0.00003	-0.00303	-0.00026	-0.00329	1.92619
A27	1.96766	-0.00020	-0.00119	-0.00064	-0.00184	1.96582
A28	2.55743	0.00057	-0.00233	0.00014	-0.00220	2.55524
A29	2.14831	0.00009	0.00252	0.00046	0.00298	2.15129
A30	1.94930	0.00018	0.00173	0.00034	0.00207	1.95137
A31	2.18470	-0.00027	-0.00425	-0.00085	-0.00511	2.17959
A32	2.08581	0.00004	-0.00155	0.00029	-0.00126	2.08455
A33	2.14436	0.00002	0.00145	0.00007	0.00151	2.14587
A34	2.05301	-0.00006	0.00011	-0.00035	-0.00025	2.05276
A35	1.89844	-0.00013	-0.00080	0.00029	-0.00051	1.89793
D1	0.00269	0.00007	-0.00024	0.00186	0.00162	0.00431
D2	3.11220	-0.00001	0.00629	-0.00170	0.00459	3.11679
D3	-3.13384	0.00008	-0.00312	0.00377	0.00065	-3.13320
D4	-0.02434	0.00001	0.00341	0.00021	0.00362	-0.02072
D5	-0.03873	-0.00006	-0.00042	-0.00089	-0.00131	-0.04005
D6	-3.01589	-0.00006	-0.00077	0.00084	0.00007	-3.01581
D7	3.09835	-0.00007	0.00215	-0.00260	-0.00045	3.09790
D8	0.12119	-0.00007	0.00180	-0.00086	0.00094	0.12213
D9	0.03400	-0.00005	0.00080	-0.00219	-0.00139	0.03261
D10	3.00852	0.00007	0.00324	0.00271	0.00597	3.01449
D11	-3.07907	0.00002	-0.00498	0.00098	-0.00400	-3.08308
D12	-0.10456	0.00013	-0.00253	0.00588	0.00336	-0.10120
D13	-0.05854	0.00001	-0.00110	0.00167	0.00058	-0.05797
D14	-3.11487	0.00006	-0.00468	0.00100	-0.00368	-3.11855
D15	-3.04171	-0.00009	-0.00368	-0.00304	-0.00670	-3.04841
D16	0.18515	-0.00004	-0.00726	-0.00371	-0.01096	0.17420
D17	0.67395	-0.00009	-0.01613	-0.00729	-0.02342	0.65053
D18	-2.42456	-0.00009	-0.01576	-0.00614	-0.02190	-2.44646
D19	-2.65760	0.00004	-0.01331	-0.00164	-0.01495	-2.67255
D20	0.52707	0.00005	-0.01295	-0.00048	-0.01343	0.51365
D21	0.06026	0.00003	0.00094	-0.00050	0.00044	0.06070
D22	3.03982	0.00002	0.00136	-0.00212	-0.00076	3.03906
D23	3.11618	-0.00003	0.00448	0.00016	0.00464	3.12081
D24	-0.18745	-0.00004	0.00490	-0.00146	0.00344	-0.18401
D25	1.35366	-0.00010	-0.01099	-0.00946	-0.02045	1.33320
D26	-2.81692	-0.00007	-0.01050	-0.01004	-0.02054	-2.83747
D27	-0.77480	-0.00011	-0.00914	-0.01025	-0.01938	-0.79418
D28	-1.59793	-0.00009	-0.01135	-0.00761	-0.01896	-1.61688
D29	0.51468	-0.00006	-0.01086	-0.00819	-0.01905	0.49563
D30	2.55681	-0.00010	-0.00950	-0.00839	-0.01789	2.53892
D31	-0.98594	0.00000	-0.00365	0.00101	-0.00264	-0.98858
D32	1.08950	0.00011	-0.00106	0.00140	0.00033	1.08983
D33	-3.06966	0.00004	-0.00067	0.00057	-0.00009	-3.06975
D34	-3.07941	-0.00007	-0.00504	0.00207	-0.00296	-3.08237

D35	-1.00397	0.00004	-0.00245	0.00246	0.00001	-1.00396
D36	1.12006	-0.00003	-0.00205	0.00164	-0.00042	1.11964
D37	1.12088	-0.00004	-0.00463	0.00155	-0.00307	1.11780
D38	-3.08687	0.00007	-0.00204	0.00194	-0.00010	-3.08697
D39	-0.96284	0.00000	-0.00165	0.00112	-0.00053	-0.96337
D40	-0.62705	0.00006	0.03346	0.01623	0.04969	-0.57737
D41	1.46415	0.00011	0.03469	0.01700	0.05169	1.51584
D42	-2.67672	-0.00005	0.03116	0.01640	0.04756	-2.62916
D43	-2.57210	-0.00004	0.03873	0.01781	0.05654	-2.51556
D44	1.63492	0.00003	0.04007	0.01664	0.05671	1.69163
D45	-0.48658	0.00017	0.04105	0.01699	0.05803	-0.42855
D46	-3.08787	-0.00001	-0.00207	0.00164	-0.00044	-3.08831
D47	0.05232	-0.00002	-0.00111	0.00034	-0.00077	0.05155
D48	0.00475	0.00000	-0.00231	0.00036	-0.00195	0.00280
D49	-3.13825	-0.00001	-0.00135	-0.00093	-0.00228	-3.14052

Item	Value	Threshold	Converged?
Maximum Force	0.000574	0.000450	NO
RMS Force	0.000100	0.000300	YES
Maximum Displacement	0.060016	0.001800	NO
RMS Displacement	0.015459	0.001200	NO

Predicted change in Energy=-1.522908D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.456298	-1.991635	-1.311725
2	6	0	-1.747199	-1.618949	-1.481051
3	7	0	-2.109414	-0.878740	-0.359098
4	6	0	-1.035426	-0.776765	0.448296
5	7	0	-0.034366	-1.485307	-0.088148
6	6	0	1.337306	-1.520567	0.432691
7	6	0	2.226922	-0.469171	-0.237762
8	1	0	0.197544	-2.563824	-1.946448
9	1	0	-2.428623	-1.787850	-2.295019
10	1	0	1.295517	-1.340589	1.506607
11	1	0	1.741230	-2.521523	0.269245
12	1	0	2.220913	-0.613309	-1.325944
13	1	0	1.838859	0.529194	-0.017134
14	35	0	-0.437457	2.100111	0.455317
15	1	0	-1.015809	-0.278848	1.399014
16	6	0	-3.317868	-0.157370	-0.146005

17	6	0	-4.503081	-0.583959	-0.562675
18	1	0	-3.139188	0.790548	0.352496
19	1	0	-5.375174	0.037613	-0.410992
20	1	0	-4.645884	-1.537895	-1.056802
21	8	0	3.538093	-0.675574	0.282777
22	1	0	3.969754	0.177531	0.379515

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.354250	0.000000			
3	N	2.208806	1.392080	0.000000		
4	C	2.215620	2.222223	1.347492	0.000000	
5	N	1.389796	2.211749	2.178798	1.338628	0.000000
6	C	2.545959	3.631289	3.594266	2.486632	1.467651
7	C	3.266643	4.319883	4.357325	3.347865	2.483614
8	H	1.076003	2.211653	3.268217	3.232428	2.161078
9	H	2.213247	1.074900	2.162444	3.238683	3.270211
10	H	3.381673	4.273372	3.909951	2.621300	2.081532
11	H	2.758510	4.005910	4.233321	3.284214	2.086676
12	H	3.011219	4.096496	4.444882	3.711925	2.716396
13	H	3.646682	4.429152	4.205720	3.191186	2.751769
14	Br	4.457036	4.392761	3.511733	2.938372	3.648706
15	H	3.254965	3.259690	2.155644	1.073392	2.151842
16	C	3.593330	2.526967	1.423428	2.438522	3.542337
17	C	4.349607	3.083749	2.420327	3.617163	4.583341
18	H	4.208096	3.332447	2.086462	2.625159	3.874739
19	H	5.396713	4.129338	3.392284	4.498334	5.563070
20	H	4.221789	2.930688	2.712002	3.984978	4.712446
21	O	4.497734	5.651138	5.687497	4.577632	3.681809
22	H	5.211094	6.274759	6.214301	5.095806	4.360816

		6	7	8	9	10
6	C	0.000000				
7	C	1.531782	0.000000			
8	H	2.836855	3.380170	0.000000		
9	H	4.657689	5.257882	2.760506	0.000000	
10	H	1.089694	2.160951	3.824321	5.340564	0.000000
11	H	1.091688	2.169124	2.700750	4.949889	1.767577
12	H	2.167182	1.097703	2.878117	4.892529	3.067351
13	H	2.157642	1.093620	3.997866	5.363661	2.472468
14	Br	4.032320	3.765699	5.284315	5.161912	3.993348
15	H	2.830688	3.637384	4.229120	4.233085	2.545800
16	C	4.885063	5.554308	4.625012	2.840331	5.041276
17	C	5.998175	6.738819	5.284938	2.958673	6.203077

18	H	5.038519	5.543503	5.260298	3.763293	5.053744
19	H	6.942414	7.620939	6.338792	3.945128	7.076352
20	H	6.165829	7.003460	5.030188	2.551843	6.473812
21	O	2.362193	1.425740	4.437815	6.594232	2.639916
22	H	3.133073	1.958754	5.211017	7.207988	3.275144

		11	12	13	14	15
11	H	0.000000				
12	H	2.532984	0.000000			
13	H	3.065685	1.778838	0.000000		
14	Br	5.112808	4.195530	2.805816	0.000000	
15	H	3.729241	4.244247	3.287481	2.623833	0.000000
16	C	5.599655	5.681394	5.203827	3.708716	2.775125
17	C	6.590726	6.767240	6.461960	4.976931	4.012778
18	H	5.898748	5.789530	4.998588	3.004143	2.597604
19	H	7.593097	7.678631	7.241481	5.420834	4.730786
20	H	6.597056	6.933989	6.885177	5.764759	4.560008
21	O	2.576127	2.080102	2.104474	4.851721	4.705465
22	H	3.501910	2.567579	2.195839	4.808905	5.109158

		16	17	18	19	20
16	C	0.000000				
17	C	1.326771	0.000000			
18	H	1.085808	2.141732	0.000000		
19	H	2.083445	1.081622	2.479811	0.000000	
20	H	2.121091	1.083766	3.110933	1.852340	0.000000
21	O	6.888875	8.086017	6.836699	8.968628	8.337599
22	H	7.314217	8.559003	7.135374	9.379348	8.901399

		21	22
21	O	0.000000	
22	H	0.960977	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.138239	-2.267499	-0.628346
2	6	0	-1.438653	-1.910315	-0.752185
3	7	0	-1.662509	-0.866151	0.140842
4	6	0	-0.500037	-0.577693	0.758244

5	7	0	0.427654	-1.447832	0.340904
6	6	0	1.851227	-1.384251	0.692186
7	6	0	2.659216	-0.603971	-0.349290
8	1	0	0.433568	-3.022129	-1.139573
9	1	0	-2.212368	-2.279629	-1.400554
10	1	0	1.937671	-0.902296	1.665675
11	1	0	2.229051	-2.404608	0.781092
12	1	0	2.523761	-1.053897	-1.341343
13	1	0	2.303907	0.429709	-0.384869
14	35	0	0.105718	2.155392	-0.134693
15	1	0	-0.365982	0.170922	1.515724
16	6	0	-2.834394	-0.068622	0.270379
17	6	0	-4.062273	-0.551486	0.130824
18	1	0	-2.594229	0.974964	0.449901
19	1	0	-4.907832	0.120124	0.193089
20	1	0	-4.266318	-1.600940	-0.046827
21	8	0	4.022015	-0.701998	0.058023
22	1	0	4.465406	0.125965	-0.145348

Rotational constants (GHZ): 0.8170900 0.5704453 0.3554057

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 866.1687251868 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 6.77D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Initial guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999991 0.000739 0.000336 0.004045 Ang= 0.47 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Keep R1 ints in memory in canonical form, NReq=1804729152.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3032.33810590 A.U. after 11 cycles

NFock= 11 Conv=0.39D-08 -V/T= 2.0017

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000232148	-0.000186707	0.000222339
2	6	-0.000459982	-0.000123255	0.000335485
3	7	0.000321799	0.000216019	-0.000319966
4	6	-0.000273418	0.000223973	0.000046856
5	7	0.000024644	-0.000128122	-0.000139615
6	6	0.000084149	0.000015900	-0.000299287
7	6	0.000283957	-0.000046370	0.000306130
8	1	0.000005217	0.000082598	-0.000032555
9	1	0.000034226	0.000215359	-0.000053645
10	1	-0.000046359	0.000049695	-0.000003268
11	1	-0.000030135	-0.000085293	0.000169868
12	1	0.000026353	-0.000003961	0.000028223
13	1	-0.000268279	-0.000098457	-0.000208949
14	35	0.000003880	-0.000017806	0.000040921
15	1	-0.000029652	-0.000120781	0.000043761
16	6	-0.000005750	0.000018141	-0.000067250
17	6	0.000030804	0.000106220	0.000073227
18	1	0.000006508	-0.000097972	-0.000017239
19	1	0.000010927	-0.000089614	-0.000073275
20	1	0.000004998	0.000051812	0.000027249
21	8	0.000028318	-0.000019330	-0.000131968
22	1	0.000015648	0.000037951	0.000052959

Cartesian Forces: Max 0.000459982 RMS 0.000150043

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000400338 RMS 0.000103157
Search for a local minimum.
Step number 14 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 10 11 12 13 14
DE= -3.41D-05 DEPred=-1.52D-05 R= 2.24D+00
TightC=F SS= 1.41D+00 RLast= 1.46D-01 DXNew= 1.8091D+00 4.3825D-01
Trust test= 2.24D+00 RLast= 1.46D-01 DXMaxT set to 1.08D+00
ITU= 1 1 1 1 1 1 1 1 1 0 0 -1 0 0

Eigenvalues ---	0.00067	0.00180	0.00496	0.00773	0.01240
Eigenvalues ---	0.01316	0.01687	0.01873	0.02073	0.02269
Eigenvalues ---	0.02381	0.02563	0.03068	0.03090	0.03531
Eigenvalues ---	0.04285	0.04758	0.05452	0.05912	0.07622
Eigenvalues ---	0.08727	0.09566	0.13777	0.14197	0.15529
Eigenvalues ---	0.15910	0.15956	0.15996	0.16012	0.16202
Eigenvalues ---	0.16660	0.20355	0.22413	0.22893	0.23140
Eigenvalues ---	0.24276	0.24841	0.25710	0.29819	0.33176
Eigenvalues ---	0.33857	0.33878	0.33912	0.34120	0.34358
Eigenvalues ---	0.34628	0.34719	0.36096	0.36312	0.36392
Eigenvalues ---	0.37281	0.42629	0.43503	0.45777	0.50533
Eigenvalues ---	0.53686	0.54938	0.56294	0.60629	2.26820

En-DIIS/RFO-DIIS IScMMF= 0 using points: 14 13 12 11 10
RFO step: Lambda=-2.24334931D-06.
DidBck=F Rises=F RFO-DIIS coefs: 1.67592 -0.66009 -0.20750 0.20053 -0.00886
Iteration 1 RMS(Cart)= 0.01481871 RMS(Int)= 0.00017615
Iteration 2 RMS(Cart)= 0.00046517 RMS(Int)= 0.00000416
Iteration 3 RMS(Cart)= 0.00000022 RMS(Int)= 0.00000415

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55916	0.00026	-0.00021	0.00034	0.00014	2.55930
R2	2.62633	-0.00014	0.00009	-0.00014	-0.00006	2.62628
R3	2.03335	-0.00002	0.00000	-0.00005	-0.00005	2.03330
R4	2.63065	-0.00029	-0.00021	-0.00021	-0.00042	2.63023
R5	2.03127	-0.00002	0.00001	-0.00004	-0.00004	2.03123
R6	2.54639	-0.00014	0.00024	-0.00003	0.00022	2.54661
R7	2.68989	-0.00008	-0.00125	-0.00038	-0.00163	2.68826
R8	2.52964	0.00022	-0.00026	0.00012	-0.00014	2.52950

R9	2.02842	-0.00002	0.00002	-0.00001	0.00000	2.02842
R10	2.77346	0.00006	-0.00053	0.00049	-0.00005	2.77341
R11	2.89465	-0.00004	0.00026	0.00021	0.00047	2.89511
R12	2.05922	0.00000	-0.00011	-0.00005	-0.00016	2.05906
R13	2.06299	0.00004	0.00016	0.00000	0.00016	2.06316
R14	2.07436	-0.00002	-0.00012	-0.00014	-0.00025	2.07410
R15	2.06664	-0.00003	-0.00016	-0.00002	-0.00017	2.06647
R16	2.69426	-0.00001	0.00038	-0.00011	0.00027	2.69453
R17	5.30222	0.00001	0.00281	0.00230	0.00511	5.30734
R18	2.50723	-0.00006	0.00012	0.00006	0.00018	2.50741
R19	2.05188	-0.00010	-0.00032	-0.00017	-0.00049	2.05139
R20	2.04397	-0.00008	0.00009	-0.00019	-0.00010	2.04387
R21	2.04802	-0.00005	0.00010	-0.00013	-0.00003	2.04799
R22	1.81598	0.00006	-0.00020	0.00004	-0.00016	1.81582
A1	1.87466	-0.00006	0.00012	0.00011	0.00023	1.87489
A2	2.28078	0.00002	-0.00013	-0.00013	-0.00026	2.28052
A3	2.12774	0.00004	0.00000	0.00001	0.00002	2.12776
A4	1.86877	0.00002	-0.00009	0.00001	-0.00007	1.86870
A5	2.28594	0.00005	-0.00029	0.00004	-0.00023	2.28571
A6	2.12811	-0.00007	0.00035	-0.00007	0.00029	2.12840
A7	1.89206	0.00009	0.00011	-0.00018	-0.00008	1.89199
A8	2.22815	-0.00011	0.00103	0.00023	0.00124	2.22940
A9	2.15149	0.00003	-0.00028	0.00022	-0.00008	2.15141
A10	1.89216	-0.00002	-0.00008	0.00030	0.00022	1.89238
A11	2.18999	0.00003	-0.00031	0.00002	-0.00029	2.18969
A12	2.19790	-0.00001	0.00055	-0.00046	0.00008	2.19799
A13	1.89506	-0.00002	-0.00005	-0.00028	-0.00034	1.89473
A14	2.19867	0.00011	0.00034	0.00034	0.00067	2.19934
A15	2.17660	-0.00009	-0.00049	-0.00025	-0.00074	2.17586
A16	1.95085	-0.00030	-0.00004	-0.00003	-0.00007	1.95078
A17	1.88592	0.00000	0.00026	-0.00099	-0.00073	1.88519
A18	1.89094	0.00015	0.00000	0.00125	0.00126	1.89219
A19	1.91799	0.00004	-0.00030	-0.00065	-0.00096	1.91704
A20	1.92722	0.00018	-0.00018	0.00043	0.00025	1.92747
A21	1.88933	-0.00007	0.00028	-0.00002	0.00027	1.88960
A22	1.91834	0.00003	0.00005	0.00008	0.00013	1.91847
A23	1.90945	-0.00040	0.00040	-0.00038	0.00002	1.90947
A24	1.84932	0.00030	0.00166	0.00101	0.00267	1.85199
A25	1.89433	0.00006	0.00111	-0.00013	0.00097	1.89530
A26	1.92619	-0.00011	-0.00199	-0.00105	-0.00305	1.92314
A27	1.96582	0.00012	-0.00121	0.00050	-0.00072	1.96511
A28	2.55524	-0.00008	-0.00094	0.00051	-0.00043	2.55480
A29	2.15129	-0.00011	0.00167	0.00017	0.00184	2.15313
A30	1.95137	0.00003	0.00160	-0.00040	0.00121	1.95257

A31	2.17959	0.00008	-0.00329	0.00027	-0.00302	2.17657
A32	2.08455	0.00014	-0.00046	0.00024	-0.00021	2.08433
A33	2.14587	-0.00007	0.00084	-0.00012	0.00072	2.14659
A34	2.05276	-0.00007	-0.00038	-0.00013	-0.00050	2.05226
A35	1.89793	0.00000	-0.00067	0.00037	-0.00030	1.89763
D1	0.00431	0.00000	0.00202	-0.00191	0.00012	0.00443
D2	3.11679	-0.00012	0.00201	-0.00257	-0.00056	3.11623
D3	-3.13320	0.00011	0.00201	0.00050	0.00251	-3.13069
D4	-0.02072	-0.00001	0.00200	-0.00016	0.00184	-0.01888
D5	-0.04005	0.00004	-0.00143	0.00102	-0.00041	-0.04046
D6	-3.01581	0.00010	-0.00008	0.00228	0.00221	-3.01361
D7	3.09790	-0.00006	-0.00142	-0.00113	-0.00255	3.09535
D8	0.12213	0.00000	-0.00007	0.00014	0.00007	0.12220
D9	0.03261	-0.00004	-0.00193	0.00215	0.00021	0.03283
D10	3.01449	0.00004	0.00384	0.00399	0.00784	3.02233
D11	-3.08308	0.00007	-0.00191	0.00273	0.00082	-3.08226
D12	-0.10120	0.00015	0.00386	0.00458	0.00845	-0.09276
D13	-0.05797	0.00007	0.00105	-0.00154	-0.00049	-0.05846
D14	-3.11855	0.00006	-0.00101	0.00035	-0.00065	-3.11920
D15	-3.04841	0.00001	-0.00457	-0.00329	-0.00784	-3.05625
D16	0.17420	0.00001	-0.00662	-0.00140	-0.00801	0.16619
D17	0.65053	-0.00002	-0.01515	-0.00165	-0.01680	0.63373
D18	-2.44646	-0.00005	-0.01476	-0.00257	-0.01733	-2.46379
D19	-2.67255	0.00007	-0.00853	0.00042	-0.00811	-2.68065
D20	0.51365	0.00003	-0.00813	-0.00050	-0.00864	0.50501
D21	0.06070	-0.00007	0.00021	0.00034	0.00055	0.06125
D22	3.03906	-0.00010	-0.00103	-0.00083	-0.00186	3.03720
D23	3.12081	-0.00006	0.00222	-0.00153	0.00069	3.12151
D24	-0.18401	-0.00010	0.00099	-0.00271	-0.00172	-0.18572
D25	1.33320	0.00004	-0.01370	-0.00784	-0.02154	1.31166
D26	-2.83747	-0.00009	-0.01393	-0.00933	-0.02325	-2.86072
D27	-0.79418	-0.00010	-0.01345	-0.00921	-0.02266	-0.81684
D28	-1.61688	0.00009	-0.01219	-0.00639	-0.01858	-1.63547
D29	0.49563	-0.00004	-0.01242	-0.00788	-0.02030	0.47533
D30	2.53892	-0.00004	-0.01194	-0.00776	-0.01970	2.51922
D31	-0.98858	-0.00005	-0.00247	-0.00350	-0.00597	-0.99454
D32	1.08983	-0.00021	-0.00084	-0.00385	-0.00469	1.08515
D33	-3.06975	-0.00011	-0.00108	-0.00287	-0.00395	-3.07370
D34	-3.08237	0.00011	-0.00257	-0.00180	-0.00437	-3.08674
D35	-1.00396	-0.00005	-0.00094	-0.00215	-0.00309	-1.00705
D36	1.11964	0.00005	-0.00119	-0.00117	-0.00235	1.11729
D37	1.11780	0.00006	-0.00261	-0.00164	-0.00425	1.11355
D38	-3.08697	-0.00010	-0.00098	-0.00198	-0.00297	-3.08994
D39	-0.96337	0.00000	-0.00123	-0.00100	-0.00223	-0.96560

D40	-0.57737	0.00017	0.03655	0.01799	0.05454	-0.52283
D41	1.51584	0.00000	0.03751	0.01778	0.05529	1.57113
D42	-2.62916	-0.00002	0.03496	0.01667	0.05164	-2.57753
D43	-2.51556	0.00015	0.03105	0.01669	0.04773	-2.46783
D44	1.69163	0.00000	0.03108	0.01656	0.04764	1.73927
D45	-0.42855	-0.00008	0.03192	0.01715	0.04907	-0.37948
D46	-3.08831	-0.00002	-0.00058	-0.00062	-0.00120	-3.08951
D47	0.05155	-0.00001	-0.00093	0.00017	-0.00076	0.05079
D48	0.00280	0.00002	-0.00088	0.00041	-0.00047	0.00233
D49	-3.14052	0.00003	-0.00122	0.00119	-0.00003	-3.14055

Item	Value	Threshold	Converged?
Maximum Force	0.000400	0.000450	YES
RMS Force	0.000103	0.000300	YES
Maximum Displacement	0.064582	0.001800	NO
RMS Displacement	0.014856	0.001200	NO

Predicted change in Energy=-8.870870D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.455013	-1.984823	-1.311520
2	6	0	-1.746080	-1.612739	-1.481488
3	7	0	-2.110284	-0.876266	-0.357996
4	6	0	-1.037186	-0.775598	0.450937
5	7	0	-0.034922	-1.481989	-0.085907
6	6	0	1.336324	-1.515024	0.436129
7	6	0	2.231164	-0.478754	-0.251272
8	1	0	0.200568	-2.552868	-1.948122
9	1	0	-2.425915	-1.779501	-2.297198
10	1	0	1.294288	-1.315398	1.506469
11	1	0	1.736478	-2.520403	0.290999
12	1	0	2.229817	-0.644449	-1.336260
13	1	0	1.844909	0.524554	-0.051309
14	35	0	-0.423885	2.096990	0.466196
15	1	0	-1.019248	-0.279875	1.402835
16	6	0	-3.321935	-0.163689	-0.139299
17	6	0	-4.504615	-0.586554	-0.567116
18	1	0	-3.150830	0.776780	0.375145
19	1	0	-5.378838	0.029971	-0.407669
20	1	0	-4.643840	-1.532370	-1.077572
21	8	0	3.541567	-0.676208	0.275037

22	1	0	3.957825	0.181334	0.396133	

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.354322	0.000000			
3	N	2.208626	1.391859	0.000000		
4	C	2.215267	2.222071	1.347607	0.000000	
5	N	1.389765	2.211968	2.179004	1.338552	0.000000
6	C	2.546346	3.631531	3.594128	2.486066	1.467627
7	C	3.256980	4.314837	4.360914	3.356088	2.483742
8	H	1.075975	2.211566	3.267955	3.232059	2.161038
9	H	2.213182	1.074881	2.162397	3.238616	3.270347
10	H	3.383674	4.273188	3.906428	2.615589	2.080917
11	H	2.767227	4.011704	4.233433	3.280722	2.087635
12	H	3.000921	4.094684	4.455021	3.726202	2.719173
13	H	3.629703	4.416858	4.207125	3.201424	2.749759
14	Br	4.452240	4.393605	3.516175	2.937368	3.642142
15	H	3.254679	3.259468	2.155590	1.073394	2.151820
16	C	3.593031	2.526764	1.422566	2.437804	3.541923
17	C	4.348398	3.081988	2.420844	3.618733	4.583832
18	H	4.211736	3.336197	2.086335	2.623568	3.876014
19	H	5.396331	4.128985	3.392223	4.498453	5.563001
20	H	4.219682	2.926879	2.714253	3.989610	4.714664
21	O	4.494696	5.649928	5.690710	4.583209	3.683862
22	H	5.203985	6.267271	6.205576	5.086144	4.352130

		6	7	8	9	10
6	C	0.000000				
7	C	1.532029	0.000000			
8	H	2.837554	3.362227	0.000000		
9	H	4.657840	5.250347	2.760139	0.000000	
10	H	1.089608	2.160408	3.829067	5.340711	0.000000
11	H	1.091775	2.169586	2.715462	4.957138	1.767749
12	H	2.167392	1.097568	2.852068	4.887493	3.067001
13	H	2.157806	1.093528	3.971433	5.347207	2.472909
14	Br	4.018194	3.768090	5.276367	5.164461	3.959631
15	H	2.829989	3.652506	4.228873	4.232947	2.536829
16	C	4.884322	5.563157	4.624721	2.840814	5.034333
17	C	5.998760	6.744041	5.283210	2.955892	6.201471
18	H	5.038912	5.561890	5.264598	3.768486	5.041446
19	H	6.942075	7.628590	6.338282	3.945156	7.071390
20	H	6.168789	7.004181	5.026685	2.543178	6.479638
21	O	2.364880	1.425884	4.430188	6.591244	2.641070
22	H	3.122738	1.958624	5.204649	7.200767	3.250766

		11	12	13	14	15
11	H	0.000000				
12	H	2.531907	0.000000			
13	H	3.066055	1.779276	0.000000		
14	Br	5.100801	4.219771	2.808521	0.000000	
15	H	3.721582	4.265206	3.311350	2.623211	0.000000
16	C	5.597035	5.699632	5.213224	3.725049	2.773814
17	C	6.589945	6.778459	6.466612	4.992144	4.015288
18	H	5.896124	5.822385	5.020248	3.031085	2.591584
19	H	7.590801	7.694723	7.249422	5.439464	4.730745
20	H	6.599822	6.935596	6.883895	5.776114	4.567146
21	O	2.580631	2.077974	2.104039	4.842725	4.714875
22	H	3.499260	2.582463	2.186874	4.782679	5.098766

		16	17	18	19	20
16	C	0.000000				
17	C	1.326866	0.000000			
18	H	1.085547	2.139922	0.000000		
19	H	2.083357	1.081569	2.476800	0.000000	
20	H	2.121573	1.083751	3.109925	1.851999	0.000000
21	O	6.895072	8.090631	6.849042	8.974319	8.340471
22	H	7.307574	8.551630	7.133580	9.372421	8.893662

		21	22
21	O	0.000000	
22	H	0.960892	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.151830	-2.262645	-0.624326
2	6	0	-1.450582	-1.900322	-0.751420
3	7	0	-1.672161	-0.854769	0.140205
4	6	0	-0.509705	-0.570456	0.759808
5	7	0	0.415353	-1.444797	0.345661
6	6	0	1.838559	-1.384374	0.698878
7	6	0	2.654584	-0.631572	-0.356823
8	1	0	0.418394	-3.018635	-1.135253
9	1	0	-2.223970	-2.266802	-1.401752

10	1	0	1.925761	-0.881439	1.661530
11	1	0	2.209671	-2.404984	0.811152
12	1	0	2.522871	-1.104436	-1.338508
13	1	0	2.303767	0.402350	-0.417959
14	35	0	0.126611	2.153886	-0.135285
15	1	0	-0.374393	0.178648	1.516582
16	6	0	-2.842858	-0.057678	0.273651
17	6	0	-4.071704	-0.534827	0.122530
18	1	0	-2.603481	0.983213	0.467704
19	1	0	-4.915270	0.138660	0.190390
20	1	0	-4.279001	-1.581053	-0.069707
21	8	0	4.016424	-0.724479	0.055373
22	1	0	4.451737	0.112504	-0.127045

Rotational constants (GHZ): 0.8182556 0.5695121 0.3553815

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 866.1168814213 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 6.75D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Initial guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999995 0.000598 0.000322 0.003243 Ang= 0.38 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.33812985 A.U. after 11 cycles
NFock= 11 Conv=0.34D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000242288	-0.000176367	0.000117333
2	6	-0.000363961	-0.000228474	0.000205825
3	7	0.000472846	0.000095037	-0.000142307
4	6	-0.000299845	0.000324950	0.000133606
5	7	-0.000088326	-0.000012096	-0.000162161
6	6	0.000176801	0.000009187	-0.000245393
7	6	0.000458552	-0.000052384	0.000243714
8	1	-0.000017027	0.000023483	-0.000022973
9	1	0.000031719	0.000191418	-0.000053254
10	1	-0.000084289	0.000038311	0.000014402
11	1	-0.000070184	-0.000056016	0.000138076
12	1	-0.000001993	0.000038139	0.000017553
13	1	-0.000358295	-0.000144743	-0.000174760
14	35	-0.000017417	-0.000101705	0.000032440
15	1	-0.000022020	-0.000186847	0.000057695
16	6	-0.000277865	0.000258206	-0.000071522
17	6	0.000065001	0.000000290	0.000061798
18	1	0.000118045	-0.000059913	-0.000015701
19	1	0.000009003	-0.000056532	-0.000080544
20	1	0.000045144	0.000051812	0.000028268
21	8	-0.000080211	0.000008374	-0.000144155
22	1	0.000062036	0.000035872	0.000062061

Cartesian Forces: Max 0.000472846 RMS 0.000161959

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000787781 RMS 0.000165329

Search for a local minimum.
Step number 15 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 10 11 12 13 14 15
DE= -2.40D-05 DEPred=-8.87D-06 R= 2.70D+00
TightC=F SS= 1.41D+00 RLast= 1.40D-01 DXNew= 1.8091D+00 4.1935D-01
Trust test= 2.70D+00 RLast= 1.40D-01 DXMaxT set to 1.08D+00
ITU= 1 1 1 1 1 1 1 1 1 1 0 0 -1 0 0

Eigenvalues ---	0.00041	0.00170	0.00504	0.00735	0.01225
Eigenvalues ---	0.01253	0.01664	0.01859	0.02073	0.02223
Eigenvalues ---	0.02382	0.02565	0.03066	0.03100	0.03567
Eigenvalues ---	0.04285	0.04721	0.05451	0.05897	0.07552
Eigenvalues ---	0.08723	0.09536	0.13714	0.14180	0.15676
Eigenvalues ---	0.15882	0.15934	0.15993	0.16000	0.16364
Eigenvalues ---	0.17220	0.20208	0.22468	0.22909	0.23155
Eigenvalues ---	0.24300	0.25347	0.25850	0.30092	0.33136
Eigenvalues ---	0.33863	0.33878	0.33931	0.34120	0.34406
Eigenvalues ---	0.34619	0.34751	0.36227	0.36312	0.36443
Eigenvalues ---	0.37300	0.42643	0.43167	0.45870	0.49631
Eigenvalues ---	0.53810	0.54746	0.56160	0.60625	2.43136

En-DIIS/RFO-DIIS IScMMF= 0 using points: 15 14 13 12 11
RFO step: Lambda=-3.42024599D-06.
DidBck=F Rises=F RFO-DIIS coefs: 1.93866 -0.90202 -0.17646 -0.06731 0.20713
Iteration 1 RMS(Cart)= 0.01692189 RMS(Int)= 0.00025787
Iteration 2 RMS(Cart)= 0.00067747 RMS(Int)= 0.00000488
Iteration 3 RMS(Cart)= 0.00000047 RMS(Int)= 0.00000486

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55930	0.00019	0.00035	-0.00009	0.00026	2.55956
R2	2.62628	-0.00008	-0.00020	0.00007	-0.00014	2.62614
R3	2.03330	-0.00001	-0.00007	0.00001	-0.00006	2.03324
R4	2.63023	-0.00008	-0.00088	0.00032	-0.00056	2.62967
R5	2.03123	-0.00001	-0.00004	0.00001	-0.00003	2.03120
R6	2.54661	-0.00020	-0.00001	-0.00009	-0.00010	2.54651
R7	2.68826	0.00010	-0.00125	0.00037	-0.00089	2.68737
R8	2.52950	0.00021	0.00017	0.00002	0.00019	2.52969
R9	2.02842	-0.00004	-0.00002	-0.00013	-0.00015	2.02827
R10	2.77341	0.00004	-0.00008	0.00021	0.00012	2.77354
R11	2.89511	-0.00008	0.00018	0.00033	0.00052	2.89563
R12	2.05906	0.00002	-0.00008	0.00002	-0.00007	2.05900

R13	2.06316	0.00000	0.00021	-0.00009	0.00012	2.06328
R14	2.07410	-0.00002	-0.00014	-0.00007	-0.00022	2.07388
R15	2.06647	-0.00010	-0.00009	-0.00010	-0.00019	2.06628
R16	2.69453	-0.00007	0.00011	-0.00037	-0.00026	2.69427
R17	5.30734	-0.00003	0.00388	0.00215	0.00604	5.31337
R18	2.50741	-0.00010	0.00005	-0.00004	0.00001	2.50743
R19	2.05139	-0.00005	-0.00056	0.00011	-0.00045	2.05094
R20	2.04387	-0.00006	-0.00015	0.00004	-0.00011	2.04376
R21	2.04799	-0.00005	-0.00003	-0.00001	-0.00004	2.04796
R22	1.81582	0.00008	-0.00008	-0.00002	-0.00010	1.81572
A1	1.87489	-0.00012	0.00014	-0.00020	-0.00006	1.87483
A2	2.28052	0.00003	-0.00020	-0.00013	-0.00032	2.28020
A3	2.12776	0.00009	0.00003	0.00033	0.00036	2.12812
A4	1.86870	0.00001	-0.00011	0.00000	-0.00009	1.86860
A5	2.28571	0.00004	0.00006	-0.00010	-0.00003	2.28568
A6	2.12840	-0.00006	-0.00009	0.00008	0.00000	2.12840
A7	1.89199	0.00012	0.00026	0.00016	0.00040	1.89238
A8	2.22940	-0.00014	0.00069	-0.00022	0.00044	2.22984
A9	2.15141	0.00002	0.00024	0.00001	0.00022	2.15163
A10	1.89238	-0.00009	0.00000	-0.00028	-0.00028	1.89211
A11	2.18969	0.00009	-0.00021	0.00039	0.00018	2.18987
A12	2.19799	0.00000	0.00010	-0.00021	-0.00011	2.19788
A13	1.89473	0.00009	-0.00029	0.00038	0.00008	1.89481
A14	2.19934	0.00013	0.00047	-0.00002	0.00045	2.19979
A15	2.17586	-0.00023	-0.00064	-0.00049	-0.00114	2.17472
A16	1.95078	-0.00057	-0.00042	-0.00035	-0.00077	1.95002
A17	1.88519	0.00004	-0.00072	-0.00057	-0.00130	1.88389
A18	1.89219	0.00024	0.00117	0.00010	0.00126	1.89346
A19	1.91704	0.00009	-0.00096	-0.00001	-0.00096	1.91607
A20	1.92747	0.00031	0.00106	0.00042	0.00149	1.92895
A21	1.88960	-0.00010	-0.00014	0.00041	0.00027	1.88987
A22	1.91847	0.00012	0.00004	0.00047	0.00052	1.91900
A23	1.90947	-0.00079	-0.00055	-0.00080	-0.00135	1.90813
A24	1.85199	0.00041	0.00264	0.00131	0.00395	1.85594
A25	1.89530	0.00010	0.00071	0.00005	0.00075	1.89606
A26	1.92314	-0.00014	-0.00227	-0.00099	-0.00326	1.91988
A27	1.96511	0.00029	-0.00056	-0.00001	-0.00057	1.96454
A28	2.55480	-0.00053	0.00053	0.00000	0.00052	2.55532
A29	2.15313	-0.00023	0.00109	-0.00046	0.00063	2.15376
A30	1.95257	-0.00002	0.00127	-0.00046	0.00081	1.95338
A31	2.17657	0.00024	-0.00230	0.00087	-0.00142	2.17514
A32	2.08433	0.00014	0.00045	0.00018	0.00063	2.08496
A33	2.14659	-0.00011	0.00030	-0.00033	-0.00003	2.14656
A34	2.05226	-0.00003	-0.00075	0.00015	-0.00060	2.05166

A35	1.89763	0.00008	-0.00064	0.00057	-0.00007	1.89756
D1	0.00443	0.00002	0.00108	-0.00032	0.00076	0.00519
D2	3.11623	-0.00013	-0.00273	-0.00093	-0.00365	3.11259
D3	-3.13069	0.00012	0.00473	-0.00072	0.00401	-3.12667
D4	-0.01888	-0.00003	0.00092	-0.00133	-0.00040	-0.01928
D5	-0.04046	0.00006	-0.00090	0.00072	-0.00018	-0.04064
D6	-3.01361	0.00015	0.00209	0.00163	0.00373	-3.00988
D7	3.09535	-0.00003	-0.00416	0.00108	-0.00309	3.09226
D8	0.12220	0.00006	-0.00117	0.00199	0.00082	0.12302
D9	0.03283	-0.00008	-0.00088	-0.00019	-0.00108	0.03175
D10	3.02233	-0.00004	0.00744	-0.00060	0.00684	3.02917
D11	-3.08226	0.00005	0.00249	0.00036	0.00285	-3.07941
D12	-0.09276	0.00009	0.01081	-0.00005	0.01077	-0.08199
D13	-0.05846	0.00013	0.00032	0.00066	0.00098	-0.05748
D14	-3.11920	0.00009	0.00166	0.00188	0.00355	-3.11566
D15	-3.05625	0.00010	-0.00760	0.00107	-0.00653	-3.06278
D16	0.16619	0.00006	-0.00625	0.00229	-0.00396	0.16223
D17	0.63373	0.00001	-0.01346	0.00084	-0.01261	0.62112
D18	-2.46379	-0.00001	-0.01472	0.00191	-0.01282	-2.47661
D19	-2.68065	0.00006	-0.00400	0.00039	-0.00360	-2.68425
D20	0.50501	0.00004	-0.00526	0.00146	-0.00381	0.50120
D21	0.06125	-0.00011	0.00034	-0.00085	-0.00051	0.06073
D22	3.03720	-0.00016	-0.00247	-0.00169	-0.00416	3.03304
D23	3.12151	-0.00007	-0.00103	-0.00205	-0.00308	3.11843
D24	-0.18572	-0.00012	-0.00384	-0.00288	-0.00673	-0.19245
D25	1.31166	0.00013	-0.01930	-0.00712	-0.02643	1.28524
D26	-2.86072	-0.00009	-0.02123	-0.00772	-0.02895	-2.88967
D27	-0.81684	-0.00006	-0.02116	-0.00750	-0.02865	-0.84549
D28	-1.63547	0.00020	-0.01590	-0.00616	-0.02207	-1.65754
D29	0.47533	-0.00002	-0.01783	-0.00676	-0.02459	0.45074
D30	2.51922	0.00001	-0.01776	-0.00654	-0.02430	2.49492
D31	-0.99454	-0.00005	-0.00601	-0.00147	-0.00748	-1.00202
D32	1.08515	-0.00033	-0.00545	-0.00161	-0.00706	1.07809
D33	-3.07370	-0.00018	-0.00486	-0.00130	-0.00616	-3.07985
D34	-3.08674	0.00021	-0.00419	-0.00052	-0.00471	-3.09145
D35	-1.00705	-0.00007	-0.00363	-0.00067	-0.00430	-1.01134
D36	1.11729	0.00008	-0.00304	-0.00035	-0.00339	1.11390
D37	1.11355	0.00008	-0.00408	-0.00129	-0.00537	1.10819
D38	-3.08994	-0.00020	-0.00352	-0.00143	-0.00495	-3.09489
D39	-0.96560	-0.00005	-0.00293	-0.00112	-0.00405	-0.96965
D40	-0.52283	0.00020	0.05124	0.01473	0.06597	-0.45686
D41	1.57113	-0.00006	0.05140	0.01486	0.06626	1.63739
D42	-2.57753	0.00002	0.04865	0.01363	0.06228	-2.51525
D43	-2.46783	0.00030	0.03266	0.02725	0.05991	-2.40792

D44	1.73927	-0.00001	0.03228	0.02646	0.05874	1.79801
D45	-0.37948	-0.00024	0.03337	0.02711	0.06048	-0.31900
D46	-3.08951	0.00001	-0.00120	0.00142	0.00023	-3.08928
D47	0.05079	0.00000	-0.00105	0.00068	-0.00036	0.05043
D48	0.00233	0.00003	0.00035	0.00018	0.00052	0.00286
D49	-3.14055	0.00002	0.00050	-0.00056	-0.00006	-3.14061

Item	Value	Threshold	Converged?
Maximum Force	0.000788	0.000450	NO
RMS Force	0.000165	0.000300	YES
Maximum Displacement	0.077432	0.001800	NO
RMS Displacement	0.016958	0.001200	NO

Predicted change in Energy=-8.581730D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.453193	-1.976969	-1.311481
2	6	0	-1.744353	-1.604960	-1.481988
3	7	0	-2.110458	-0.873092	-0.356475
4	6	0	-1.039260	-0.775790	0.455293
5	7	0	-0.035623	-1.479338	-0.082967
6	6	0	1.335397	-1.509509	0.440021
7	6	0	2.235020	-0.490783	-0.267670
8	1	0	0.204379	-2.539480	-1.950882
9	1	0	-2.421766	-1.766001	-2.300837
10	1	0	1.293052	-1.286499	1.505687
11	1	0	1.730726	-2.519799	0.316968
12	1	0	2.238921	-0.681741	-1.348374
13	1	0	1.848353	0.516846	-0.092284
14	35	0	-0.408701	2.092604	0.480808
15	1	0	-1.024068	-0.286579	1.410513
16	6	0	-3.325317	-0.168372	-0.133210
17	6	0	-4.505094	-0.589622	-0.570547
18	1	0	-3.160756	0.765891	0.394018
19	1	0	-5.382257	0.021424	-0.406610
20	1	0	-4.639272	-1.529019	-1.094002
21	8	0	3.544833	-0.674378	0.264720
22	1	0	3.939790	0.188290	0.416452

Distance matrix (angstroms):

	1	2	3	4	5

1	C	0.000000				
2	C	1.354458	0.000000			
3	N	2.208417	1.391562	0.000000		
4	C	2.215354	2.222102	1.347554	0.000000	
5	N	1.389693	2.211967	2.178825	1.338653	0.000000
6	C	2.546631	3.631541	3.593515	2.485472	1.467693
7	C	3.244191	4.307130	4.363166	3.365236	2.483380
8	H	1.075944	2.211503	3.267638	3.232170	2.161159
9	H	2.213281	1.074865	2.162115	3.238533	3.270290
10	H	3.385640	4.272406	3.901594	2.608415	2.079997
11	H	2.777772	4.018626	4.233186	3.276206	2.088659
12	H	2.987717	4.091046	4.465151	3.742797	2.722309
13	H	3.605921	4.397826	4.204035	3.210772	2.744850
14	Br	4.446988	4.394146	3.520280	2.936995	3.635354
15	H	3.254622	3.259371	2.155571	1.073314	2.151785
16	C	3.592831	2.526348	1.422097	2.437488	3.541643
17	C	4.346449	3.079501	2.420840	3.619256	4.583176
18	H	4.214606	3.338642	2.086296	2.623220	3.877502
19	H	5.395186	4.127458	3.392247	4.498894	5.562690
20	H	4.215592	2.921790	2.714607	3.990960	4.713623
21	O	4.490586	5.647341	5.692775	4.589173	3.686260
22	H	5.193496	6.255342	6.191078	5.071676	4.339852

		6	7	8	9	10
6	C	0.000000				
7	C	1.532303	0.000000			
8	H	2.838390	3.339740	0.000000		
9	H	4.657721	5.238855	2.759960	0.000000	
10	H	1.089573	2.159922	3.834455	5.340358	0.000000
11	H	1.091839	2.170949	2.733728	4.966318	1.767948
12	H	2.167929	1.097453	2.820207	4.879017	3.066931
13	H	2.156986	1.093429	3.936771	5.321937	2.472635
14	Br	4.002344	3.771388	5.267370	5.165154	3.919780
15	H	2.829220	3.671464	4.228903	4.232773	2.525459
16	C	4.883594	5.571298	4.624374	2.840322	5.026482
17	C	5.998231	6.747639	5.280759	2.952630	6.197974
18	H	5.039340	5.579557	5.267653	3.770786	5.028372
19	H	6.941715	7.635742	6.336680	3.943030	7.065925
20	H	6.168491	7.001189	5.021577	2.535733	6.481487
21	O	2.368498	1.425748	4.421100	6.585896	2.642954
22	H	3.109010	1.958419	5.195988	7.188345	3.219729

		11	12	13	14	15
11	H	0.000000				
12	H	2.531814	0.000000			
13	H	3.066355	1.779583	0.000000		

14	Br	5.087067	4.248859	2.811715	0.000000	
15	H	3.711065	4.291236	3.339864	2.627458	0.000000
16	C	5.594233	5.718471	5.219009	3.741080	2.773589
17	C	6.587771	6.789348	6.466784	5.008006	4.016712
18	H	5.893072	5.855603	5.038818	3.056388	2.589670
19	H	7.587879	7.711272	7.254376	5.460179	4.731872
20	H	6.599194	6.934849	6.875921	5.787392	4.570115
21	O	2.588298	2.075460	2.103452	4.830457	4.726318
22	H	3.496227	2.600869	2.177354	4.747623	5.084638

		16	17	18	19	20
16	C	0.000000				
17	C	1.326872	0.000000			
18	H	1.085310	2.138936	0.000000		
19	H	2.083692	1.081512	2.475945	0.000000	
20	H	2.121547	1.083732	3.109152	1.851596	0.000000
21	O	6.900242	8.093589	6.859739	8.979296	8.340031
22	H	7.294594	8.537879	7.124035	9.359799	8.878678

		21	22
21	O	0.000000	
22	H	0.960838	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.166314	-2.257502	-0.619243
2	6	0	-1.463114	-1.889175	-0.750406
3	7	0	-1.682085	-0.841788	0.139244
4	6	0	-0.520584	-0.562859	0.762955
5	7	0	0.401632	-1.441880	0.352067
6	6	0	1.824584	-1.384215	0.707039
7	6	0	2.648105	-0.663899	-0.365765
8	1	0	0.402321	-3.014645	-1.130166
9	1	0	-2.235428	-2.250345	-1.404946
10	1	0	1.912605	-0.856042	1.655963
11	1	0	2.187904	-2.404168	0.847782
12	1	0	2.520589	-1.164011	-1.334285
13	1	0	2.299578	0.368470	-0.457032

14	35	0	0.149660	2.151798	-0.135574
15	1	0	-0.384767	0.184139	1.521606
16	6	0	-2.851480	-0.043871	0.274155
17	6	0	-4.080857	-0.516655	0.113848
18	1	0	-2.611927	0.994839	0.478097
19	1	0	-4.923400	0.157843	0.183426
20	1	0	-4.289871	-1.560647	-0.088313
21	8	0	4.009208	-0.746924	0.050485
22	1	0	4.431767	0.101778	-0.105588

Rotational constants (GHZ): 0.8196319 0.5687503 0.3554912

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 866.1335830727 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 6.76D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Initial guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999993 0.000709 0.000361 0.003549 Ang= 0.42 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Keep R1 ints in memory in canonical form, NReq=1804729152.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3032.33815396 A.U. after 11 cycles

NFock= 11 Conv=0.38D-08 -V/T= 2.0017

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000134286	-0.000084948	0.000064674
2	6	-0.000143037	-0.000161605	-0.000010359
3	7	0.000232012	-0.000042784	0.000137202
4	6	-0.000114415	0.000332756	-0.000034767
5	7	-0.000106813	0.000088080	-0.000047614
6	6	0.000143969	-0.000090811	-0.000131471
7	6	0.000481879	0.000007648	0.000191264
8	1	-0.000026973	-0.000040081	0.000013892
9	1	0.000016334	0.000105205	-0.000026882
10	1	-0.000069066	0.000026975	0.000004064
11	1	-0.000040505	-0.000015066	0.000067839
12	1	0.000007725	0.000033086	0.000058278
13	1	-0.000389019	-0.000135891	-0.000151658
14	35	-0.000049222	-0.000247456	0.000032983
15	1	-0.000005963	-0.000149633	0.000041478
16	6	-0.000321444	0.000371258	-0.000103342
17	6	0.000015268	-0.000068415	-0.000017651
18	1	0.000162027	-0.000008602	-0.000003970
19	1	0.000020002	-0.000010482	-0.000028705
20	1	0.000060722	0.000041538	0.000031393
21	8	-0.000081259	0.000032230	-0.000165007
22	1	0.000073492	0.000016998	0.000078358

Cartesian Forces: Max 0.000481879 RMS 0.000138324

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.001300076 RMS 0.000262775

Search for a local minimum.

Step number 16 out of a maximum of 116

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.
Update second derivatives using D2CorX and points 11 12 13 14 15
16
DE= -2.41D-05 DEPred=-8.58D-06 R= 2.81D+00
TightC=F SS= 1.41D+00 RLast= 1.69D-01 DXNew= 1.8091D+00 5.0581D-01
Trust test= 2.81D+00 RLast= 1.69D-01 DXMaxT set to 1.08D+00
ITU= 1 1 1 1 1 1 1 1 1 1 1 0 0 -1 0 0
Eigenvalues --- 0.00032 0.00179 0.00525 0.00705 0.01212
Eigenvalues --- 0.01324 0.01658 0.01862 0.02073 0.02165
Eigenvalues --- 0.02394 0.02537 0.03066 0.03088 0.03480
Eigenvalues --- 0.04291 0.04703 0.05451 0.05876 0.07124
Eigenvalues --- 0.08727 0.09301 0.13646 0.14215 0.15702
Eigenvalues --- 0.15734 0.15918 0.15994 0.16000 0.16328
Eigenvalues --- 0.17159 0.20007 0.21153 0.22846 0.22955
Eigenvalues --- 0.24177 0.24943 0.25616 0.29904 0.33144
Eigenvalues --- 0.33863 0.33878 0.33963 0.34119 0.34378
Eigenvalues --- 0.34454 0.34684 0.36205 0.36312 0.36468
Eigenvalues --- 0.37280 0.42621 0.43206 0.45955 0.49813
Eigenvalues --- 0.53619 0.54512 0.55782 0.60549 2.52117
En-DIIS/RFO-DIIS IScMMF= 0 using points: 16 15 14 13 12
RFO step: Lambda=-6.08886884D-06.
DidBck=F Rises=F RFO-DIIS coefs: 2.40544 -2.06782 -0.50176 2.10416 -0.94002
Iteration 1 RMS(Cart)= 0.01138088 RMS(Int)= 0.00016975
Iteration 2 RMS(Cart)= 0.00022944 RMS(Int)= 0.00000941
Iteration 3 RMS(Cart)= 0.00000004 RMS(Int)= 0.00000941

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55956	0.00014	0.00028	-0.00001	0.00027	2.55983
R2	2.62614	-0.00005	-0.00013	0.00002	-0.00010	2.62604
R3	2.03324	0.00000	-0.00007	0.00002	-0.00005	2.03319
R4	2.62967	0.00010	-0.00004	-0.00007	-0.00012	2.62955
R5	2.03120	-0.00001	-0.00003	0.00001	-0.00003	2.03118
R6	2.54651	-0.00015	-0.00008	-0.00021	-0.00031	2.54620
R7	2.68737	0.00018	0.00118	-0.00065	0.00053	2.68790
R8	2.52969	0.00011	0.00041	0.00005	0.00046	2.53015
R9	2.02827	-0.00003	-0.00016	-0.00018	-0.00034	2.02793
R10	2.77354	0.00006	0.00085	-0.00023	0.00061	2.77415
R11	2.89563	-0.00015	0.00016	0.00064	0.00081	2.89644
R12	2.05900	0.00001	0.00002	-0.00002	0.00000	2.05899
R13	2.06328	-0.00001	-0.00011	0.00010	-0.00001	2.06327
R14	2.07388	-0.00006	-0.00017	-0.00014	-0.00031	2.07358
R15	2.06628	-0.00020	0.00001	-0.00009	-0.00008	2.06620
R16	2.69427	-0.00006	-0.00092	0.00009	-0.00083	2.69344

R17	5.31337	-0.00008	0.00159	0.00071	0.00230	5.31568
R18	2.50743	-0.00006	-0.00023	0.00007	-0.00016	2.50727
R19	2.05094	0.00001	0.00028	-0.00038	-0.00010	2.05084
R20	2.04376	-0.00003	-0.00009	-0.00009	-0.00018	2.04358
R21	2.04796	-0.00005	-0.00004	-0.00012	-0.00016	2.04779
R22	1.81572	0.00007	0.00003	0.00003	0.00006	1.81578
A1	1.87483	-0.00009	0.00008	-0.00023	-0.00014	1.87468
A2	2.28020	0.00003	-0.00028	0.00006	-0.00022	2.27997
A3	2.12812	0.00006	0.00020	0.00017	0.00036	2.12848
A4	1.86860	0.00001	-0.00003	0.00007	0.00003	1.86863
A5	2.28568	0.00002	0.00023	0.00012	0.00033	2.28601
A6	2.12840	-0.00003	-0.00026	-0.00025	-0.00052	2.12789
A7	1.89238	0.00002	0.00003	0.00012	0.00018	1.89256
A8	2.22984	-0.00005	-0.00093	0.00006	-0.00082	2.22902
A9	2.15163	0.00002	0.00059	-0.00017	0.00047	2.15210
A10	1.89211	-0.00001	0.00006	-0.00018	-0.00014	1.89197
A11	2.18987	0.00006	0.00047	-0.00015	0.00031	2.19018
A12	2.19788	-0.00004	-0.00093	0.00017	-0.00077	2.19711
A13	1.89481	0.00008	-0.00012	0.00017	0.00006	1.89487
A14	2.19979	0.00023	0.00001	0.00003	0.00004	2.19983
A15	2.17472	-0.00033	-0.00018	-0.00058	-0.00077	2.17396
A16	1.95002	-0.00093	-0.00055	-0.00020	-0.00075	1.94926
A17	1.88389	0.00012	-0.00096	-0.00064	-0.00160	1.88229
A18	1.89346	0.00041	0.00063	0.00050	0.00113	1.89458
A19	1.91607	0.00010	-0.00061	-0.00044	-0.00104	1.91503
A20	1.92895	0.00044	0.00132	0.00070	0.00202	1.93097
A21	1.88987	-0.00013	0.00015	0.00006	0.00021	1.89009
A22	1.91900	0.00022	-0.00004	0.00033	0.00029	1.91928
A23	1.90813	-0.00130	-0.00137	-0.00022	-0.00159	1.90653
A24	1.85594	0.00058	0.00231	0.00158	0.00389	1.85983
A25	1.89606	0.00020	-0.00045	0.00011	-0.00034	1.89571
A26	1.91988	-0.00022	-0.00131	-0.00116	-0.00247	1.91742
A27	1.96454	0.00051	0.00089	-0.00061	0.00028	1.96482
A28	2.55532	-0.00127	0.00150	-0.00002	0.00148	2.55681
A29	2.15376	-0.00017	-0.00143	-0.00004	-0.00147	2.15229
A30	1.95338	-0.00008	-0.00088	-0.00007	-0.00095	1.95243
A31	2.17514	0.00025	0.00234	0.00009	0.00243	2.17757
A32	2.08496	0.00007	0.00087	0.00005	0.00092	2.08588
A33	2.14656	-0.00009	-0.00090	-0.00022	-0.00112	2.14545
A34	2.05166	0.00003	0.00003	0.00017	0.00020	2.05186
A35	1.89756	0.00012	0.00047	0.00015	0.00061	1.89817
D1	0.00519	0.00002	-0.00067	0.00097	0.00030	0.00549
D2	3.11259	-0.00010	-0.00349	-0.00116	-0.00466	3.10792
D3	-3.12667	0.00009	-0.00033	0.00150	0.00117	-3.12550

D4	-0.01928	-0.00003	-0.00316	-0.00063	-0.00379	-0.02308
D5	-0.04064	0.00005	0.00080	-0.00118	-0.00038	-0.04102
D6	-3.00988	0.00019	0.00252	0.00125	0.00378	-3.00610
D7	3.09226	-0.00001	0.00049	-0.00165	-0.00116	3.09110
D8	0.12302	0.00013	0.00222	0.00078	0.00299	0.12601
D9	0.03175	-0.00008	0.00032	-0.00044	-0.00011	0.03164
D10	3.02917	-0.00011	-0.00088	-0.00042	-0.00130	3.02786
D11	-3.07941	0.00003	0.00284	0.00145	0.00429	-3.07512
D12	-0.08199	0.00000	0.00164	0.00147	0.00309	-0.07889
D13	-0.05748	0.00011	0.00017	-0.00029	-0.00012	-0.05760
D14	-3.11566	0.00005	0.00541	0.00163	0.00705	-3.10861
D15	-3.06278	0.00014	0.00148	-0.00033	0.00114	-3.06164
D16	0.16223	0.00008	0.00672	0.00159	0.00831	0.17053
D17	0.62112	0.00006	0.00578	0.00486	0.01064	0.63176
D18	-2.47661	0.00004	0.00499	0.00529	0.01028	-2.46633
D19	-2.68425	0.00003	0.00433	0.00491	0.00924	-2.67501
D20	0.50120	0.00001	0.00354	0.00534	0.00888	0.51008
D21	0.06073	-0.00010	-0.00059	0.00090	0.00031	0.06104
D22	3.03304	-0.00017	-0.00226	-0.00141	-0.00367	3.02937
D23	3.11843	-0.00003	-0.00578	-0.00105	-0.00683	3.11160
D24	-0.19245	-0.00010	-0.00745	-0.00336	-0.01081	-0.20326
D25	1.28524	0.00026	-0.00802	-0.00354	-0.01157	1.27367
D26	-2.88967	-0.00010	-0.00974	-0.00463	-0.01437	-2.90404
D27	-0.84549	0.00003	-0.00975	-0.00464	-0.01438	-0.85987
D28	-1.65754	0.00038	-0.00604	-0.00083	-0.00687	-1.66441
D29	0.45074	0.00002	-0.00776	-0.00191	-0.00967	0.44107
D30	2.49492	0.00015	-0.00777	-0.00192	-0.00969	2.48523
D31	-1.00202	-0.00008	-0.00692	-0.00271	-0.00963	-1.01165
D32	1.07809	-0.00050	-0.00834	-0.00251	-0.01085	1.06723
D33	-3.07985	-0.00027	-0.00667	-0.00243	-0.00910	-3.08895
D34	-3.09145	0.00030	-0.00496	-0.00149	-0.00645	-3.09790
D35	-1.01134	-0.00012	-0.00638	-0.00129	-0.00767	-1.01901
D36	1.11390	0.00010	-0.00471	-0.00120	-0.00592	1.10799
D37	1.10819	0.00011	-0.00558	-0.00173	-0.00731	1.10087
D38	-3.09489	-0.00030	-0.00700	-0.00153	-0.00853	-3.10343
D39	-0.96965	-0.00008	-0.00533	-0.00144	-0.00678	-0.97643
D40	-0.45686	0.00024	0.02654	0.01004	0.03657	-0.42028
D41	1.63739	-0.00014	0.02540	0.01037	0.03578	1.67317
D42	-2.51525	0.00006	0.02401	0.00858	0.03260	-2.48265
D43	-2.40792	0.00049	0.02034	0.03145	0.05179	-2.35613
D44	1.79801	0.00001	0.01977	0.03076	0.05052	1.84854
D45	-0.31900	-0.00044	0.02066	0.03185	0.05251	-0.26649
D46	-3.08928	-0.00001	0.00014	0.00065	0.00078	-3.08850
D47	0.05043	0.00000	0.00025	0.00052	0.00077	0.05120

D48	0.00286	0.00001	0.00092	0.00016	0.00109	0.00394
D49	-3.14061	0.00002	0.00104	0.00003	0.00107	-3.13954

Item	Value	Threshold	Converged?
Maximum Force	0.001300	0.000450	NO
RMS Force	0.000263	0.000300	YES
Maximum Displacement	0.056138	0.001800	NO
RMS Displacement	0.011326	0.001200	NO

Predicted change in Energy=-5.433097D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.452412	-1.974096	-1.313627
2	6	0	-1.743146	-1.599957	-1.483855
3	7	0	-2.109101	-0.871065	-0.356440
4	6	0	-1.038626	-0.777503	0.456453
5	7	0	-0.035344	-1.480958	-0.083193
6	6	0	1.336289	-1.510358	0.439146
7	6	0	2.236686	-0.497281	-0.276547
8	1	0	0.204982	-2.534674	-1.954864
9	1	0	-2.419253	-1.754063	-2.305097
10	1	0	1.293665	-1.277449	1.502679
11	1	0	1.729678	-2.522496	0.325458
12	1	0	2.246973	-0.701177	-1.354678
13	1	0	1.844028	0.510399	-0.115620
14	35	0	-0.412047	2.081017	0.480937
15	1	0	-1.024946	-0.296628	1.415721
16	6	0	-3.323282	-0.164530	-0.133454
17	6	0	-4.503663	-0.589644	-0.565139
18	1	0	-3.155801	0.772460	0.387874
19	1	0	-5.381385	0.021155	-0.403936
20	1	0	-4.637130	-1.532898	-1.081613
21	8	0	3.545917	-0.666656	0.260789
22	1	0	3.918269	0.199523	0.446159

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.354604	0.000000			
3	N	2.208507	1.391500	0.000000		
4	C	2.215551	2.222066	1.347392	0.000000	

5	N	1.389640	2.211923	2.178785	1.338897	0.000000
6	C	2.546904	3.631650	3.593378	2.485478	1.468018
7	C	3.238482	4.302621	4.362564	3.368009	2.483370
8	H	1.075918	2.211503	3.267650	3.232439	2.161302
9	H	2.213569	1.074852	2.161745	3.238202	3.270239
10	H	3.386102	4.271489	3.898755	2.604634	2.079103
11	H	2.783677	4.023083	4.234198	3.275006	2.089760
12	H	2.984742	4.092132	4.472217	3.752490	2.726481
13	H	3.589091	4.381037	4.194481	3.208685	2.738356
14	Br	4.434640	4.379704	3.506563	2.926489	3.625992
15	H	3.254387	3.259144	2.155440	1.073136	2.151440
16	C	3.592942	2.526038	1.422375	2.437904	3.542040
17	C	4.346214	3.079810	2.420058	3.617378	4.581767
18	H	4.212717	3.335765	2.085846	2.624788	3.877763
19	H	5.394752	4.126866	3.392073	4.498631	5.562318
20	H	4.214303	2.922575	2.711979	3.985662	4.709138
21	O	4.491640	5.647037	5.692275	4.590056	3.688745
22	H	5.188866	6.246176	6.174101	5.052277	4.328428

		6	7	8	9	10
6	C	0.000000				
7	C	1.532729	0.000000			
8	H	2.839078	3.330997	0.000000		
9	H	4.657720	5.231852	2.760185	0.000000	
10	H	1.089571	2.159536	3.836724	5.339670	0.000000
11	H	1.091835	2.172778	2.743121	4.972316	1.768078
12	H	2.168392	1.097290	2.809210	4.877041	3.066818
13	H	2.156159	1.093387	3.916856	5.300675	2.473497
14	Br	3.994546	3.773220	5.255327	5.147689	3.902910
15	H	2.828828	3.679983	4.228760	4.232338	2.519033
16	C	4.883720	5.571754	4.624258	2.838999	5.023119
17	C	5.996778	6.747157	5.280702	2.954334	6.193380
18	H	5.039122	5.579660	5.265018	3.765357	5.024207
19	H	6.941431	7.636754	6.336019	3.942086	7.062425
20	H	6.164005	6.997856	5.021172	2.542599	6.474423
21	O	2.371941	1.425309	4.422721	6.584032	2.643482
22	H	3.096832	1.958460	5.198967	7.179839	3.191587

		11	12	13	14	15
11	H	0.000000				
12	H	2.531334	0.000000			
13	H	3.066932	1.779198	0.000000		
14	Br	5.079714	4.263857	2.812935	0.000000	
15	H	3.705551	4.306300	3.350718	2.627292	0.000000
16	C	5.594909	5.727750	5.211233	3.727633	2.774841
17	C	6.586624	6.797566	6.457968	4.996802	4.013868

18	H	5.893091	5.864985	5.031945	3.041244	2.596143
19	H	7.587450	7.721239	7.247695	5.451638	4.731881
20	H	6.595104	6.939539	6.863936	5.775229	4.562117
21	O	2.597508	2.073206	2.103228	4.823242	4.729015
22	H	3.494838	2.616774	2.171340	4.721533	5.061778

		16	17	18	19	20
16	C	0.000000				
17	C	1.326790	0.000000			
18	H	1.085257	2.140162	0.000000		
19	H	2.084089	1.081415	2.478840	0.000000	
20	H	2.120762	1.083645	3.109406	1.851552	0.000000
21	O	6.898801	8.092208	6.855671	8.978401	8.337547
22	H	7.273827	8.519064	7.097473	9.340132	8.861729

		21	22
21	O	0.000000	
22	H	0.960872	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.158731	-2.254059	-0.618546
2	6	0	-1.455946	-1.887357	-0.751636
3	7	0	-1.677956	-0.841198	0.138608
4	6	0	-0.518238	-0.561202	0.764804
5	7	0	0.406081	-1.438813	0.354831
6	6	0	1.829186	-1.376163	0.709688
7	6	0	2.651221	-0.663425	-0.369905
8	1	0	0.411888	-3.009311	-1.130001
9	1	0	-2.225771	-2.245961	-1.410482
10	1	0	1.914774	-0.837172	1.652730
11	1	0	2.194299	-2.393776	0.862194
12	1	0	2.532154	-1.177550	-1.331957
13	1	0	2.292339	0.363883	-0.476378
14	35	0	0.141116	2.144031	-0.135919
15	1	0	-0.386033	0.180876	1.528652
16	6	0	-2.848909	-0.044552	0.270414
17	6	0	-4.076892	-0.522910	0.116783

18	1	0	-2.610031	0.995892	0.465855
19	1	0	-4.922164	0.148436	0.182117
20	1	0	-4.281498	-1.569478	-0.075879
21	8	0	4.012449	-0.726972	0.047858
22	1	0	4.414387	0.136928	-0.076227

Rotational constants (GHZ): 0.8244192 0.5690358 0.3565924

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 867.0098347454 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 6.86D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Initial guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999999 0.000348 0.000001 -0.001443 Ang= 0.17 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Keep R1 ints in memory in canonical form, NReq=1804729152.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3032.33817051 A.U. after 11 cycles

NFock= 11 Conv=0.40D-08 -V/T= 2.0017

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1

NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000047987	-0.000025028	-0.000038601
2	6	0.000075570	-0.000039524	-0.000099880
3	7	-0.000085709	-0.000211096	0.000135606
4	6	0.000059927	0.000277306	0.000010086
5	7	0.000093481	-0.000004448	0.000020154
6	6	-0.000118380	-0.000028035	-0.000002561
7	6	0.000232647	0.000037138	0.000078810
8	1	-0.000007717	-0.000040053	0.000017912
9	1	-0.000019367	-0.000011523	0.000001457
10	1	-0.000006365	-0.000025929	0.000040944
11	1	-0.000020936	0.000015884	-0.000008365
12	1	0.000041741	0.000000542	0.000083146
13	1	-0.000317572	-0.000111644	-0.000129224
14	35	0.000131457	0.000062828	0.000018213
15	1	-0.000056218	-0.000190028	0.000040396
16	6	-0.000084602	0.000168467	-0.000115231
17	6	-0.000010829	-0.000018181	-0.000027577
18	1	0.000036755	0.000082587	0.000029710
19	1	-0.000024634	0.000045229	0.000010073
20	1	0.000017879	-0.000007529	-0.000019564
21	8	0.000103140	0.000069840	-0.000100847
22	1	0.000007717	-0.000046805	0.000055343

Cartesian Forces: Max 0.000317572 RMS 0.000091999

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000619246 RMS 0.000078240

Search for a local minimum.

Step number 17 out of a maximum of 116

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 13 14 15 16 17

DE= -1.66D-05 DEPred=-5.43D-07 R= 3.05D+01

TightC=F SS= 1.41D+00 RLast= 1.18D-01 DXNew= 1.8091D+00 3.5356D-01

Trust test= 3.05D+01 RLast= 1.18D-01 DXMaxT set to 1.08D+00

ITU= 1 1 1 1 1 1 1 1 1 1 1 1 0 0 -1 0 0

Eigenvalues ---	0.00008	0.00181	0.00472	0.00733	0.01224
Eigenvalues ---	0.01541	0.01585	0.01923	0.02027	0.02092
Eigenvalues ---	0.02306	0.02437	0.03071	0.03103	0.03470
Eigenvalues ---	0.04295	0.04820	0.05450	0.05853	0.06796
Eigenvalues ---	0.08736	0.09318	0.13657	0.14221	0.15410
Eigenvalues ---	0.15737	0.15897	0.15989	0.15998	0.16094
Eigenvalues ---	0.16649	0.19153	0.20863	0.22799	0.22951
Eigenvalues ---	0.24305	0.25328	0.25583	0.29711	0.33267
Eigenvalues ---	0.33865	0.33879	0.33934	0.34120	0.34364
Eigenvalues ---	0.34681	0.34978	0.36120	0.36313	0.36426
Eigenvalues ---	0.37234	0.42801	0.43328	0.45880	0.50710
Eigenvalues ---	0.53677	0.54370	0.55752	0.60652	2.39081

Eigenvalue 1 is 8.23D-05 Eigenvector:

	D45	D43	D44	D40	D41
1	-0.43167	-0.42135	-0.41587	-0.35468	-0.35441
	D42	D26	D27	D25	D29
1	-0.32572	0.13418	0.13144	0.12128	0.10689

En-DIIS/RFO-DIIS IScMMF= 0 using points: 17 16 15 14 13

RFO step: Lambda=-1.93658433D-06.

DidBck=F Rises=F RFO-DIIS coefs: 1.90397 0.69222 -1.57278 0.21018 -0.23359

Iteration 1 RMS(Cart)= 0.04639147 RMS(Int)= 0.00424246

Iteration 2 RMS(Cart)= 0.00740395 RMS(Int)= 0.00006766

Iteration 3 RMS(Cart)= 0.00005934 RMS(Int)= 0.00001990

Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00001990

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55983	-0.00001	0.00055	-0.00004	0.00050	2.56032
R2	2.62604	0.00007	-0.00025	0.00022	-0.00003	2.62601
R3	2.03319	0.00001	-0.00014	0.00000	-0.00013	2.03306
R4	2.62955	0.00010	-0.00097	0.00076	-0.00020	2.62935
R5	2.03118	0.00001	-0.00007	0.00002	-0.00005	2.03113
R6	2.54620	0.00011	-0.00031	0.00037	0.00006	2.54627
R7	2.68790	0.00015	-0.00147	0.00060	-0.00087	2.68703
R8	2.53015	0.00010	0.00056	-0.00001	0.00056	2.53070
R9	2.02793	-0.00005	-0.00054	-0.00025	-0.00079	2.02715
R10	2.77415	0.00004	0.00058	0.00058	0.00116	2.77532
R11	2.89644	0.00017	0.00171	0.00151	0.00322	2.89966
R12	2.05899	0.00003	-0.00016	-0.00001	-0.00017	2.05882
R13	2.06327	-0.00002	0.00023	-0.00010	0.00012	2.06339
R14	2.07358	-0.00008	-0.00069	-0.00069	-0.00137	2.07220
R15	2.06620	0.00002	-0.00044	-0.00013	-0.00058	2.06563

R16	2.69344	0.00007	-0.00099	-0.00012	-0.00111	2.69233
R17	5.31568	-0.00006	0.01301	-0.00021	0.01279	5.32847
R18	2.50727	0.00003	-0.00004	0.00009	0.00004	2.50731
R19	2.05084	0.00008	-0.00091	0.00029	-0.00062	2.05022
R20	2.04358	0.00004	-0.00030	0.00009	-0.00021	2.04337
R21	2.04779	0.00002	-0.00017	0.00000	-0.00018	2.04762
R22	1.81578	-0.00001	-0.00019	-0.00018	-0.00037	1.81542
A1	1.87468	0.00003	-0.00018	0.00029	0.00011	1.87480
A2	2.27997	-0.00002	-0.00077	-0.00023	-0.00102	2.27896
A3	2.12848	-0.00002	0.00092	-0.00004	0.00086	2.12934
A4	1.86863	0.00001	-0.00014	0.00007	-0.00008	1.86855
A5	2.28601	0.00000	0.00009	-0.00013	-0.00008	2.28594
A6	2.12789	-0.00001	-0.00026	0.00012	-0.00018	2.12771
A7	1.89256	-0.00002	0.00077	-0.00058	0.00019	1.89275
A8	2.22902	-0.00002	0.00045	-0.00003	0.00038	2.22940
A9	2.15210	0.00004	0.00061	-0.00026	0.00031	2.15241
A10	1.89197	-0.00001	-0.00055	0.00056	0.00001	1.89198
A11	2.19018	0.00001	0.00045	-0.00021	0.00017	2.19036
A12	2.19711	0.00000	-0.00068	-0.00067	-0.00141	2.19571
A13	1.89487	-0.00002	0.00017	-0.00033	-0.00017	1.89470
A14	2.19983	-0.00007	0.00092	0.00025	0.00111	2.20094
A15	2.17396	0.00009	-0.00272	-0.00037	-0.00314	2.17081
A16	1.94926	0.00008	-0.00185	-0.00030	-0.00216	1.94710
A17	1.88229	0.00000	-0.00347	-0.00070	-0.00419	1.87809
A18	1.89458	-0.00005	0.00309	0.00083	0.00392	1.89850
A19	1.91503	0.00001	-0.00259	-0.00001	-0.00263	1.91240
A20	1.93097	-0.00004	0.00396	-0.00035	0.00362	1.93459
A21	1.89009	0.00001	0.00082	0.00055	0.00138	1.89147
A22	1.91928	-0.00005	0.00117	-0.00025	0.00096	1.92024
A23	1.90653	0.00008	-0.00337	0.00047	-0.00291	1.90362
A24	1.85983	0.00011	0.01038	0.00416	0.01454	1.87437
A25	1.89571	-0.00001	0.00134	-0.00064	0.00068	1.89639
A26	1.91742	-0.00005	-0.00827	-0.00377	-0.01207	1.90535
A27	1.96482	-0.00008	-0.00110	0.00010	-0.00103	1.96379
A28	2.55681	0.00062	0.00165	0.00159	0.00324	2.56004
A29	2.15229	-0.00004	0.00041	0.00008	0.00049	2.15278
A30	1.95243	0.00000	0.00094	-0.00070	0.00025	1.95268
A31	2.17757	0.00004	-0.00134	0.00066	-0.00068	2.17689
A32	2.08588	0.00000	0.00153	-0.00021	0.00132	2.08720
A33	2.14545	-0.00002	-0.00069	-0.00015	-0.00084	2.14460
A34	2.05186	0.00002	-0.00085	0.00037	-0.00048	2.05138
A35	1.89817	0.00006	0.00032	0.00089	0.00121	1.89938
D1	0.00549	-0.00001	0.00187	-0.00119	0.00068	0.00618
D2	3.10792	0.00000	-0.00898	0.00052	-0.00846	3.09946

D3	-3.12550	-0.00002	0.00768	-0.00290	0.00479	-3.12072
D4	-0.02308	-0.00001	-0.00318	-0.00118	-0.00436	-0.02744
D5	-0.04102	0.00002	-0.00094	0.00097	0.00003	-0.04099
D6	-3.00610	-0.00001	0.00943	0.00371	0.01317	-2.99293
D7	3.09110	0.00003	-0.00614	0.00250	-0.00366	3.08744
D8	0.12601	0.00000	0.00423	0.00523	0.00948	0.13549
D9	0.03164	0.00000	-0.00214	0.00099	-0.00115	0.03049
D10	3.02786	-0.00003	0.01132	-0.00562	0.00570	3.03357
D11	-3.07512	-0.00001	0.00751	-0.00052	0.00698	-3.06814
D12	-0.07889	-0.00004	0.02097	-0.00713	0.01383	-0.06506
D13	-0.05760	0.00002	0.00158	-0.00041	0.00117	-0.05642
D14	-3.10861	0.00007	0.01116	0.00330	0.01448	-3.09413
D15	-3.06164	0.00005	-0.01114	0.00582	-0.00532	-3.06696
D16	0.17053	0.00011	-0.00156	0.00953	0.00799	0.17852
D17	0.63176	0.00003	-0.01638	0.00526	-0.01113	0.62064
D18	-2.46633	0.00002	-0.01669	0.00421	-0.01248	-2.47881
D19	-2.67501	-0.00001	-0.00108	-0.00228	-0.00335	-2.67836
D20	0.51008	-0.00002	-0.00139	-0.00332	-0.00470	0.50538
D21	0.06104	-0.00002	-0.00042	-0.00033	-0.00075	0.06029
D22	3.02937	-0.00001	-0.01018	-0.00293	-0.01309	3.01628
D23	3.11160	-0.00008	-0.00999	-0.00403	-0.01401	3.09760
D24	-0.20326	-0.00007	-0.01974	-0.00663	-0.02634	-0.22960
D25	1.27367	-0.00002	-0.05792	-0.01104	-0.06896	1.20471
D26	-2.90404	0.00003	-0.06454	-0.01169	-0.07622	-2.98026
D27	-0.85987	0.00001	-0.06380	-0.01098	-0.07478	-0.93465
D28	-1.66441	-0.00005	-0.04630	-0.00791	-0.05421	-1.71862
D29	0.44107	0.00001	-0.05292	-0.00856	-0.06148	0.37959
D30	2.48523	-0.00001	-0.05218	-0.00785	-0.06003	2.42520
D31	-1.01165	0.00004	-0.02140	-0.00756	-0.02895	-1.04060
D32	1.06723	0.00004	-0.02111	-0.00821	-0.02932	1.03791
D33	-3.08895	0.00006	-0.01816	-0.00534	-0.02351	-3.11246
D34	-3.09790	-0.00002	-0.01415	-0.00649	-0.02063	-3.11853
D35	-1.01901	-0.00001	-0.01386	-0.00713	-0.02100	-1.04002
D36	1.10799	0.00000	-0.01091	-0.00427	-0.01519	1.09280
D37	1.10087	-0.00001	-0.01600	-0.00694	-0.02293	1.07795
D38	-3.10343	0.00000	-0.01571	-0.00759	-0.02330	-3.12673
D39	-0.97643	0.00001	-0.01276	-0.00472	-0.01749	-0.99392
D40	-0.42028	0.00010	0.15124	0.04859	0.19982	-0.22047
D41	1.67317	0.00008	0.15147	0.04818	0.19966	1.87283
D42	-2.48265	-0.00004	0.14120	0.04303	0.18423	-2.29842
D43	-2.35613	-0.00002	0.15677	0.06158	0.21829	-2.13783
D44	1.84854	0.00000	0.15380	0.06151	0.21538	2.06392
D45	-0.26649	0.00010	0.15871	0.06491	0.22361	-0.04288
D46	-3.08850	-0.00002	0.00094	-0.00153	-0.00060	-3.08909

D47	0.05120	-0.00001	-0.00008	-0.00017	-0.00024	0.05096
D48	0.00394	-0.00001	0.00135	-0.00039	0.00096	0.00490
D49	-3.13954	0.00000	0.00034	0.00097	0.00131	-3.13823

Item	Value	Threshold	Converged?
Maximum Force	0.000619	0.000450	NO
RMS Force	0.000078	0.000300	YES
Maximum Displacement	0.221590	0.001800	NO
RMS Displacement	0.047928	0.001200	NO

Predicted change in Energy=-3.407302D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.447780	-1.957293	-1.316461
2	6	0	-1.738981	-1.583851	-1.486755
3	7	0	-2.110442	-0.869707	-0.351859
4	6	0	-1.043533	-0.784946	0.466724
5	7	0	-0.036333	-1.479205	-0.078239
6	6	0	1.336189	-1.497566	0.443997
7	6	0	2.244289	-0.527048	-0.322772
8	1	0	0.213489	-2.505226	-1.964490
9	1	0	-2.409490	-1.722958	-2.315197
10	1	0	1.293614	-1.206076	1.492896
11	1	0	1.720805	-2.517816	0.385648
12	1	0	2.273737	-0.799817	-1.384458
13	1	0	1.841760	0.485236	-0.232881
14	35	0	-0.349219	2.091126	0.523073
15	1	0	-1.037598	-0.327365	1.436937
16	6	0	-3.328954	-0.173980	-0.121576
17	6	0	-4.505059	-0.595366	-0.568392
18	1	0	-3.169538	0.752060	0.420744
19	1	0	-5.387195	0.006812	-0.399766
20	1	0	-4.630510	-1.528385	-1.104883
21	8	0	3.553470	-0.644423	0.226864
22	1	0	3.837628	0.218915	0.537997

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.354866	0.000000			
3	N	2.208561	1.391392	0.000000		

4	C	2.215641	2.222156	1.347426	0.000000	
5	N	1.389622	2.212211	2.179055	1.339190	0.000000
6	C	2.548157	3.632068	3.592612	2.484234	1.468634
7	C	3.206283	4.282305	4.368289	3.391105	2.483473
8	H	1.075849	2.211177	3.267439	3.232688	2.161730
9	H	2.213751	1.074825	2.161518	3.238022	3.270363
10	H	3.389581	4.268216	3.886369	2.587013	2.076493
11	H	2.813205	4.043304	4.235402	3.263583	2.093189
12	H	2.958214	4.089876	4.504683	3.798865	2.739380
13	H	3.518819	4.321462	4.179704	3.229199	2.722164
14	Br	4.447841	4.413196	3.554426	2.959229	3.634107
15	H	3.253575	3.258630	2.155208	1.072721	2.150587
16	C	3.592927	2.525760	1.421914	2.437730	3.542152
17	C	4.344648	3.077609	2.419988	3.617951	4.581586
18	H	4.215025	3.337892	2.085361	2.623813	3.878723
19	H	5.394058	4.125678	3.392299	4.499454	5.562674
20	H	4.209983	2.917163	2.711391	3.986107	4.707746
21	O	4.485028	5.641724	5.697857	4.605401	3.698193
22	H	5.151660	6.200657	6.111994	4.983828	4.274451

		6	7	8	9	10
6	C	0.000000				
7	C	1.534433	0.000000			
8	H	2.841945	3.276062	0.000000		
9	H	4.657689	5.201694	2.759521	0.000000	
10	H	1.089480	2.159053	3.848114	5.336827	0.000000
11	H	1.091899	2.176936	2.792009	4.998570	1.768941
12	H	2.170046	1.096562	2.736691	4.863238	3.066733
13	H	2.155289	1.093083	3.820027	5.223533	2.477762
14	Br	3.965547	3.781081	5.256526	5.181480	3.809330
15	H	2.826688	3.729240	4.228239	4.231818	2.491950
16	C	4.882143	5.588039	4.623846	2.838437	5.003987
17	C	5.996589	6.754162	5.278386	2.951983	6.184374
18	H	5.036162	5.612349	5.267269	3.766797	4.990344
19	H	6.941108	7.650522	6.334537	3.940521	7.048863
20	H	6.164533	6.991226	5.015722	2.536858	6.476695
21	O	2.385652	1.424721	4.406824	6.571317	2.650516
22	H	3.035183	1.958599	5.178587	7.137091	3.068295

		11	12	13	14	15
11	H	0.000000				
12	H	2.527950	0.000000			
13	H	3.068474	1.778791	0.000000		
14	Br	5.054328	4.344667	2.819705	0.000000	
15	H	3.675877	4.375891	3.426268	2.675464	0.000000
16	C	5.590252	5.777257	5.213755	3.798039	2.775393

17	C	6.585392	6.830801	6.446889	5.067498	4.014531
18	H	5.882922	5.941071	5.060783	3.123742	2.596724
19	H	7.583817	7.765961	7.246691	5.529665	4.733302
20	H	6.598474	6.948208	6.834130	5.837855	4.562052
21	O	2.625542	2.063546	2.101773	4.775139	4.758435
22	H	3.463212	2.679440	2.156077	4.586402	4.987418

		16	17	18	19	20
16	C	0.000000				
17	C	1.326813	0.000000			
18	H	1.084930	2.139523	0.000000		
19	H	2.084809	1.081303	2.479240	0.000000	
20	H	2.120224	1.083552	3.108441	1.851106	0.000000
21	O	6.907278	8.097822	6.869250	8.986226	8.338613
22	H	7.207586	8.455032	7.028397	9.274790	8.801219

		21	22
21	O	0.000000	
22	H	0.960678	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.230855	-2.247247	-0.607789
2	6	0	-1.517964	-1.849187	-0.751177
3	7	0	-1.721823	-0.798652	0.138086
4	6	0	-0.561251	-0.547978	0.775104
5	7	0	0.345352	-1.447190	0.371468
6	6	0	1.769271	-1.407019	0.728857
7	6	0	2.614316	-0.785008	-0.390735
8	1	0	0.325730	-3.013311	-1.118483
9	1	0	-2.288609	-2.183668	-1.421608
10	1	0	1.865091	-0.808299	1.634019
11	1	0	2.104753	-2.422176	0.950562
12	1	0	2.504643	-1.368866	-1.312435
13	1	0	2.264578	0.233485	-0.578311
14	35	0	0.244111	2.149908	-0.135849
15	1	0	-0.420491	0.181026	1.549357
16	6	0	-2.876052	0.021900	0.265728

17	6	0	-4.112809	-0.427520	0.095771
18	1	0	-2.616935	1.054562	0.474395
19	1	0	-4.944413	0.260666	0.159417
20	1	0	-4.337795	-1.467542	-0.108732
21	8	0	3.974939	-0.825899	0.029816
22	1	0	4.327420	0.067773	0.026577

Rotational constants (GHZ): 0.8186181 0.5666829 0.3549945

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 865.0957244764 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 6.98D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Initial guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999867 0.001420 0.001150 0.016196 Ang= 1.87 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Keep R1 ints in memory in canonical form, NReq=1804729152.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3032.33816582 A.U. after 11 cycles

NFock= 11 Conv=0.87D-08 -V/T= 2.0017

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000153152	0.000078360	0.000217024
2	6	0.000273414	0.000254801	-0.000201547
3	7	0.000252544	-0.000113743	0.000334139
4	6	0.000420477	-0.000231095	-0.000690815
5	7	-0.000208805	0.000576788	0.000019979
6	6	-0.000071944	-0.000141499	0.000238169
7	6	0.000266247	0.000176647	0.000090173
8	1	-0.000007914	-0.000104619	0.000051697
9	1	-0.000080755	-0.000190168	0.000050684
10	1	0.000023666	-0.000079286	0.000095744
11	1	-0.000011274	0.000067174	-0.000218293
12	1	0.000295359	-0.000092334	0.000288008
13	1	-0.000365929	0.000023282	0.000045366
14	35	-0.000399007	-0.001660710	0.000130448
15	1	0.000185999	0.000831430	-0.000067710
16	6	-0.000114446	0.000368866	-0.000027164
17	6	0.000041999	-0.000038803	-0.000018006
18	1	-0.000110840	0.000193607	0.000020551
19	1	-0.000011973	0.000136054	0.000067396
20	1	0.000022880	-0.000023492	-0.000058670
21	8	-0.000117986	-0.000304452	-0.000575891
22	1	-0.000128560	0.000273189	0.000208718

Cartesian Forces: Max 0.001660710 RMS 0.000317020

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.008513194 RMS 0.001347858

Search for a local minimum.

Step number 18 out of a maximum of 116

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 13 14 15 16 18 17

DE= 4.68D-06 DEPred=-3.41D-05 R=-1.37D-01

Trust test=-1.37D-01 RLast= 5.40D-01 DXMaxT set to 5.38D-01

ITU= -1 1 1 1 1 1 1 1 1 1 1 1 1 0 0 -1 0 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.39324.

Iteration 1 RMS(Cart)= 0.01917354 RMS(Int)= 0.00046577

Iteration 2 RMS(Cart)= 0.00094808 RMS(Int)= 0.00000302

Iteration 3 RMS(Cart)= 0.00000096 RMS(Int)= 0.00000290

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56032	0.00006	-0.00019	0.00000	-0.00019	2.56013
R2	2.62601	-0.00025	0.00001	0.00000	0.00001	2.62602
R3	2.03306	0.00002	0.00005	0.00000	0.00005	2.03311
R4	2.62935	0.00024	0.00008	0.00000	0.00008	2.62943
R5	2.03113	0.00003	0.00002	0.00000	0.00002	2.03115
R6	2.54627	-0.00037	-0.00003	0.00000	-0.00003	2.54624
R7	2.68703	0.00044	0.00034	0.00000	0.00034	2.68737
R8	2.53070	-0.00039	-0.00022	0.00000	-0.00022	2.53048
R9	2.02715	0.00030	0.00031	0.00000	0.00031	2.02746
R10	2.77532	-0.00037	-0.00046	0.00000	-0.00046	2.77486
R11	2.89966	-0.00131	-0.00127	0.00000	-0.00127	2.89839
R12	2.05882	0.00007	0.00007	0.00000	0.00007	2.05889
R13	2.06339	-0.00006	-0.00005	0.00000	-0.00005	2.06334
R14	2.07220	-0.00024	0.00054	0.00000	0.00054	2.07274
R15	2.06563	-0.00121	0.00023	0.00000	0.00023	2.06585
R16	2.69233	-0.00038	0.00044	0.00000	0.00044	2.69277
R17	5.32847	-0.00060	-0.00503	0.00000	-0.00503	5.32344
R18	2.50731	-0.00006	-0.00002	0.00000	-0.00002	2.50730
R19	2.05022	0.00016	0.00024	0.00000	0.00024	2.05046
R20	2.04337	0.00009	0.00008	0.00000	0.00008	2.04345
R21	2.04762	0.00005	0.00007	0.00000	0.00007	2.04769
R22	1.81542	0.00028	0.00014	0.00000	0.00014	1.81556
A1	1.87480	-0.00014	-0.00005	0.00000	-0.00005	1.87475
A2	2.27896	0.00009	0.00040	0.00000	0.00040	2.27936
A3	2.12934	0.00005	-0.00034	0.00000	-0.00033	2.12900
A4	1.86855	-0.00003	0.00003	0.00000	0.00003	1.86859
A5	2.28594	-0.00001	0.00003	0.00000	0.00003	2.28597
A6	2.12771	0.00003	0.00007	0.00000	0.00007	2.12778
A7	1.89275	-0.00016	-0.00007	0.00000	-0.00008	1.89267
A8	2.22940	0.00020	-0.00015	0.00000	-0.00015	2.22925
A9	2.15241	-0.00006	-0.00012	0.00000	-0.00012	2.15230
A10	1.89198	0.00018	0.00000	0.00000	0.00000	1.89198
A11	2.19036	-0.00013	-0.00007	0.00000	-0.00006	2.19030
A12	2.19571	0.00000	0.00055	0.00000	0.00056	2.19627

A13	1.89470	0.00014	0.00006	0.00000	0.00007	1.89477
A14	2.20094	0.00121	-0.00044	0.00000	-0.00043	2.20051
A15	2.17081	-0.00144	0.00124	0.00000	0.00124	2.17206
A16	1.94710	-0.00420	0.00085	0.00000	0.00085	1.94795
A17	1.87809	0.00081	0.00165	0.00000	0.00165	1.87974
A18	1.89850	0.00180	-0.00154	0.00000	-0.00154	1.89696
A19	1.91240	0.00024	0.00103	0.00000	0.00104	1.91344
A20	1.93459	0.00191	-0.00142	0.00000	-0.00142	1.93317
A21	1.89147	-0.00050	-0.00054	0.00000	-0.00055	1.89092
A22	1.92024	0.00132	-0.00038	0.00000	-0.00038	1.91986
A23	1.90362	-0.00631	0.00115	0.00000	0.00115	1.90476
A24	1.87437	0.00229	-0.00572	0.00000	-0.00572	1.86865
A25	1.89639	0.00133	-0.00027	0.00000	-0.00026	1.89613
A26	1.90535	-0.00108	0.00475	0.00000	0.00475	1.91010
A27	1.96379	0.00245	0.00040	0.00000	0.00041	1.96420
A28	2.56004	-0.00851	-0.00127	0.00000	-0.00127	2.55877
A29	2.15278	0.00004	-0.00019	0.00000	-0.00019	2.15258
A30	1.95268	0.00013	-0.00010	0.00000	-0.00010	1.95258
A31	2.17689	-0.00017	0.00027	0.00000	0.00027	2.17716
A32	2.08720	-0.00013	-0.00052	0.00000	-0.00052	2.08668
A33	2.14460	0.00004	0.00033	0.00000	0.00033	2.14494
A34	2.05138	0.00009	0.00019	0.00000	0.00019	2.05157
A35	1.89938	-0.00030	-0.00048	0.00000	-0.00048	1.89891
D1	0.00618	0.00019	-0.00027	0.00000	-0.00027	0.00591
D2	3.09946	0.00003	0.00333	0.00000	0.00333	3.10279
D3	-3.12072	0.00020	-0.00188	0.00000	-0.00188	-3.12260
D4	-0.02744	0.00004	0.00171	0.00000	0.00171	-0.02572
D5	-0.04099	-0.00009	-0.00001	0.00000	-0.00001	-0.04100
D6	-2.99293	0.00059	-0.00518	0.00000	-0.00518	-2.99812
D7	3.08744	-0.00011	0.00144	0.00000	0.00144	3.08888
D8	0.13549	0.00058	-0.00373	0.00000	-0.00373	0.13176
D9	0.03049	-0.00022	0.00045	0.00000	0.00045	0.03094
D10	3.03357	-0.00037	-0.00224	0.00000	-0.00224	3.03132
D11	-3.06814	-0.00008	-0.00275	0.00000	-0.00275	-3.07088
D12	-0.06506	-0.00023	-0.00544	0.00000	-0.00544	-0.07050
D13	-0.05642	0.00016	-0.00046	0.00000	-0.00046	-0.05689
D14	-3.09413	-0.00038	-0.00569	0.00000	-0.00570	-3.09983
D15	-3.06696	0.00028	0.00209	0.00000	0.00209	-3.06487
D16	0.17852	-0.00026	-0.00314	0.00000	-0.00314	0.17538
D17	0.62064	0.00008	0.00437	0.00000	0.00438	0.62501
D18	-2.47881	0.00011	0.00491	0.00000	0.00491	-2.47390
D19	-2.67836	-0.00009	0.00132	0.00000	0.00132	-2.67705
D20	0.50538	-0.00006	0.00185	0.00000	0.00185	0.50723
D21	0.06029	-0.00003	0.00030	0.00000	0.00030	0.06059

D22	3.01628	-0.00035	0.00515	0.00000	0.00514	3.02142
D23	3.09760	0.00050	0.00551	0.00000	0.00551	3.10310
D24	-0.22960	0.00018	0.01036	0.00000	0.01035	-0.21925
D25	1.20471	0.00143	0.02712	0.00000	0.02712	1.23183
D26	-2.98026	-0.00026	0.02997	0.00000	0.02997	-2.95029
D27	-0.93465	0.00055	0.02941	0.00000	0.02941	-0.90525
D28	-1.71862	0.00200	0.02132	0.00000	0.02132	-1.69730
D29	0.37959	0.00030	0.02418	0.00000	0.02417	0.40376
D30	2.42520	0.00111	0.02361	0.00000	0.02361	2.44881
D31	-1.04060	-0.00042	0.01138	0.00000	0.01138	-1.02922
D32	1.03791	-0.00185	0.01153	0.00000	0.01153	1.04944
D33	-3.11246	-0.00121	0.00925	0.00000	0.00925	-3.10322
D34	-3.11853	0.00105	0.00811	0.00000	0.00811	-3.11042
D35	-1.04002	-0.00039	0.00826	0.00000	0.00826	-1.03175
D36	1.09280	0.00026	0.00597	0.00000	0.00597	1.09877
D37	1.07795	0.00032	0.00902	0.00000	0.00901	1.08696
D38	-3.12673	-0.00111	0.00916	0.00000	0.00916	-3.11756
D39	-0.99392	-0.00047	0.00688	0.00000	0.00688	-0.98704
D40	-0.22047	0.00037	-0.07858	0.00000	-0.07857	-0.29904
D41	1.87283	-0.00096	-0.07852	0.00000	-0.07852	1.79431
D42	-2.29842	0.00018	-0.07245	0.00000	-0.07245	-2.37087
D43	-2.13783	0.00247	-0.08584	0.00000	-0.08583	-2.22367
D44	2.06392	0.00017	-0.08470	0.00000	-0.08471	1.97921
D45	-0.04288	-0.00235	-0.08793	0.00000	-0.08793	-0.13081
D46	-3.08909	0.00000	0.00023	0.00000	0.00023	-3.08886
D47	0.05096	-0.00001	0.00010	0.00000	0.00010	0.05105
D48	0.00490	-0.00002	-0.00038	0.00000	-0.00038	0.00453
D49	-3.13823	-0.00003	-0.00052	0.00000	-0.00052	-3.13875

Item	Value	Threshold	Converged?
Maximum Force	0.008513	0.000450	NO
RMS Force	0.001348	0.000300	NO
Maximum Displacement	0.085834	0.001800	NO
RMS Displacement	0.019028	0.001200	NO

Predicted change in Energy=-5.590759D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.449637	-1.964129	-1.315184
2	6	0	-1.740583	-1.590190	-1.485511
3	7	0	-2.109713	-0.869899	-0.353692

4	6	0	-1.041368	-0.781696	0.462629
5	7	0	-0.035861	-1.479908	-0.080117
6	6	0	1.336339	-1.502781	0.442109
7	6	0	2.241614	-0.515575	-0.305106
8	1	0	0.209985	-2.517333	-1.960453
9	1	0	-2.413340	-1.735266	-2.311116
10	1	0	1.293817	-1.233985	1.497090
11	1	0	1.724184	-2.520313	0.362149
12	1	0	2.263461	-0.761647	-1.373772
13	1	0	1.843155	0.495603	-0.187459
14	35	0	-0.378502	2.082050	0.507634
15	1	0	-1.032274	-0.314700	1.428503
16	6	0	-3.326379	-0.169604	-0.126388
17	6	0	-4.504266	-0.592359	-0.567149
18	1	0	-3.163586	0.760890	0.407494
19	1	0	-5.384542	0.013445	-0.401538
20	1	0	-4.633075	-1.529553	-1.095581
21	8	0	3.550825	-0.653666	0.240226
22	1	0	3.870097	0.213735	0.502388

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.354763	0.000000			
3	N	2.208542	1.391435	0.000000		
4	C	2.215606	2.222119	1.347412	0.000000	
5	N	1.389629	2.212097	2.178949	1.339074	0.000000
6	C	2.547671	3.631915	3.592925	2.484728	1.468392
7	C	3.218912	4.290227	4.366000	3.382042	2.483435
8	H	1.075876	2.211307	3.267525	3.232591	2.161563
9	H	2.213682	1.074836	2.161610	3.238095	3.270316
10	H	3.388454	4.269704	3.891268	2.593793	2.077523
11	H	2.801479	4.035293	4.234981	3.268205	2.091841
12	H	2.968214	4.090395	4.491874	3.780829	2.734287
13	H	3.546680	4.344956	4.185379	3.220959	2.728529
14	Br	4.438388	4.394683	3.528877	2.939806	3.626349
15	H	3.253905	3.258842	2.155305	1.072884	2.150926
16	C	3.592937	2.525872	1.422095	2.437800	3.542111
17	C	4.345265	3.078474	2.420015	3.617727	4.581658
18	H	4.214127	3.337062	2.085552	2.624199	3.878351
19	H	5.394333	4.126146	3.392210	4.499132	5.562536
20	H	4.211678	2.919286	2.711622	3.985933	4.708291
21	O	4.487795	5.643956	5.695716	4.599358	3.694538
22	H	5.167858	6.219776	6.137203	5.011482	4.297004

		6	7	8	9	10
6	C	0.000000				
7	C	1.533763	0.000000			
8	H	2.840826	3.297685	0.000000		
9	H	4.657723	5.213475	2.759787	0.000000	
10	H	1.089516	2.159246	3.843992	5.338232	0.000000
11	H	1.091874	2.175302	2.772596	4.988161	1.768600
12	H	2.169391	1.096848	2.764668	4.868163	3.066784
13	H	2.155634	1.093202	3.858567	5.253993	2.476076
14	Br	3.974417	3.777991	5.252818	5.163121	3.843405
15	H	2.827514	3.710000	4.228454	4.232032	2.502097
16	C	4.882774	5.581593	4.624013	2.838657	5.011466
17	C	5.996677	6.751404	5.279297	2.952902	6.187934
18	H	5.037334	5.599406	5.266394	3.766233	5.003517
19	H	6.941248	7.645091	6.335123	3.941132	7.054172
20	H	6.164341	6.993879	5.017862	2.539107	6.475905
21	O	2.380273	1.424952	4.413327	6.576508	2.647747
22	H	3.061044	1.958544	5.188520	7.155137	3.118099

		11	12	13	14	15
11	H	0.000000				
12	H	2.529258	0.000000			
13	H	3.067893	1.778954	0.000000		
14	Br	5.062035	4.313499	2.817043	0.000000	
15	H	3.687805	4.349067	3.396471	2.649496	0.000000
16	C	5.592199	5.757846	5.212515	3.763231	2.775186
17	C	6.585908	6.817729	6.451168	5.032847	4.014280
18	H	5.887160	5.911334	5.048941	3.084183	2.596506
19	H	7.585324	7.748416	7.246924	5.492372	4.732754
20	H	6.597069	6.944730	6.845984	5.806493	4.562086
21	O	2.614546	2.067355	2.102349	4.795338	4.746757
22	H	3.478451	2.655678	2.159591	4.641252	5.016988

		16	17	18	19	20
16	C	0.000000				
17	C	1.326804	0.000000			
18	H	1.085059	2.139775	0.000000		
19	H	2.084526	1.081347	2.479083	0.000000	
20	H	2.120436	1.083589	3.108820	1.851281	0.000000
21	O	6.903959	8.095684	6.863837	8.983189	8.338331
22	H	7.234056	8.480781	7.055571	9.300835	8.825898

		21	22
21	O	0.000000	
22	H	0.960754	0.000000

Stoichiometry C7H11BrN2O

Framework group C1[X(C7H11BrN2O)]

Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.196092	-2.250126	-0.610464
2	6	0	-1.488112	-1.867296	-0.750136
3	7	0	-1.701268	-0.817814	0.138258
4	6	0	-0.541428	-0.552372	0.770580
5	7	0	0.374065	-1.441671	0.365441
6	6	0	1.797636	-1.389186	0.721624
7	6	0	2.632545	-0.730660	-0.383681
8	1	0	0.367605	-3.011392	-1.120590
9	1	0	-2.257873	-2.213707	-1.415522
10	1	0	1.887924	-0.812312	1.641465
11	1	0	2.146967	-2.404975	0.917403
12	1	0	2.520689	-1.288791	-1.321260
13	1	0	2.277003	0.291109	-0.540743
14	35	0	0.195339	2.145416	-0.135828
15	1	0	-0.405431	0.183020	1.539855
16	6	0	-2.863849	-0.008945	0.266676
17	6	0	-4.096288	-0.472607	0.103830
18	1	0	-2.614833	1.027620	0.468858
19	1	0	-4.934752	0.207282	0.167404
20	1	0	-4.311096	-1.515966	-0.094727
21	8	0	3.993390	-0.776984	0.036371
22	1	0	4.363752	0.107990	-0.015600

Rotational constants (GHZ): 0.8226282 0.5678583 0.3560149
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 358 symmetry adapted cartesian basis functions of A symmetry.
There are 345 symmetry adapted basis functions of A symmetry.
345 basis functions, 553 primitive gaussians, 358 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 866.2315215003 Hartrees.
NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.
NBasis= 345 RedAO= T EigKep= 6.93D-06 NBF= 345
NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345
Lowest energy guess from the checkpoint file: "."
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999963 0.001018 0.000643 0.008492 Ang= 0.98 deg.
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999970 -0.000404 -0.000509 -0.007702 Ang= -0.89 deg.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.33819882 A.U. after 9 cycles
NFock= 9 Conv=0.72D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000135200	0.000039715	0.000060406
2	6	0.000224677	0.000122599	-0.000187946
3	7	0.000021101	-0.000191107	0.000256114
4	6	0.000273330	0.000026955	-0.000328222
5	7	-0.000042187	0.000272126	0.000034981
6	6	-0.000136969	-0.000076793	0.000144983
7	6	0.000222030	0.000121783	0.000055672
8	1	-0.000004106	-0.000074606	0.000039974
9	1	-0.000055660	-0.000122312	0.000032909
10	1	0.000026577	-0.000065233	0.000063212
11	1	-0.000011290	0.000049465	-0.000130570
12	1	0.000164719	-0.000055659	0.000180894
13	1	-0.000338028	-0.000057204	-0.000009987
14	35	-0.000126259	-0.000745069	0.000062919
15	1	0.000052680	0.000298581	-0.000014585
16	6	-0.000075086	0.000259786	-0.000069089
17	6	0.000008984	-0.000034855	-0.000027694
18	1	-0.000035116	0.000149323	0.000024732
19	1	-0.000017679	0.000101106	0.000042512
20	1	0.000019503	-0.000019818	-0.000042545
21	8	0.000034050	-0.000084799	-0.000328338
22	1	-0.000070071	0.000086017	0.000139669

Cartesian Forces: Max 0.000745069 RMS 0.000163748

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.003710213 RMS 0.000616277

Search for a local minimum.

Step number 19 out of a maximum of 116

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 16 18 17 19

ITU= 0 -1 1 1 1 1 1 1 1 1 1 1 1 0 0 -1 0 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00017	0.00224	0.00492	0.00851	0.01017
Eigenvalues ---	0.01273	0.01603	0.01772	0.01994	0.02078
Eigenvalues ---	0.02224	0.02426	0.03069	0.03093	0.03478
Eigenvalues ---	0.04287	0.04774	0.05451	0.05822	0.06847
Eigenvalues ---	0.08769	0.09312	0.13658	0.14265	0.15486
Eigenvalues ---	0.15729	0.15882	0.15972	0.15997	0.16060
Eigenvalues ---	0.16674	0.18800	0.20929	0.22799	0.22967
Eigenvalues ---	0.24244	0.25107	0.25590	0.29721	0.33107
Eigenvalues ---	0.33837	0.33869	0.33879	0.34119	0.34318
Eigenvalues ---	0.34576	0.34683	0.36107	0.36312	0.36378
Eigenvalues ---	0.37239	0.42690	0.43116	0.45815	0.49537
Eigenvalues ---	0.53631	0.54397	0.55759	0.60582	3.06059

RFO step: Lambda=-6.46927218D-05 EMin= 1.67988332D-04

Quartic linear search produced a step of -0.12128.

Iteration 1 RMS(Cart)= 0.02856576 RMS(Int)= 0.00196687

Iteration 2 RMS(Cart)= 0.00217183 RMS(Int)= 0.00000943

Iteration 3 RMS(Cart)= 0.00000784 RMS(Int)= 0.00000772

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000772

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56013	0.00000	-0.00004	0.00016	0.00012	2.56025
R2	2.62602	-0.00006	0.00000	0.00029	0.00029	2.62631
R3	2.03311	0.00001	0.00001	-0.00002	-0.00001	2.03310
R4	2.62943	0.00020	0.00001	0.00096	0.00098	2.63041
R5	2.03115	0.00002	0.00000	0.00005	0.00006	2.03120
R6	2.54624	-0.00011	0.00000	-0.00009	-0.00008	2.54616
R7	2.68737	0.00028	0.00006	0.00208	0.00215	2.68952
R8	2.53048	-0.00016	-0.00004	0.00047	0.00043	2.53091
R9	2.02746	0.00012	0.00006	-0.00059	-0.00053	2.02693

R10	2.77486	-0.00016	-0.00009	0.00148	0.00140	2.77626
R11	2.89839	-0.00054	-0.00024	0.00356	0.00333	2.90172
R12	2.05889	0.00004	0.00001	0.00011	0.00012	2.05901
R13	2.06334	-0.00004	-0.00001	-0.00026	-0.00027	2.06307
R14	2.07274	-0.00016	0.00010	-0.00164	-0.00154	2.07120
R15	2.06585	-0.00056	0.00004	-0.00053	-0.00049	2.06536
R16	2.69277	-0.00012	0.00008	-0.00142	-0.00133	2.69144
R17	5.32344	-0.00030	-0.00094	0.00094	-0.00001	5.32343
R18	2.50730	-0.00001	0.00000	-0.00019	-0.00019	2.50710
R19	2.05046	0.00013	0.00005	0.00051	0.00056	2.05102
R20	2.04345	0.00007	0.00002	-0.00001	0.00001	2.04346
R21	2.04769	0.00004	0.00001	-0.00010	-0.00009	2.04760
R22	1.81556	0.00010	0.00003	-0.00012	-0.00009	1.81547
A1	1.87475	-0.00004	-0.00001	0.00002	0.00001	1.87477
A2	2.27936	0.00004	0.00007	-0.00052	-0.00045	2.27891
A3	2.12900	0.00000	-0.00006	0.00052	0.00046	2.12946
A4	1.86859	-0.00001	0.00001	0.00009	0.00010	1.86869
A5	2.28597	0.00000	0.00001	0.00038	0.00038	2.28635
A6	2.12778	0.00001	0.00001	-0.00058	-0.00057	2.12721
A7	1.89267	-0.00009	-0.00001	-0.00028	-0.00030	1.89237
A8	2.22925	0.00011	-0.00003	-0.00142	-0.00148	2.22777
A9	2.15230	-0.00003	-0.00002	0.00016	0.00010	2.15240
A10	1.89198	0.00009	0.00000	0.00034	0.00034	1.89231
A11	2.19030	-0.00007	-0.00001	0.00011	0.00008	2.19038
A12	2.19627	0.00000	0.00010	-0.00142	-0.00133	2.19494
A13	1.89477	0.00006	0.00001	-0.00006	-0.00005	1.89471
A14	2.20051	0.00056	-0.00008	0.00029	0.00019	2.20070
A15	2.17206	-0.00066	0.00023	-0.00171	-0.00149	2.17056
A16	1.94795	-0.00201	0.00016	-0.00110	-0.00094	1.94701
A17	1.87974	0.00042	0.00031	-0.00279	-0.00248	1.87726
A18	1.89696	0.00084	-0.00029	0.00182	0.00153	1.89850
A19	1.91344	0.00013	0.00019	-0.00056	-0.00037	1.91307
A20	1.93317	0.00089	-0.00027	0.00158	0.00131	1.93448
A21	1.89092	-0.00024	-0.00010	0.00101	0.00091	1.89183
A22	1.91986	0.00057	-0.00007	0.00052	0.00047	1.92033
A23	1.90476	-0.00295	0.00021	-0.00120	-0.00100	1.90376
A24	1.86865	0.00118	-0.00107	0.01228	0.01121	1.87986
A25	1.89613	0.00063	-0.00005	-0.00104	-0.00110	1.89503
A26	1.91010	-0.00054	0.00089	-0.01030	-0.00941	1.90068
A27	1.96420	0.00110	0.00007	-0.00011	-0.00006	1.96415
A28	2.55877	-0.00371	-0.00024	0.00246	0.00222	2.56099
A29	2.15258	0.00003	-0.00004	-0.00243	-0.00247	2.15012
A30	1.95258	0.00005	-0.00002	-0.00185	-0.00187	1.95071
A31	2.17716	-0.00008	0.00005	0.00431	0.00436	2.18152

A32	2.08668	-0.00008	-0.00010	0.00092	0.00082	2.08751
A33	2.14494	0.00002	0.00006	-0.00180	-0.00174	2.14319
A34	2.05157	0.00006	0.00004	0.00088	0.00092	2.05249
A35	1.89891	-0.00011	-0.00009	0.00122	0.00113	1.90004
D1	0.00591	0.00008	-0.00005	-0.00086	-0.00091	0.00500
D2	3.10279	0.00002	0.00062	-0.00383	-0.00321	3.09958
D3	-3.12260	0.00008	-0.00035	-0.00304	-0.00339	-3.12599
D4	-0.02572	0.00002	0.00032	-0.00601	-0.00569	-0.03141
D5	-0.04100	-0.00003	0.00000	0.00162	0.00162	-0.03938
D6	-2.99812	0.00028	-0.00097	0.01040	0.00943	-2.98869
D7	3.08888	-0.00003	0.00027	0.00356	0.00383	3.09271
D8	0.13176	0.00028	-0.00070	0.01234	0.01165	0.14341
D9	0.03094	-0.00011	0.00008	-0.00019	-0.00010	0.03084
D10	3.03132	-0.00021	-0.00042	-0.01225	-0.01266	3.01866
D11	-3.07088	-0.00005	-0.00051	0.00243	0.00191	-3.06897
D12	-0.07050	-0.00016	-0.00102	-0.00964	-0.01065	-0.08115
D13	-0.05689	0.00009	-0.00009	0.00120	0.00111	-0.05577
D14	-3.09983	-0.00015	-0.00106	0.01152	0.01046	-3.08936
D15	-3.06487	0.00017	0.00039	0.01277	0.01317	-3.05170
D16	0.17538	-0.00006	-0.00059	0.02310	0.02252	0.19789
D17	0.62501	0.00006	0.00082	0.02493	0.02574	0.65075
D18	-2.47390	0.00008	0.00092	0.02417	0.02509	-2.44881
D19	-2.67705	-0.00006	0.00025	0.01116	0.01141	-2.66564
D20	0.50723	-0.00004	0.00035	0.01040	0.01075	0.51799
D21	0.06059	-0.00003	0.00006	-0.00172	-0.00167	0.05892
D22	3.02142	-0.00018	0.00096	-0.01007	-0.00910	3.01232
D23	3.10310	0.00020	0.00103	-0.01199	-0.01095	3.09215
D24	-0.21925	0.00005	0.00194	-0.02033	-0.01838	-0.23763
D25	1.23183	0.00067	0.00507	-0.02641	-0.02134	1.21049
D26	-2.95029	-0.00010	0.00561	-0.02957	-0.02396	-2.97425
D27	-0.90525	0.00029	0.00550	-0.02893	-0.02342	-0.92867
D28	-1.69730	0.00093	0.00399	-0.01651	-0.01252	-1.70982
D29	0.40376	0.00015	0.00452	-0.01967	-0.01514	0.38862
D30	2.44881	0.00055	0.00442	-0.01903	-0.01461	2.43420
D31	-1.02922	-0.00017	0.00213	-0.02091	-0.01878	-1.04800
D32	1.04944	-0.00085	0.00216	-0.02261	-0.02046	1.02898
D33	-3.10322	-0.00053	0.00173	-0.01604	-0.01431	-3.11753
D34	-3.11042	0.00049	0.00152	-0.01637	-0.01485	-3.12527
D35	-1.03175	-0.00020	0.00155	-0.01807	-0.01653	-1.04829
D36	1.09877	0.00013	0.00112	-0.01150	-0.01038	1.08839
D37	1.08696	0.00015	0.00169	-0.01825	-0.01656	1.07040
D38	-3.11756	-0.00054	0.00171	-0.01994	-0.01824	-3.13580
D39	-0.98704	-0.00021	0.00129	-0.01338	-0.01209	-0.99913
D40	-0.29904	0.00030	-0.01470	0.10548	0.09077	-0.20827

D41	1.79431	-0.00037	-0.01469	0.10478	0.09009	1.88440
D42	-2.37087	0.00010	-0.01356	0.09100	0.07745	-2.29342
D43	-2.22367	0.00117	-0.01606	0.18758	0.17149	-2.05218
D44	1.97921	0.00010	-0.01585	0.18553	0.16971	2.14892
D45	-0.13081	-0.00105	-0.01645	0.19408	0.17762	0.04681
D46	-3.08886	0.00000	0.00004	0.00079	0.00083	-3.08803
D47	0.05105	-0.00001	0.00002	0.00098	0.00100	0.05205
D48	0.00453	-0.00001	-0.00007	0.00146	0.00139	0.00591
D49	-3.13875	-0.00002	-0.00010	0.00165	0.00156	-3.13719

Item	Value	Threshold	Converged?
Maximum Force	0.003710	0.000450	NO
RMS Force	0.000616	0.000300	NO
Maximum Displacement	0.175509	0.001800	NO
RMS Displacement	0.028080	0.001200	NO

Predicted change in Energy=-2.180078D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.448350	-1.965025	-1.318422
2	6	0	-1.739244	-1.589940	-1.487124
3	7	0	-2.108522	-0.874468	-0.351666
4	6	0	-1.040133	-0.790556	0.464976
5	7	0	-0.034096	-1.485526	-0.081501
6	6	0	1.340664	-1.500701	0.436334
7	6	0	2.242646	-0.521677	-0.329023
8	1	0	0.209971	-2.517842	-1.965343
9	1	0	-2.411732	-1.729231	-2.313981
10	1	0	1.299360	-1.214885	1.486947
11	1	0	1.729429	-2.518792	0.371317
12	1	0	2.275768	-0.793209	-1.390372
13	1	0	1.831216	0.486978	-0.240346
14	35	0	-0.364966	2.076016	0.526112
15	1	0	-1.032979	-0.336213	1.436573
16	6	0	-3.320905	-0.163156	-0.128625
17	6	0	-4.501882	-0.587941	-0.558730
18	1	0	-3.148085	0.773636	0.391520
19	1	0	-5.379646	0.023370	-0.400153
20	1	0	-4.634425	-1.533167	-1.071609
21	8	0	3.554771	-0.625799	0.215005
22	1	0	3.801492	0.221248	0.595263

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.354827	0.000000			
3	N	2.209096	1.391952	0.000000		
4	C	2.215873	2.222266	1.347368	0.000000	
5	N	1.389784	2.212285	2.179363	1.339303	0.000000
6	C	2.548595	3.632284	3.593048	2.484617	1.469132
7	C	3.209926	4.282270	4.365506	3.388122	2.484719
8	H	1.075872	2.211139	3.268034	3.233069	2.161969
9	H	2.213957	1.074865	2.161767	3.238055	3.270552
10	H	3.389292	4.268358	3.887164	2.587993	2.076387
11	H	2.811512	4.043299	4.237496	3.265892	2.093491
12	H	2.966336	4.094443	4.506386	3.799675	2.743705
13	H	3.517241	4.314653	4.169828	3.220904	2.719447
14	Br	4.442889	4.402384	3.537773	2.945644	3.628119
15	H	3.253432	3.258626	2.155066	1.072604	2.150171
16	C	3.593595	2.526437	1.423231	2.438835	3.543162
17	C	4.347944	3.081896	2.419327	3.615623	4.581977
18	H	4.208650	3.331760	2.085488	2.625938	3.876143
19	H	5.395796	4.127566	3.392450	4.499144	5.563561
20	H	4.215524	2.925397	2.707838	3.978881	4.705912
21	O	4.491091	5.643882	5.697003	4.604647	3.702298
22	H	5.148119	6.190032	6.084861	4.947935	4.252390

		6	7	8	9	10
6	C	0.000000				
7	C	1.535523	0.000000			
8	H	2.842727	3.285420	0.000000		
9	H	4.657997	5.202066	2.759853	0.000000	
10	H	1.089580	2.160572	3.847438	5.337023	0.000000
11	H	1.091731	2.177690	2.787245	4.998345	1.769114
12	H	2.170673	1.096033	2.751812	4.868455	3.067597
13	H	2.156248	1.092943	3.825310	5.216719	2.482489
14	Br	3.963601	3.778744	5.257512	5.170617	3.810933
15	H	2.826781	3.725781	4.228176	4.231799	2.492871
16	C	4.882462	5.578692	4.624410	2.838127	5.006302
17	C	5.996551	6.748764	5.282484	2.958407	6.183224
18	H	5.032244	5.590796	5.259769	3.758496	4.993390
19	H	6.941546	7.642086	6.336513	3.942443	7.050074
20	H	6.162518	6.990612	5.023596	2.553878	6.469723
21	O	2.390964	1.424247	4.418306	6.573621	2.655511
22	H	3.007664	1.958633	5.192142	7.132477	3.019643

		11	12	13	14	15

11	H	0.000000				
12	H	2.525801	0.000000			
13	H	3.069063	1.777376	0.000000		
14	Br	5.052001	4.344979	2.817040	0.000000	
15	H	3.678223	4.375874	3.419549	2.663462	0.000000
16	C	5.595073	5.771631	5.194181	3.765653	2.777481
17	C	6.589568	6.831567	6.431559	5.038612	4.009724
18	H	5.884780	5.920163	5.027412	3.075721	2.607216
19	H	7.589249	7.762261	7.227517	5.497120	4.732481
20	H	6.599404	6.957005	6.824698	5.814395	4.549076
21	O	2.634336	2.059395	2.101490	4.770841	4.756421
22	H	3.442588	2.701796	2.156581	4.561175	4.938692

		16	17	18	19	20
16	C	0.000000				
17	C	1.326702	0.000000			
18	H	1.085355	2.142342	0.000000		
19	H	2.084930	1.081350	2.483849	0.000000	
20	H	2.119312	1.083543	3.109869	1.851760	0.000000
21	O	6.899786	8.093809	6.849661	8.979067	8.339162
22	H	7.169402	8.422143	6.974473	9.237061	8.776168

		21	22
21	O	0.000000	
22	H	0.960706	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.213505	-2.254737	-0.600943
2	6	0	-1.502399	-1.863115	-0.745660
3	7	0	-1.711186	-0.809661	0.139875
4	6	0	-0.551476	-0.551203	0.775226
5	7	0	0.359644	-1.447157	0.374154
6	6	0	1.784811	-1.395461	0.727106
7	6	0	2.621227	-0.762982	-0.394593
8	1	0	0.345264	-3.023103	-1.105811
9	1	0	-2.272215	-2.204126	-1.413815
10	1	0	1.877490	-0.798127	1.633631

11	1	0	2.129808	-2.408066	0.945012
12	1	0	2.519621	-1.349507	-1.314893
13	1	0	2.256231	0.249486	-0.584885
14	35	0	0.219105	2.142373	-0.134539
15	1	0	-0.414574	0.178473	1.549378
16	6	0	-2.864847	0.016276	0.251589
17	6	0	-4.101628	-0.439118	0.099516
18	1	0	-2.601275	1.053678	0.431375
19	1	0	-4.934086	0.249382	0.147466
20	1	0	-4.324642	-1.485021	-0.074890
21	8	0	3.984439	-0.783394	0.017374
22	1	0	4.301873	0.120779	0.085657

Rotational constants (GHZ): 0.8229262 0.5682294 0.3562302

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 866.1565126859 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 7.12D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Initial guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999993 0.000816 0.000198 0.003751 Ang= 0.44 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Keep R1 ints in memory in canonical form, NReq=1804729152.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.33823892 A.U. after 11 cycles
NFock= 11 Conv=0.66D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000170307	0.000071297	0.000207776
2	6	0.000178959	0.000335964	0.000058040
3	7	0.000110463	0.000010846	-0.000058891
4	6	0.000370996	-0.000247415	-0.000538858
5	7	-0.000035283	0.000263494	0.000088407
6	6	-0.000330517	-0.000063985	0.000067129
7	6	0.000033756	0.000144308	0.000192045
8	1	0.000050175	0.000029392	0.000005605
9	1	-0.000074252	-0.000180249	0.000056643
10	1	0.000049375	-0.000111659	0.000095448
11	1	0.000009561	0.000007905	-0.000175762
12	1	0.000384183	-0.000224730	0.000298264
13	1	-0.000312101	0.000108679	0.000050882
14	35	-0.000189781	-0.001060230	0.000102325
15	1	0.000116189	0.000749134	-0.000068677
16	6	0.000350598	-0.000099810	0.000057440
17	6	0.000041208	0.000124118	0.000040366
18	1	-0.000309371	0.000112209	-0.000010334
19	1	-0.000032171	0.000101025	0.000040215
20	1	-0.000054475	-0.000031519	-0.000082020
21	8	-0.000028410	-0.000409358	-0.000617048
22	1	-0.000158796	0.000370586	0.000191006

Cartesian Forces: Max 0.001060230 RMS 0.000254335

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.005302272 RMS 0.000857726
Search for a local minimum.

Step number 20 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 18 19 20
DE= -4.01D-05 DEPred=-2.18D-05 R= 1.84D+00
TightC=F SS= 1.41D+00 RLast= 3.47D-01 DXNew= 9.0455D-01 1.0408D+00
Trust test= 1.84D+00 RLast= 3.47D-01 DXMaxT set to 9.05D-01
ITU= 1 0 -1 1 1 1 1 1 1 1 1 1 1 1 0 0 -1 0 0

Eigenvalues ---	0.00022	0.00260	0.00469	0.00731	0.01134
Eigenvalues ---	0.01342	0.01600	0.01767	0.02046	0.02084
Eigenvalues ---	0.02232	0.02444	0.03069	0.03093	0.03510
Eigenvalues ---	0.04312	0.04797	0.05455	0.05809	0.06989
Eigenvalues ---	0.08820	0.09306	0.13697	0.14315	0.15667
Eigenvalues ---	0.15739	0.15866	0.15984	0.15997	0.16111
Eigenvalues ---	0.16913	0.18812	0.21146	0.22799	0.22991
Eigenvalues ---	0.24247	0.25148	0.25634	0.29741	0.33084
Eigenvalues ---	0.33799	0.33878	0.33898	0.34120	0.34427
Eigenvalues ---	0.34543	0.34682	0.36245	0.36315	0.36450
Eigenvalues ---	0.37255	0.42827	0.43098	0.45964	0.49574
Eigenvalues ---	0.53661	0.54536	0.55844	0.60576	2.54668

En-DIIS/RFO-DIIS IScMMF= 0 using points: 20 19
RFO step: Lambda=-5.56281080D-05.
DidBck=F Rises=F RFO-DIIS coefs: 1.22727 -0.22727
Iteration 1 RMS(Cart)= 0.03706089 RMS(Int)= 0.00451377
Iteration 2 RMS(Cart)= 0.00479247 RMS(Int)= 0.00006879
Iteration 3 RMS(Cart)= 0.00006031 RMS(Int)= 0.00002101
Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00002101

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56025	-0.00001	0.00003	-0.00036	-0.00034	2.55991
R2	2.62631	-0.00025	0.00007	0.00036	0.00041	2.62672
R3	2.03310	0.00001	0.00000	0.00008	0.00008	2.03319
R4	2.63041	-0.00009	0.00022	0.00072	0.00095	2.63136
R5	2.03120	0.00002	0.00001	0.00006	0.00007	2.03127
R6	2.54616	-0.00023	-0.00002	-0.00005	-0.00005	2.54610
R7	2.68952	0.00010	0.00049	0.00144	0.00192	2.69144
R8	2.53091	-0.00031	0.00010	0.00036	0.00046	2.53138
R9	2.02693	0.00026	-0.00012	-0.00007	-0.00019	2.02674
R10	2.77626	-0.00044	0.00032	0.00044	0.00076	2.77702
R11	2.90172	-0.00090	0.00076	0.00397	0.00472	2.90644
R12	2.05901	0.00006	0.00003	0.00037	0.00040	2.05940
R13	2.06307	0.00000	-0.00006	-0.00029	-0.00035	2.06272
R14	2.07120	-0.00022	-0.00035	-0.00258	-0.00293	2.06827

R15	2.06536	-0.00067	-0.00011	0.00006	-0.00005	2.06531
R16	2.69144	-0.00034	-0.00030	-0.00214	-0.00244	2.68900
R17	5.32343	-0.00042	0.00000	-0.01557	-0.01557	5.30786
R18	2.50710	-0.00001	-0.00004	-0.00020	-0.00025	2.50686
R19	2.05102	0.00004	0.00013	0.00032	0.00044	2.05147
R20	2.04346	0.00008	0.00000	-0.00010	-0.00010	2.04336
R21	2.04760	0.00008	-0.00002	-0.00012	-0.00014	2.04746
R22	1.81547	0.00037	-0.00002	0.00116	0.00114	1.81661
A1	1.87477	-0.00006	0.00000	-0.00014	-0.00014	1.87462
A2	2.27891	0.00007	-0.00010	0.00004	-0.00007	2.27884
A3	2.12946	-0.00001	0.00010	0.00015	0.00025	2.12971
A4	1.86869	-0.00001	0.00002	0.00032	0.00036	1.86905
A5	2.28635	-0.00001	0.00009	0.00057	0.00065	2.28700
A6	2.12721	0.00001	-0.00013	-0.00070	-0.00084	2.12637
A7	1.89237	-0.00008	-0.00007	-0.00046	-0.00055	1.89182
A8	2.22777	0.00016	-0.00034	-0.00173	-0.00215	2.22562
A9	2.15240	-0.00008	0.00002	-0.00020	-0.00027	2.15213
A10	1.89231	0.00011	0.00008	0.00009	0.00017	1.89248
A11	2.19038	-0.00014	0.00002	-0.00067	-0.00070	2.18968
A12	2.19494	0.00007	-0.00030	-0.00055	-0.00090	2.19403
A13	1.89471	0.00004	-0.00001	-0.00009	-0.00011	1.89461
A14	2.20070	0.00074	0.00004	-0.00071	-0.00068	2.20002
A15	2.17056	-0.00085	-0.00034	-0.00019	-0.00054	2.17002
A16	1.94701	-0.00275	-0.00021	0.00041	0.00020	1.94721
A17	1.87726	0.00056	-0.00056	-0.00253	-0.00309	1.87417
A18	1.89850	0.00117	0.00035	0.00073	0.00108	1.89957
A19	1.91307	0.00020	-0.00008	0.00069	0.00061	1.91367
A20	1.93448	0.00120	0.00030	0.00022	0.00051	1.93499
A21	1.89183	-0.00034	0.00021	0.00040	0.00061	1.89244
A22	1.92033	0.00075	0.00011	-0.00044	-0.00028	1.92005
A23	1.90376	-0.00402	-0.00023	0.00096	0.00070	1.90446
A24	1.87986	0.00167	0.00255	0.01328	0.01582	1.89568
A25	1.89503	0.00099	-0.00025	0.00164	0.00136	1.89638
A26	1.90068	-0.00083	-0.00214	-0.01494	-0.01708	1.88361
A27	1.96415	0.00146	-0.00001	-0.00052	-0.00061	1.96353
A28	2.56099	-0.00530	0.00050	0.00373	0.00423	2.56522
A29	2.15012	0.00019	-0.00056	-0.00239	-0.00295	2.14717
A30	1.95071	0.00024	-0.00043	-0.00071	-0.00113	1.94958
A31	2.18152	-0.00043	0.00099	0.00307	0.00406	2.18558
A32	2.08751	-0.00012	0.00019	-0.00029	-0.00010	2.08740
A33	2.14319	0.00011	-0.00040	-0.00107	-0.00146	2.14173
A34	2.05249	0.00001	0.00021	0.00135	0.00156	2.05405
A35	1.90004	-0.00043	0.00026	-0.00184	-0.00159	1.89846
D1	0.00500	0.00015	-0.00021	-0.00171	-0.00192	0.00309

D2	3.09958	0.00009	-0.00073	0.00314	0.00241	3.10199
D3	-3.12599	0.00014	-0.00077	-0.00637	-0.00714	-3.13313
D4	-0.03141	0.00008	-0.00129	-0.00153	-0.00281	-0.03422
D5	-0.03938	-0.00014	0.00037	-0.00132	-0.00095	-0.04034
D6	-2.98869	0.00031	0.00214	0.00416	0.00630	-2.98238
D7	3.09271	-0.00013	0.00087	0.00285	0.00373	3.09644
D8	0.14341	0.00031	0.00265	0.00833	0.01098	0.15440
D9	0.03084	-0.00011	-0.00002	0.00414	0.00412	0.03496
D10	3.01866	-0.00017	-0.00288	-0.01298	-0.01584	3.00282
D11	-3.06897	-0.00005	0.00043	-0.00020	0.00023	-3.06874
D12	-0.08115	-0.00012	-0.00242	-0.01732	-0.01973	-0.10088
D13	-0.05577	0.00001	0.00025	-0.00500	-0.00475	-0.06052
D14	-3.08936	-0.00032	0.00238	0.00595	0.00833	-3.08104
D15	-3.05170	0.00005	0.00299	0.01138	0.01438	-3.03732
D16	0.19789	-0.00028	0.00512	0.02233	0.02746	0.22536
D17	0.65075	-0.00001	0.00585	0.03134	0.03719	0.68794
D18	-2.44881	0.00002	0.00570	0.03198	0.03768	-2.41113
D19	-2.66564	-0.00008	0.00259	0.01183	0.01443	-2.65121
D20	0.51799	-0.00005	0.00244	0.01247	0.01492	0.53291
D21	0.05892	0.00008	-0.00038	0.00395	0.00357	0.06249
D22	3.01232	-0.00014	-0.00207	-0.00149	-0.00355	3.00877
D23	3.09215	0.00040	-0.00249	-0.00705	-0.00953	3.08262
D24	-0.23763	0.00018	-0.00418	-0.01248	-0.01666	-0.25429
D25	1.21049	0.00087	-0.00485	0.00475	-0.00010	1.21040
D26	-2.97425	-0.00017	-0.00544	0.00423	-0.00122	-2.97546
D27	-0.92867	0.00036	-0.00532	0.00371	-0.00161	-0.93028
D28	-1.70982	0.00125	-0.00285	0.01106	0.00821	-1.70161
D29	0.38862	0.00022	-0.00344	0.01054	0.00709	0.39571
D30	2.43420	0.00074	-0.00332	0.01002	0.00670	2.44090
D31	-1.04800	-0.00032	-0.00427	-0.03600	-0.04026	-1.08826
D32	1.02898	-0.00112	-0.00465	-0.03368	-0.03835	0.99063
D33	-3.11753	-0.00073	-0.00325	-0.02559	-0.02883	3.13682
D34	-3.12527	0.00057	-0.00338	-0.03356	-0.03693	3.12098
D35	-1.04829	-0.00022	-0.00376	-0.03124	-0.03502	-1.08330
D36	1.08839	0.00017	-0.00236	-0.02316	-0.02550	1.06289
D37	1.07040	0.00011	-0.00376	-0.03464	-0.03840	1.03201
D38	-3.13580	-0.00068	-0.00414	-0.03232	-0.03648	3.11090
D39	-0.99913	-0.00029	-0.00275	-0.02423	-0.02696	-1.02609
D40	-0.20827	0.00033	0.02063	0.05043	0.07104	-0.13723
D41	1.88440	-0.00053	0.02047	0.05143	0.07192	1.95632
D42	-2.29342	0.00003	0.01760	0.03346	0.05107	-2.24235
D43	-2.05218	0.00152	0.03897	0.17456	0.21348	-1.83870
D44	2.14892	0.00014	0.03857	0.17583	0.21447	2.36339
D45	0.04681	-0.00147	0.04037	0.18430	0.22465	0.27146

D46	-3.08803	0.00000	0.00019	0.00260	0.00279	-3.08524
D47	0.05205	-0.00002	0.00023	0.00086	0.00109	0.05315
D48	0.00591	-0.00002	0.00031	0.00176	0.00208	0.00799
D49	-3.13719	-0.00003	0.00035	0.00003	0.00038	-3.13681

Item	Value	Threshold	Converged?
Maximum Force	0.005302	0.000450	NO
RMS Force	0.000858	0.000300	NO
Maximum Displacement	0.253601	0.001800	NO
RMS Displacement	0.037914	0.001200	NO

Predicted change in Energy=-6.121680D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.448812	-1.969295	-1.324793
2	6	0	-1.739255	-1.591174	-1.488638
3	7	0	-2.104525	-0.878332	-0.349620
4	6	0	-1.032129	-0.794815	0.461746
5	7	0	-0.029495	-1.492304	-0.088362
6	6	0	1.348766	-1.504827	0.421312
7	6	0	2.244748	-0.518942	-0.347296
8	1	0	0.204799	-2.526324	-1.972948
9	1	0	-2.415919	-1.729178	-2.312347
10	1	0	1.309635	-1.221096	1.472791
11	1	0	1.740751	-2.521238	0.352533
12	1	0	2.305152	-0.810628	-1.400465
13	1	0	1.810229	0.482019	-0.286143
14	35	0	-0.379352	2.054724	0.502328
15	1	0	-1.023097	-0.348869	1.437100
16	6	0	-3.309379	-0.151071	-0.130754
17	6	0	-4.496807	-0.579866	-0.538116
18	1	0	-3.121785	0.797195	0.363313
19	1	0	-5.369066	0.041494	-0.388856
20	1	0	-4.638259	-1.537751	-1.024275
21	8	0	3.557292	-0.577173	0.199181
22	1	0	3.706859	0.210573	0.729463

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.354645	0.000000			

3	N	2.209649	1.392454	0.000000		
4	C	2.216164	2.222209	1.347339	0.000000	
5	N	1.390003	2.212199	2.179671	1.339547	0.000000
6	C	2.548705	3.631974	3.593334	2.484836	1.469533
7	C	3.211587	4.280727	4.364097	3.386529	2.487300
8	H	1.075916	2.210975	3.268647	3.233551	2.162350
9	H	2.214143	1.074903	2.161759	3.237824	3.270663
10	H	3.387981	4.266468	3.885249	2.586075	2.074614
11	H	2.812872	4.045414	4.240083	3.268230	2.094484
12	H	2.988739	4.119983	4.533665	3.821718	2.763489
13	H	3.491562	4.282869	4.144863	3.204473	2.705856
14	Br	4.419947	4.371024	3.507828	2.923635	3.612855
15	H	3.253250	3.258243	2.154573	1.072504	2.149820
16	C	3.593676	2.526467	1.424249	2.439535	3.543775
17	C	4.351509	3.087123	2.418186	3.612467	4.581669
18	H	4.200947	3.323465	2.085781	2.628849	3.874026
19	H	5.397050	4.129244	3.391880	4.497995	5.563618
20	H	4.222322	2.936446	2.703665	3.970439	4.703053
21	O	4.506592	5.650694	5.696319	4.602076	3.712841
22	H	5.122636	6.150319	6.010184	4.851854	4.186761

		6	7	8	9	10
6	C	0.000000				
7	C	1.538022	0.000000			
8	H	2.843343	3.291462	0.000000		
9	H	4.657905	5.200761	2.760217	0.000000	
10	H	1.089790	2.163371	3.846739	5.335276	0.000000
11	H	1.091547	2.180130	2.786940	5.000685	1.769522
12	H	2.171511	1.094484	2.771793	4.895282	3.068409
13	H	2.158935	1.092917	3.804320	5.182203	2.499009
14	Br	3.957697	3.772468	5.239678	5.136917	3.811230
15	H	2.827330	3.727171	4.228176	4.231260	2.490721
16	C	4.882187	5.570507	4.624387	2.836906	5.005158
17	C	5.995563	6.744530	5.287016	2.966295	6.178162
18	H	5.028767	5.571073	5.250720	3.746994	4.994189
19	H	6.940947	7.634525	6.338061	3.944131	7.047333
20	H	6.159162	6.990855	5.033137	2.575765	6.458565
21	O	2.405717	1.422955	4.444834	6.581348	2.662458
22	H	2.932262	1.956878	5.201736	7.106592	2.889445

		11	12	13	14	15
11	H	0.000000				
12	H	2.513511	0.000000			
13	H	3.071204	1.776963	0.000000		
14	Br	5.045464	4.363190	2.808799	0.000000	
15	H	3.678903	4.397981	3.418725	2.658095	0.000000

16	C	5.599560	5.793975	5.160944	3.721745	2.779277
17	C	6.593125	6.860287	6.400765	4.997702	4.002687
18	H	5.886966	5.928546	4.984566	3.020206	2.621254
19	H	7.593862	7.787367	7.193531	5.453856	4.730111
20	H	6.599592	6.991509	6.797596	5.777083	4.532241
21	O	2.665095	2.044803	2.099919	4.745098	4.750214
22	H	3.386805	2.746675	2.168488	4.488831	4.815205

		16	17	18	19	20
16	C	0.000000				
17	C	1.326572	0.000000			
18	H	1.085589	2.144658	0.000000		
19	H	2.084708	1.081297	2.487391	0.000000	
20	H	2.118297	1.083468	3.110799	1.852526	0.000000
21	O	6.887786	8.087776	6.820990	8.967074	8.341860
22	H	7.078019	8.338566	6.863568	9.146127	8.704782

		21	22
21	O	0.000000	
22	H	0.961309	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.196265	-2.254319	-0.603062
2	6	0	-1.485927	-1.865652	-0.747181
3	7	0	-1.699232	-0.816982	0.143729
4	6	0	-0.539582	-0.555279	0.777800
5	7	0	0.374127	-1.448289	0.375241
6	6	0	1.800537	-1.389139	0.723643
7	6	0	2.630381	-0.743470	-0.398847
8	1	0	0.363584	-3.022393	-1.107271
9	1	0	-2.255493	-2.207331	-1.415343
10	1	0	1.889209	-0.795043	1.632945
11	1	0	2.153674	-2.399909	0.936042
12	1	0	2.562422	-1.346955	-1.309387
13	1	0	2.233705	0.252913	-0.609411
14	35	0	0.192728	2.123622	-0.135902
15	1	0	-0.407218	0.166607	1.559865

16	6	0	-2.850625	0.015307	0.244095
17	6	0	-4.088174	-0.443488	0.110778
18	1	0	-2.581687	1.055859	0.397155
19	1	0	-4.920131	0.246340	0.145225
20	1	0	-4.310656	-1.493603	-0.036407
21	8	0	3.994440	-0.712405	0.005106
22	1	0	4.225259	0.189113	0.246149

Rotational constants (GHZ): 0.8336526 0.5698641 0.3589627

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 868.2138986408 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 7.33D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Initial guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999991 0.000188 -0.000271 -0.004201 Ang= 0.48 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Keep R1 ints in memory in canonical form, NReq=1804729152.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3032.33829576 A.U. after 11 cycles

NFock= 11 Conv=0.10D-07 -V/T= 2.0017

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000183733	-0.000020920	0.000186955
2	6	-0.000083909	0.000195609	0.000329986
3	7	0.000078001	0.000299088	-0.000558615
4	6	0.000224764	-0.000387666	-0.000121026
5	7	0.000410913	0.000062881	-0.000020703
6	6	-0.000365939	0.000247757	-0.000026482
7	6	-0.000025495	-0.000043232	0.000081459
8	1	0.000103817	0.000190452	-0.000038196
9	1	-0.000049344	-0.000143162	0.000037905
10	1	0.000108976	-0.000169505	0.000169466
11	1	-0.000040001	-0.000058646	-0.000065625
12	1	0.000156785	-0.000263418	0.000067277
13	1	-0.000270291	0.000167943	-0.000039242
14	35	0.000091784	-0.000324577	0.000190176
15	1	0.000068893	0.000538500	-0.000129293
16	6	0.000576889	-0.000632377	0.000025163
17	6	0.000078089	0.000334738	0.000017652
18	1	-0.000415284	0.000118974	0.000040805
19	1	-0.000153568	0.000047729	0.000058747
20	1	-0.000159051	-0.000082991	-0.000117067
21	8	-0.000027543	-0.000427506	-0.000206459
22	1	-0.000124752	0.000350330	0.000117116

Cartesian Forces: Max 0.000632377 RMS 0.000231348

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.001526710 RMS 0.000288680

Search for a local minimum.

Step number 21 out of a maximum of 116

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 18 20 21

DE= -5.68D-05 DEPred=-6.12D-05 R= 9.29D-01
TightC=F SS= 1.41D+00 RLast= 4.15D-01 DXNew= 1.5213D+00 1.2450D+00
Trust test= 9.29D-01 RLast= 4.15D-01 DXMaxT set to 1.25D+00
ITU= 1 1 0 -1 1 1 1 1 1 1 1 1 1 1 1 0 0 -1 0
ITU= 0

Eigenvalues ---	0.00026	0.00264	0.00518	0.00678	0.01217
Eigenvalues ---	0.01369	0.01633	0.01755	0.02036	0.02090
Eigenvalues ---	0.02262	0.02446	0.03070	0.03098	0.03505
Eigenvalues ---	0.04297	0.04816	0.05456	0.05765	0.07103
Eigenvalues ---	0.08927	0.09318	0.13710	0.14387	0.15739
Eigenvalues ---	0.15748	0.15840	0.15990	0.15999	0.16169
Eigenvalues ---	0.16984	0.18590	0.21136	0.22789	0.23084
Eigenvalues ---	0.24203	0.25230	0.25577	0.29881	0.33056
Eigenvalues ---	0.33811	0.33879	0.33895	0.34122	0.34444
Eigenvalues ---	0.34532	0.34685	0.36264	0.36315	0.36513
Eigenvalues ---	0.37253	0.42767	0.43109	0.46035	0.49610
Eigenvalues ---	0.53706	0.54545	0.55772	0.60575	2.19889

En-DIIS/RFO-DIIS IScMMF= 0 using points: 21 20 19
RFO step: Lambda=-1.10906442D-05.
DidBck=F Rises=F RFO-DIIS coefs: 0.91363 -0.42300 0.50937
Iteration 1 RMS(Cart)= 0.01244537 RMS(Int)= 0.00036811
Iteration 2 RMS(Cart)= 0.00036918 RMS(Int)= 0.00001502
Iteration 3 RMS(Cart)= 0.00000038 RMS(Int)= 0.00001502

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55991	-0.00003	-0.00003	-0.00015	-0.00018	2.55973
R2	2.62672	-0.00014	-0.00018	0.00021	0.00003	2.62676
R3	2.03319	-0.00001	0.00000	0.00000	0.00000	2.03318
R4	2.63136	-0.00041	-0.00058	0.00020	-0.00039	2.63097
R5	2.03127	0.00002	-0.00003	0.00003	0.00000	2.03127
R6	2.54610	0.00018	0.00005	0.00060	0.00064	2.54674
R7	2.69144	-0.00006	-0.00126	-0.00018	-0.00144	2.69000
R8	2.53138	-0.00010	-0.00026	0.00010	-0.00016	2.53122
R9	2.02674	0.00011	0.00029	-0.00007	0.00022	2.02696
R10	2.77702	-0.00038	-0.00078	-0.00029	-0.00106	2.77595
R11	2.90644	-0.00052	-0.00210	0.00042	-0.00168	2.90476
R12	2.05940	0.00011	-0.00010	0.00027	0.00018	2.05958
R13	2.06272	0.00004	0.00017	-0.00007	0.00009	2.06282
R14	2.06827	0.00002	0.00104	-0.00032	0.00072	2.06899
R15	2.06531	-0.00005	0.00025	0.00023	0.00049	2.06580
R16	2.68900	-0.00018	0.00089	-0.00053	0.00036	2.68935
R17	5.30786	-0.00019	0.00135	-0.00583	-0.00448	5.30338
R18	2.50686	0.00013	0.00012	0.00025	0.00037	2.50723
R19	2.05147	0.00005	-0.00032	0.00020	-0.00012	2.05134

R20	2.04336	0.00015	0.00001	0.00022	0.00022	2.04358
R21	2.04746	0.00015	0.00006	0.00016	0.00021	2.04767
R22	1.81661	0.00034	-0.00005	0.00052	0.00047	1.81707
A1	1.87462	0.00012	0.00001	0.00021	0.00022	1.87484
A2	2.27884	0.00001	0.00023	-0.00003	0.00020	2.27905
A3	2.12971	-0.00013	-0.00025	-0.00018	-0.00043	2.12928
A4	1.86905	0.00000	-0.00008	0.00003	-0.00007	1.86898
A5	2.28700	-0.00002	-0.00025	-0.00017	-0.00042	2.28658
A6	2.12637	0.00001	0.00036	0.00021	0.00058	2.12695
A7	1.89182	-0.00003	0.00020	-0.00007	0.00015	1.89197
A8	2.22562	0.00001	0.00094	0.00020	0.00119	2.22681
A9	2.15213	0.00003	-0.00003	0.00016	0.00019	2.15231
A10	1.89248	0.00004	-0.00019	-0.00001	-0.00020	1.89229
A11	2.18968	-0.00011	0.00002	-0.00007	-0.00001	2.18967
A12	2.19403	0.00008	0.00076	0.00008	0.00087	2.19490
A13	1.89461	-0.00015	0.00004	-0.00004	0.00000	1.89461
A14	2.20002	0.00004	-0.00004	-0.00009	-0.00011	2.19990
A15	2.17002	0.00010	0.00081	0.00057	0.00139	2.17141
A16	1.94721	-0.00093	0.00046	0.00009	0.00056	1.94776
A17	1.87417	0.00038	0.00153	0.00028	0.00181	1.87598
A18	1.89957	0.00021	-0.00087	-0.00060	-0.00147	1.89810
A19	1.91367	0.00011	0.00014	0.00070	0.00084	1.91451
A20	1.93499	0.00041	-0.00071	-0.00021	-0.00092	1.93407
A21	1.89244	-0.00017	-0.00051	-0.00026	-0.00078	1.89166
A22	1.92005	0.00005	-0.00021	-0.00004	-0.00029	1.91975
A23	1.90446	-0.00118	0.00045	-0.00075	-0.00027	1.90419
A24	1.89568	0.00056	-0.00708	0.00191	-0.00516	1.89052
A25	1.89638	0.00053	0.00044	0.00179	0.00226	1.89864
A26	1.88361	-0.00021	0.00627	-0.00229	0.00399	1.88759
A27	1.96353	0.00025	0.00008	-0.00065	-0.00051	1.96302
A28	2.56522	-0.00153	-0.00149	0.00083	-0.00066	2.56456
A29	2.14717	0.00037	0.00151	0.00096	0.00247	2.14964
A30	1.94958	0.00026	0.00105	0.00038	0.00143	1.95101
A31	2.18558	-0.00063	-0.00257	-0.00134	-0.00391	2.18167
A32	2.08740	-0.00005	-0.00041	-0.00042	-0.00083	2.08658
A33	2.14173	0.00017	0.00101	0.00054	0.00156	2.14329
A34	2.05405	-0.00012	-0.00060	-0.00013	-0.00073	2.05332
A35	1.89846	-0.00038	-0.00044	-0.00069	-0.00113	1.89732
D1	0.00309	0.00012	0.00063	-0.00027	0.00036	0.00345
D2	3.10199	0.00014	0.00142	0.00174	0.00316	3.10515
D3	-3.13313	0.00007	0.00234	-0.00009	0.00225	-3.13088
D4	-0.03422	0.00009	0.00314	0.00191	0.00505	-0.02917
D5	-0.04034	-0.00016	-0.00074	0.00129	0.00055	-0.03979
D6	-2.98238	-0.00011	-0.00535	-0.00114	-0.00649	-2.98887

D7	3.09644	-0.00012	-0.00227	0.00113	-0.00114	3.09530
D8	0.15440	-0.00007	-0.00688	-0.00130	-0.00818	0.14621
D9	0.03496	-0.00004	-0.00030	-0.00085	-0.00115	0.03381
D10	3.00282	0.00005	0.00782	0.00097	0.00878	3.01160
D11	-3.06874	-0.00006	-0.00099	-0.00262	-0.00361	-3.07235
D12	-0.10088	0.00003	0.00713	-0.00080	0.00632	-0.09456
D13	-0.06052	-0.00006	-0.00016	0.00167	0.00151	-0.05901
D14	-3.08104	-0.00019	-0.00605	0.00166	-0.00439	-3.08543
D15	-3.03732	-0.00015	-0.00795	-0.00006	-0.00802	-3.04534
D16	0.22536	-0.00027	-0.01384	-0.00007	-0.01393	0.21143
D17	0.68794	-0.00014	-0.01632	-0.00668	-0.02301	0.66494
D18	-2.41113	-0.00014	-0.01603	-0.00669	-0.02272	-2.43386
D19	-2.65121	-0.00004	-0.00706	-0.00464	-0.01170	-2.66290
D20	0.53291	-0.00004	-0.00677	-0.00465	-0.01142	0.52149
D21	0.06249	0.00013	0.00054	-0.00184	-0.00129	0.06119
D22	3.00877	0.00007	0.00494	0.00045	0.00540	3.01416
D23	3.08262	0.00024	0.00640	-0.00184	0.00455	3.08717
D24	-0.25429	0.00018	0.01080	0.00045	0.01125	-0.24304
D25	1.21040	0.00022	0.01088	0.00026	0.01114	1.22154
D26	-2.97546	0.00005	0.01231	0.00136	0.01366	-2.96180
D27	-0.93028	0.00017	0.01207	0.00088	0.01295	-0.91733
D28	-1.70161	0.00031	0.00567	-0.00245	0.00322	-1.69839
D29	0.39571	0.00014	0.00710	-0.00136	0.00574	0.40146
D30	2.44090	0.00026	0.00686	-0.00183	0.00503	2.44593
D31	-1.08826	0.00005	0.01304	-0.00858	0.00446	-1.08380
D32	0.99063	0.00002	0.01373	-0.00686	0.00689	0.99752
D33	3.13682	-0.00005	0.00978	-0.00692	0.00285	3.13968
D34	3.12098	0.00009	0.01076	-0.00943	0.00132	3.12230
D35	-1.08330	0.00005	0.01145	-0.00772	0.00374	-1.07957
D36	1.06289	-0.00002	0.00749	-0.00778	-0.00029	1.06259
D37	1.03201	-0.00003	0.01175	-0.00942	0.00232	1.03433
D38	3.11090	-0.00007	0.01244	-0.00771	0.00475	3.11565
D39	-1.02609	-0.00014	0.00849	-0.00777	0.00071	-1.02538
D40	-0.13723	0.00029	-0.05237	0.03131	-0.02105	-0.15828
D41	1.95632	-0.00003	-0.05210	0.03189	-0.02022	1.93610
D42	-2.24235	0.00022	-0.04386	0.02982	-0.01404	-2.25639
D43	-1.83870	0.00037	-0.10579	0.03344	-0.07230	-1.91100
D44	2.36339	0.00012	-0.10497	0.03371	-0.07132	2.29207
D45	0.27146	-0.00056	-0.10988	0.03339	-0.07647	0.19499
D46	-3.08524	-0.00008	-0.00066	-0.00112	-0.00179	-3.08702
D47	0.05315	-0.00004	-0.00060	-0.00009	-0.00070	0.05245
D48	0.00799	-0.00005	-0.00089	-0.00106	-0.00195	0.00604
D49	-3.13681	-0.00001	-0.00083	-0.00003	-0.00085	-3.13767

Item	Value	Threshold	Converged?

Maximum Force	0.001527	0.000450	NO
RMS Force	0.000289	0.000300	YES
Maximum Displacement	0.069907	0.001800	NO
RMS Displacement	0.012491	0.001200	NO

Predicted change in Energy=-1.420910D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.450815	-1.970874	-1.322053
2	6	0	-1.741430	-1.593852	-1.486296
3	7	0	-2.105406	-0.875534	-0.350559
4	6	0	-1.032292	-0.788940	0.460097
5	7	0	-0.030052	-1.488167	-0.088315
6	6	0	1.347131	-1.505166	0.422521
7	6	0	2.245817	-0.518677	-0.340359
8	1	0	0.202887	-2.529414	-1.968813
9	1	0	-2.419374	-1.738268	-2.307848
10	1	0	1.309109	-1.228180	1.475935
11	1	0	1.736625	-2.522169	0.347800
12	1	0	2.303272	-0.803942	-1.395844
13	1	0	1.816773	0.484296	-0.269644
14	35	0	-0.374157	2.055721	0.509128
15	1	0	-1.021564	-0.334995	1.431863
16	6	0	-3.313123	-0.155474	-0.128635
17	6	0	-4.498647	-0.580348	-0.546162
18	1	0	-3.132677	0.787412	0.378085
19	1	0	-5.372062	0.037951	-0.390247
20	1	0	-4.638661	-1.531476	-1.046062
21	8	0	3.556269	-0.589827	0.210091
22	1	0	3.732726	0.223045	0.692470

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.354551	0.000000			
3	N	2.209353	1.392249	0.000000		
4	C	2.216109	2.222432	1.347677	0.000000	
5	N	1.390021	2.212314	2.179721	1.339462	0.000000
6	C	2.548143	3.631894	3.593619	2.485165	1.468971
7	C	3.216275	4.285710	4.365843	3.385228	2.486567

8	H	1.075914	2.210988	3.268376	3.233345	2.162112
9	H	2.213848	1.074901	2.161913	3.238324	3.270740
10	H	3.387870	4.267823	3.888360	2.589791	2.075529
11	H	2.806640	4.040117	4.237961	3.268577	2.092965
12	H	2.992018	4.122106	4.531466	3.817162	2.760832
13	H	3.503909	4.296481	4.152008	3.204812	2.708182
14	Br	4.424090	4.378417	3.511201	2.920212	3.610330
15	H	3.253599	3.258616	2.154977	1.072619	2.150312
16	C	3.593429	2.526340	1.423488	2.439278	3.543480
17	C	4.349771	3.084361	2.419297	3.615478	4.582805
18	H	4.206066	3.328949	2.086048	2.627399	3.875831
19	H	5.396509	4.128630	3.392207	4.498937	5.563925
20	H	4.219869	2.931151	2.707650	3.978162	4.707275
21	O	4.506826	5.652558	5.696535	4.599678	3.709145
22	H	5.135524	6.165592	6.031465	4.876834	4.206705

		6	7	8	9	10
6	C	0.000000				
7	C	1.537134	0.000000			
8	H	2.841980	3.296738	0.000000		
9	H	4.657876	5.207919	2.759911	0.000000	
10	H	1.089884	2.163270	3.844895	5.336552	0.000000
11	H	1.091597	2.178719	2.778326	4.993926	1.769143
12	H	2.170800	1.094863	2.777978	4.899807	3.068460
13	H	2.158151	1.093176	3.817623	5.199905	2.497467
14	Br	3.956040	3.770069	5.243723	5.149041	3.814722
15	H	2.828213	3.721597	4.228398	4.231842	2.496348
16	C	4.882971	5.574815	4.624302	2.837780	5.009029
17	C	5.997228	6.747884	5.284620	2.961029	6.183735
18	H	5.032550	5.581238	5.256924	3.755276	4.999734
19	H	6.941855	7.638350	6.337451	3.943414	7.051507
20	H	6.163370	6.994270	5.028712	2.561270	6.467490
21	O	2.400680	1.423145	4.444636	6.585381	2.656987
22	H	2.958150	1.956473	5.207515	7.120182	2.931517

		11	12	13	14	15
11	H	0.000000				
12	H	2.512705	0.000000			
13	H	3.070259	1.778922	0.000000		
14	Br	5.043659	4.356056	2.806428	0.000000	
15	H	3.683277	4.389803	3.409182	2.643123	0.000000
16	C	5.597159	5.793982	5.171559	3.732780	2.778242
17	C	6.591544	6.858429	6.410496	5.007386	4.007853
18	H	5.887643	5.935383	5.000849	3.038949	2.612861
19	H	7.591597	7.786576	7.203688	5.464368	4.731385
20	H	6.600651	6.988712	6.807261	5.785551	4.544786

21	O	2.657821	2.048138	2.099935	4.747272	4.744915
22	H	3.411659	2.731134	2.159813	4.500978	4.843695

		16	17	18	19	20
16	C	0.000000				
17	C	1.326768	0.000000			
18	H	1.085523	2.142633	0.000000		
19	H	2.084486	1.081414	2.483319	0.000000	
20	H	2.119459	1.083582	3.110214	1.852315	0.000000
21	O	6.891440	8.090344	6.831325	8.970484	8.343950
22	H	7.103625	8.362723	6.895731	9.170806	8.728171

		21	22
21	O	0.000000	
22	H	0.961555	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.205759	-2.255681	-0.599597
2	6	0	-1.494886	-1.865110	-0.742479
3	7	0	-1.703298	-0.810720	0.142498
4	6	0	-0.541425	-0.548501	0.772994
5	7	0	0.369257	-1.445391	0.372486
6	6	0	1.795206	-1.393220	0.721513
7	6	0	2.628527	-0.748838	-0.397921
8	1	0	0.351693	-3.026779	-1.101838
9	1	0	-2.267412	-2.211011	-1.405025
10	1	0	1.887710	-0.804126	1.633796
11	1	0	2.142914	-2.406841	0.929492
12	1	0	2.554831	-1.347679	-1.311531
13	1	0	2.240671	0.252777	-0.601314
14	35	0	0.202525	2.125065	-0.135976
15	1	0	-0.404697	0.180381	1.547944
16	6	0	-2.855169	0.018862	0.248819
17	6	0	-4.093211	-0.436512	0.106696
18	1	0	-2.589210	1.058160	0.414608
19	1	0	-4.923858	0.254654	0.148776
20	1	0	-4.318485	-1.484143	-0.054149

```
      21                8                0            3.991197     -0.731613       0.012171
      22                1                0            4.246498      0.177021       0.195999
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.8330085           0.5693385           0.3584418
 Standard basis: 6-311++G(d,p) (5D, 7F)
 There are     358 symmetry adapted cartesian basis functions of A      symmetry.
 There are     345 symmetry adapted basis functions of A      symmetry.
    345 basis functions,      553 primitive gaussians,      358 cartesian basis functions
     55 alpha electrons              55 beta electrons
          nuclear repulsion energy             868.0314302318 Hartrees.
 NAtoms=       22 NActive=       22 NUniq=       22 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      345 RedAO= T EigKep=    7.21D-06    NBF=      345
 NBsUse=      345 1.00D-06 EigRej= -1.00D+00 NBFU=      345
 Initial guess from the checkpoint file:    "."
 B after Tr=          0.000000        0.000000        0.000000
             Rot=        0.999999        0.000181      -0.000004        0.001650 Ang=      0.19 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn=                5 AccDes=
0.00D+00
 Harris functional with IExCor=    402 and IRadAn=             5 diagonalized for initial guess.
 HarFok:    IExCor=    402 AccDes= 0.00D+00 IRadAn=                5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=    3500011 ScaDFX=    1.000000    1.000000    1.000000    1.000000
 FoFCou: FMM=F IPFlag=                  0 FMFlag=           100000 FMFlg1=                  0
             NFxFlg=                   0 DoJE=T BraDBF=F KetDBF=T FulRan=T
             wScrn=      0.000000 ICntrl=             500 IOpCl=      0 I1Cent=        200000004 NGrid=
0
             NMat0=        1 NMatS0=            1 NMatT0=        0 NMatD0=        1 NMtDS0=        0
NMtDT0=        0
 Petite list used in FoFCou.
 Keep R1 ints in memory in canonical form, NReq=1804729152.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                       energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3032.33831386          A.U. after      11 cycles
                  NFock= 11    Conv=0.35D-08         -V/T= 2.0017
 Calling FoFJK, ICntrl=              2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 ---------------------------------------------------------------------
```

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000057369	0.000032425	0.000164523
2	6	-0.000110979	0.000087860	0.000195143
3	7	0.000132807	0.000172604	-0.000313308
4	6	0.000128268	-0.000370763	-0.000130537
5	7	0.000027738	-0.000055825	-0.000113763
6	6	-0.000278415	0.000075002	0.000133587
7	6	-0.000086786	0.000041327	0.000182620
8	1	0.000064590	0.000123834	-0.000029891
9	1	-0.000012431	-0.000053101	0.000009697
10	1	0.000102317	-0.000064999	0.000003951
11	1	-0.000015276	-0.000063751	-0.000010119
12	1	-0.000023909	-0.000078109	0.000014200
13	1	-0.000249214	-0.000063603	-0.000227945
14	35	0.000121681	-0.000035832	0.000110882
15	1	0.000036908	0.000308739	-0.000095618
16	6	0.000291703	-0.000320090	0.000012686
17	6	0.000095438	0.000213289	0.000059650
18	1	-0.000233362	0.000015502	0.000019659
19	1	-0.000066463	0.000015488	0.000001359
20	1	-0.000079379	-0.000011905	-0.000060237
21	8	0.000290179	0.000166217	0.000090430
22	1	-0.000078045	-0.000134309	-0.000016969

Cartesian Forces: Max 0.000370763 RMS 0.000141869

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000405091 RMS 0.000104254
Search for a local minimum.
Step number 22 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 18 20 21 22
DE= -1.81D-05 DEPred=-1.42D-05 R= 1.27D+00
TightC=F SS= 1.41D+00 RLast= 1.42D-01 DXNew= 2.0938D+00 4.2488D-01
Trust test= 1.27D+00 RLast= 1.42D-01 DXMaxT set to 1.25D+00
ITU= 1 1 1 0 -1 1 1 1 1 1 1 1 1 1 1 1 0 0 -1
ITU= 0 0

Eigenvalues --- 0.00038 0.00233 0.00461 0.00701 0.01013
Eigenvalues --- 0.01336 0.01594 0.01749 0.01943 0.02079
Eigenvalues --- 0.02229 0.02417 0.03066 0.03091 0.03508
Eigenvalues --- 0.04272 0.04777 0.05449 0.05760 0.06952
Eigenvalues --- 0.08842 0.09315 0.13646 0.14288 0.15140
Eigenvalues --- 0.15764 0.15835 0.15987 0.15993 0.16085
Eigenvalues --- 0.16583 0.17582 0.20819 0.22761 0.22813
Eigenvalues --- 0.23980 0.24775 0.26079 0.29675 0.33088
Eigenvalues --- 0.33826 0.33877 0.33880 0.34137 0.34376
Eigenvalues --- 0.34472 0.34700 0.36127 0.36315 0.36401
Eigenvalues --- 0.37236 0.43041 0.43459 0.45788 0.49805
Eigenvalues --- 0.53376 0.54427 0.56489 0.60630 2.40644
En-DIIS/RFO-DIIS IScMMF= 0 using points: 22 21 20 19
RFO step: Lambda=-4.49943065D-06.
DidBck=T Rises=F RFO-DIIS coefs: 0.47671 0.61099 -1.07655 0.98885
Iteration 1 RMS(Cart)= 0.01080146 RMS(Int)= 0.00006719
Iteration 2 RMS(Cart)= 0.00011644 RMS(Int)= 0.00002087
Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00002087

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55973	0.00001	-0.00006	-0.00035	-0.00039	2.55934
R2	2.62676	-0.00014	-0.00027	0.00048	0.00022	2.62698
R3	2.03318	-0.00001	0.00002	-0.00001	0.00001	2.03319
R4	2.63097	-0.00025	-0.00068	0.00038	-0.00031	2.63066
R5	2.03127	0.00001	-0.00005	0.00007	0.00002	2.03129
R6	2.54674	-0.00003	-0.00026	0.00143	0.00116	2.54790
R7	2.69000	-0.00006	-0.00120	-0.00078	-0.00198	2.68802
R8	2.53122	-0.00022	-0.00030	0.00006	-0.00025	2.53097
R9	2.02696	0.00004	0.00039	-0.00014	0.00025	2.02721
R10	2.77595	-0.00012	-0.00076	-0.00070	-0.00146	2.77449
R11	2.90476	-0.00011	-0.00200	0.00141	-0.00058	2.90418
R12	2.05958	-0.00002	-0.00018	0.00062	0.00044	2.06003
R13	2.06282	0.00005	0.00019	-0.00013	0.00006	2.06288
R14	2.06899	0.00001	0.00089	-0.00097	-0.00007	2.06892
R15	2.06580	-0.00004	0.00022	0.00049	0.00071	2.06652
R16	2.68935	0.00021	0.00092	-0.00126	-0.00034	2.68901
R17	5.30338	-0.00008	0.00098	-0.01495	-0.01396	5.28942
R18	2.50723	-0.00002	-0.00002	0.00061	0.00059	2.50781
R19	2.05134	-0.00002	-0.00045	0.00035	-0.00010	2.05125
R20	2.04358	0.00006	-0.00013	0.00051	0.00038	2.04395
R21	2.04767	0.00006	-0.00004	0.00037	0.00033	2.04800
R22	1.81707	-0.00013	-0.00005	0.00125	0.00120	1.81827
A1	1.87484	0.00005	-0.00014	0.00055	0.00041	1.87525
A2	2.27905	0.00001	0.00033	-0.00011	0.00022	2.27927

A3	2.12928	-0.00006	-0.00021	-0.00045	-0.00065	2.12863
A4	1.86898	-0.00005	-0.00003	0.00001	-0.00004	1.86894
A5	2.28658	0.00001	-0.00010	-0.00045	-0.00056	2.28602
A6	2.12695	0.00004	0.00019	0.00061	0.00079	2.12774
A7	1.89197	0.00000	0.00017	-0.00017	0.00002	1.89199
A8	2.22681	0.00007	0.00065	0.00077	0.00148	2.22830
A9	2.15231	-0.00006	-0.00022	0.00032	0.00017	2.15248
A10	1.89229	0.00006	-0.00021	0.00007	-0.00015	1.89214
A11	2.18967	-0.00009	-0.00014	-0.00019	-0.00028	2.18939
A12	2.19490	0.00003	0.00079	0.00032	0.00115	2.19605
A13	1.89461	-0.00006	0.00005	-0.00015	-0.00011	1.89450
A14	2.19990	0.00005	-0.00019	-0.00009	-0.00027	2.19963
A15	2.17141	0.00000	0.00070	0.00110	0.00181	2.17322
A16	1.94776	-0.00041	0.00066	0.00013	0.00078	1.94855
A17	1.87598	0.00024	0.00124	0.00052	0.00176	1.87774
A18	1.89810	0.00005	-0.00065	-0.00126	-0.00192	1.89619
A19	1.91451	0.00002	-0.00002	0.00154	0.00152	1.91603
A20	1.93407	0.00017	-0.00077	-0.00032	-0.00109	1.93298
A21	1.89166	-0.00007	-0.00044	-0.00062	-0.00105	1.89061
A22	1.91975	-0.00010	-0.00034	-0.00031	-0.00071	1.91905
A23	1.90419	-0.00020	0.00119	-0.00170	-0.00047	1.90372
A24	1.89052	0.00026	-0.00700	0.00627	-0.00072	1.88981
A25	1.89864	0.00013	0.00003	0.00465	0.00471	1.90335
A26	1.88759	-0.00003	0.00572	-0.00703	-0.00130	1.88630
A27	1.96302	-0.00006	0.00027	-0.00193	-0.00157	1.96145
A28	2.56456	-0.00004	-0.00147	0.00185	0.00038	2.56493
A29	2.14964	0.00020	0.00089	0.00272	0.00360	2.15324
A30	1.95101	0.00014	0.00100	0.00124	0.00224	1.95325
A31	2.18167	-0.00034	-0.00191	-0.00395	-0.00586	2.17581
A32	2.08658	-0.00001	-0.00039	-0.00109	-0.00148	2.08509
A33	2.14329	0.00008	0.00078	0.00150	0.00228	2.14557
A34	2.05332	-0.00008	-0.00039	-0.00041	-0.00080	2.05252
A35	1.89732	-0.00007	-0.00066	-0.00178	-0.00244	1.89488
D1	0.00345	0.00006	0.00054	-0.00037	0.00016	0.00361
D2	3.10515	0.00005	0.00173	0.00444	0.00616	3.11131
D3	-3.13088	0.00006	0.00155	0.00076	0.00230	-3.12857
D4	-0.02917	0.00005	0.00274	0.00557	0.00830	-0.02087
D5	-0.03979	-0.00008	-0.00197	0.00306	0.00109	-0.03869
D6	-2.98887	-0.00003	-0.00538	-0.00183	-0.00721	-2.99608
D7	3.09530	-0.00008	-0.00287	0.00205	-0.00082	3.09448
D8	0.14621	-0.00004	-0.00627	-0.00285	-0.00912	0.13709
D9	0.03381	-0.00003	0.00107	-0.00244	-0.00138	0.03243
D10	3.01160	0.00001	0.00654	0.00379	0.01032	3.02191
D11	-3.07235	-0.00002	0.00002	-0.00669	-0.00667	-3.07902

D12	-0.09456	0.00002	0.00549	-0.00046	0.00502	-0.08954
D13	-0.05901	-0.00002	-0.00231	0.00438	0.00207	-0.05694
D14	-3.08543	-0.00011	-0.00732	0.00261	-0.00470	-3.09013
D15	-3.04534	-0.00008	-0.00756	-0.00158	-0.00915	-3.05449
D16	0.21143	-0.00017	-0.01257	-0.00334	-0.01592	0.19551
D17	0.66494	-0.00008	-0.01016	-0.02021	-0.03037	0.63457
D18	-2.43386	-0.00009	-0.00962	-0.02020	-0.02981	-2.46367
D19	-2.66290	-0.00003	-0.00389	-0.01316	-0.01706	-2.67996
D20	0.52149	-0.00003	-0.00335	-0.01315	-0.01651	0.50498
D21	0.06119	0.00006	0.00264	-0.00462	-0.00198	0.05921
D22	3.01416	0.00002	0.00586	0.00002	0.00589	3.02005
D23	3.08717	0.00014	0.00761	-0.00289	0.00470	3.09188
D24	-0.24304	0.00010	0.01083	0.00174	0.01257	-0.23047
D25	1.22154	0.00005	0.01526	-0.00277	0.01249	1.23403
D26	-2.96180	-0.00001	0.01643	-0.00047	0.01596	-2.94584
D27	-0.91733	0.00006	0.01624	-0.00159	0.01466	-0.90267
D28	-1.69839	0.00010	0.01142	-0.00826	0.00316	-1.69522
D29	0.40146	0.00004	0.01259	-0.00595	0.00664	0.40809
D30	2.44593	0.00011	0.01240	-0.00707	0.00534	2.45126
D31	-1.08380	0.00010	0.01270	-0.02385	-0.01116	-1.09495
D32	0.99752	0.00008	0.01326	-0.01939	-0.00611	0.99141
D33	3.13968	0.00004	0.01013	-0.01889	-0.00877	3.13091
D34	3.12230	0.00004	0.01076	-0.02559	-0.01484	3.10747
D35	-1.07957	0.00002	0.01132	-0.02113	-0.00979	-1.08936
D36	1.06259	-0.00002	0.00819	-0.02062	-0.01245	1.05014
D37	1.03433	0.00001	0.01179	-0.02560	-0.01382	1.02051
D38	3.11565	-0.00001	0.01235	-0.02114	-0.00877	3.10688
D39	-1.02538	-0.00005	0.00922	-0.02064	-0.01143	-1.03681
D40	-0.15828	0.00024	-0.07251	0.09139	0.01890	-0.13938
D41	1.93610	0.00008	-0.07220	0.09279	0.02058	1.95668
D42	-2.25639	0.00009	-0.06476	0.08590	0.02113	-2.23527
D43	-1.91100	0.00007	-0.11302	0.10922	-0.00372	-1.91473
D44	2.29207	0.00006	-0.11169	0.11003	-0.00175	2.29032
D45	0.19499	-0.00004	-0.11592	0.11012	-0.00578	0.18920
D46	-3.08702	-0.00003	0.00036	-0.00272	-0.00236	-3.08938
D47	0.05245	-0.00003	-0.00053	-0.00034	-0.00087	0.05158
D48	0.00604	-0.00001	-0.00017	-0.00257	-0.00274	0.00331
D49	-3.13767	-0.00001	-0.00106	-0.00019	-0.00125	-3.13892

Item	Value	Threshold	Converged?
Maximum Force	0.000405	0.000450	YES
RMS Force	0.000104	0.000300	YES
Maximum Displacement	0.046822	0.001800	NO
RMS Displacement	0.010793	0.001200	NO

Predicted change in Energy=-6.926954D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.453947	-1.974612	-1.319371
2	6	0	-1.744958	-1.599166	-1.482401
3	7	0	-2.105503	-0.872586	-0.351034
4	6	0	-1.029886	-0.781184	0.456789
5	7	0	-0.029003	-1.483013	-0.090454
6	6	0	1.347897	-1.504102	0.418763
7	6	0	2.248676	-0.518187	-0.341766
8	1	0	0.198637	-2.536191	-1.964634
9	1	0	-2.426447	-1.754323	-2.299063
10	1	0	1.312966	-1.233165	1.474098
11	1	0	1.734152	-2.521941	0.338355
12	1	0	2.313649	-0.808029	-1.395526
13	1	0	1.818424	0.484834	-0.273265
14	35	0	-0.358506	2.054999	0.520577
15	1	0	-1.015725	-0.316665	1.423651
16	6	0	-3.315907	-0.160638	-0.124353
17	6	0	-4.500034	-0.578683	-0.553559
18	1	0	-3.143715	0.775120	0.398099
19	1	0	-5.373745	0.037010	-0.387913
20	1	0	-4.640296	-1.520635	-1.070839
21	8	0	3.555859	-0.586340	0.216317
22	1	0	3.727761	0.230618	0.694682

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.354344	0.000000			
3	N	2.209021	1.392086	0.000000		
4	C	2.216015	2.222810	1.348290	0.000000	
5	N	1.390138	2.212580	2.179995	1.339330	0.000000
6	C	2.547377	3.631696	3.594075	2.485540	1.468196
7	C	3.221965	4.291699	4.368588	3.384646	2.486336
8	H	1.075919	2.210911	3.268081	3.233050	2.161841
9	H	2.213386	1.074913	2.162240	3.239152	3.270979
10	H	3.387505	4.269162	3.891922	2.593869	2.076325
11	H	2.799179	4.033717	4.235396	3.268664	2.090924
12	H	3.004380	4.135908	4.541369	3.822435	2.765290

13	H	3.508116	4.301483	4.152811	3.201351	2.705333
14	Br	4.430833	4.391708	3.518872	2.915262	3.605477
15	H	3.254006	3.259100	2.155499	1.072754	2.150930
16	C	3.592963	2.526171	1.422439	2.438995	3.543101
17	C	4.348092	3.081328	2.420986	3.619909	4.585019
18	H	4.212550	3.336171	2.086629	2.625605	3.878051
19	H	5.396170	4.128326	3.392658	4.500231	5.564640
20	H	4.218220	2.925497	2.713533	3.989424	4.714509
21	O	4.512669	5.657749	5.696916	4.596177	3.708014
22	H	5.138690	6.167532	6.028064	4.869860	4.203123

		6	7	8	9	10
6	C	0.000000				
7	C	1.536827	0.000000			
8	H	2.840174	3.302832	0.000000		
9	H	4.657774	5.216879	2.759389	0.000000	
10	H	1.090118	2.164280	3.842458	5.337749	0.000000
11	H	1.091629	2.177689	2.767990	4.985559	1.768687
12	H	2.169986	1.094824	2.789928	4.917353	3.068687
13	H	2.157815	1.093554	3.822438	5.209281	2.502056
14	Br	3.948339	3.763286	5.250306	5.170850	3.809861
15	H	2.829578	3.716668	4.228646	4.232683	2.503062
16	C	4.883742	5.580295	4.624058	2.839073	5.013166
17	C	6.000009	6.752304	5.282091	2.954434	6.191180
18	H	5.036850	5.594455	5.264846	3.766596	5.005296
19	H	6.943070	7.642753	6.337102	3.943087	7.056382
20	H	6.170709	6.999599	5.024490	2.542494	6.480793
21	O	2.399660	1.422965	4.453022	6.593884	2.651596
22	H	2.957894	1.955154	5.213628	7.125783	2.929400

		11	12	13	14	15
11	H	0.000000				
12	H	2.505923	0.000000			
13	H	3.069507	1.782193	0.000000		
14	Br	5.035951	4.359907	2.799040	0.000000	
15	H	3.688215	4.390208	3.399165	2.621502	0.000000
16	C	5.594010	5.807486	5.176887	3.751160	2.776959
17	C	6.590663	6.869336	6.413466	5.024172	4.014776
18	H	5.887934	5.958713	5.015756	3.067650	2.602325
19	H	7.589328	7.799064	7.207009	5.481811	4.732778
20	H	6.604698	6.997898	6.809779	5.800991	4.561748
21	O	2.660838	2.047015	2.098996	4.731966	4.736007
22	H	3.417313	2.729006	2.155717	4.478421	4.830277

		16	17	18	19	20
16	C	0.000000				
17	C	1.327078	0.000000			

18	H	1.085472	2.139635	0.000000		
19	H	2.084040	1.081613	2.477025	0.000000	
20	H	2.121187	1.083755	3.109345	1.852186	0.000000
21	O	6.893363	8.092601	6.838926	8.971705	8.349050
22	H	7.101912	8.361201	6.899393	9.167710	8.729739

		21	22
21	O	0.000000	
22	H	0.962187	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.232539	-2.259350	-0.591048
2	6	0	-1.518757	-1.859709	-0.733094
3	7	0	-1.714964	-0.794565	0.141477
4	6	0	-0.548421	-0.536415	0.766314
5	7	0	0.353387	-1.444077	0.370464
6	6	0	1.779212	-1.406909	0.718659
7	6	0	2.619768	-0.772994	-0.400919
8	1	0	0.317315	-3.038969	-1.088500
9	1	0	-2.297679	-2.209766	-1.385917
10	1	0	1.879955	-0.821036	1.632421
11	1	0	2.114699	-2.425006	0.925011
12	1	0	2.548311	-1.378494	-1.310261
13	1	0	2.238657	0.230576	-0.609392
14	35	0	0.231818	2.123548	-0.136227
15	1	0	-0.402197	0.202060	1.530561
16	6	0	-2.862322	0.038806	0.252814
17	6	0	-4.103871	-0.404033	0.099236
18	1	0	-2.594332	1.075111	0.433100
19	1	0	-4.928010	0.294655	0.149391
20	1	0	-4.339797	-1.446938	-0.077435
21	8	0	3.980450	-0.760254	0.015267
22	1	0	4.238458	0.149794	0.191473

Rotational constants (GHZ): 0.8333669 0.5687012 0.3579649
Standard basis: 6-311++G(d,p) (5D, 7F)

```
 There are      358 symmetry adapted cartesian basis functions of A      symmetry.
 There are      345 symmetry adapted basis functions of A      symmetry.
    345 basis functions,      553 primitive gaussians,      358 cartesian basis functions
     55 alpha electrons              55 beta electrons
          nuclear repulsion energy             867.9053079340 Hartrees.
 NAtoms=       22 NActive=       22 NUniq=       22 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      345 RedAO= T EigKep=    7.07D-06    NBF=      345
 NBsUse=      345 1.00D-06 EigRej= -1.00D+00 NBFU=      345
 Initial guess from the checkpoint file:    "."
 B after Tr=          0.000000        0.000000        0.000000
             Rot=        0.999988        0.000584        0.000077        0.004825 Ang=      0.56 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn=                5 AccDes=
0.00D+00
 Harris functional with IExCor=    402 and IRadAn=             5 diagonalized for initial guess.
 HarFok:    IExCor=    402 AccDes= 0.00D+00 IRadAn=                5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=    3500011 ScaDFX=    1.000000    1.000000    1.000000    1.000000
 FoFCou: FMM=F IPFlag=                  0 FMFlag=           100000 FMFlg1=                  0
             NFxFlg=                    0 DoJE=T BraDBF=F KetDBF=T FulRan=T
             wScrn=      0.000000  ICntrl=             500  IOpCl=      0  I1Cent=        200000004  NGrid=
0
             NMat0=         1 NMatS0=            1 NMatT0=         0 NMatD0=         1 NMtDS0=         0
NMtDT0=        0
 Petite list used in FoFCou.
 Keep R1 ints in memory in canonical form, NReq=1804729152.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                      energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3032.33832583          A.U. after      11 cycles
                  NFock= 11    Conv=0.23D-08         -V/T= 2.0017
 Calling FoFJK, ICntrl=             2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center         Atomic                             Forces (Hartrees/Bohr)
 Number          Number                       X                      Y                      Z
 -------------------------------------------------------------------
        1              6                  0.000201753       0.000096914       0.000157714
        2              6                 -0.000249685      -0.000093756       0.000075750
```

3	7	0.000378812	0.000046944	-0.000014992
4	6	-0.000122111	-0.000416683	-0.000129430
5	7	-0.000557111	-0.000222229	-0.000311912
6	6	-0.000009548	-0.000202935	0.000317045
7	6	-0.000093371	0.000123656	0.000408845
8	1	0.000005865	0.000041781	-0.000027109
9	1	0.000062988	0.000117405	-0.000049748
10	1	0.000044030	0.000101856	-0.000228014
11	1	0.000017129	-0.000088800	0.000112066
12	1	-0.000273423	0.000225596	-0.000096388
13	1	-0.000225266	-0.000355932	-0.000571465
14	35	0.000140408	0.000400349	0.000037302
15	1	0.000000986	0.000032566	-0.000041993
16	6	-0.000197074	0.000114605	0.000004218
17	6	0.000151856	0.000061047	0.000131434
18	1	0.000042266	-0.000161281	-0.000000378
19	1	0.000057634	-0.000059500	-0.000094366
20	1	0.000027455	0.000100449	0.000028074
21	8	0.000592689	0.000875956	0.000527722
22	1	0.000003717	-0.000738007	-0.000234374

Cartesian Forces: Max 0.000875956 RMS 0.000257374

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.002011132 RMS 0.000297927
Search for a local minimum.
Step number 23 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 18 20 21 22 23
DE= -1.20D-05 DEPred=-6.93D-06 R= 1.73D+00
TightC=F SS= 1.41D+00 RLast= 8.25D-02 DXNew= 2.0938D+00 2.4764D-01
Trust test= 1.73D+00 RLast= 8.25D-02 DXMaxT set to 1.25D+00
ITU= 1 1 1 1 0 -1 1 1 1 1 1 1 1 1 1 1 1 0 0
ITU= -1 0 0
Eigenvalues --- 0.00037 0.00213 0.00447 0.00734 0.00989
Eigenvalues --- 0.01336 0.01605 0.01779 0.01928 0.02073
Eigenvalues --- 0.02231 0.02441 0.03066 0.03096 0.03506
Eigenvalues --- 0.04263 0.04773 0.05446 0.05779 0.07295
Eigenvalues --- 0.08856 0.09317 0.13660 0.14250 0.15221

Eigenvalues --- 0.15758 0.15850 0.15991 0.15996 0.16087
Eigenvalues --- 0.16679 0.17538 0.20869 0.22770 0.22849
Eigenvalues --- 0.24031 0.24832 0.26695 0.29669 0.33092
Eigenvalues --- 0.33822 0.33878 0.33880 0.34141 0.34412
Eigenvalues --- 0.34564 0.34742 0.36150 0.36315 0.36400
Eigenvalues --- 0.37234 0.43060 0.43595 0.45995 0.50055
Eigenvalues --- 0.53511 0.54422 0.57057 0.60831 2.21524
En-DIIS/RFO-DIIS IScMMF= 0 using points: 23 22 21 20 19
RFO step: Lambda=-1.11453937D-05.
DidBck=F Rises=F RFO-DIIS coefs: 2.36002 -4.39767 2.60215 -0.19955 0.63505
Iteration 1 RMS(Cart)= 0.00905882 RMS(Int)= 0.00008514
Iteration 2 RMS(Cart)= 0.00021025 RMS(Int)= 0.00003038
Iteration 3 RMS(Cart)= 0.00000005 RMS(Int)= 0.00003038

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55934	0.00010	0.00008	-0.00002	0.00007	2.55941
R2	2.62698	-0.00017	-0.00017	-0.00007	-0.00022	2.62676
R3	2.03319	0.00000	-0.00001	0.00002	0.00001	2.03320
R4	2.63066	-0.00008	-0.00028	0.00017	-0.00011	2.63055
R5	2.03129	-0.00002	-0.00002	0.00000	-0.00003	2.03126
R6	2.54790	-0.00040	-0.00029	0.00000	-0.00030	2.54760
R7	2.68802	-0.00004	-0.00053	0.00016	-0.00037	2.68765
R8	2.53097	-0.00036	-0.00033	-0.00010	-0.00044	2.53053
R9	2.02721	-0.00002	0.00010	0.00005	0.00015	2.02736
R10	2.77449	0.00025	0.00002	0.00006	0.00008	2.77457
R11	2.90418	0.00044	0.00014	0.00068	0.00081	2.90500
R12	2.06003	-0.00020	-0.00019	0.00008	-0.00011	2.05991
R13	2.06288	0.00008	0.00012	0.00001	0.00013	2.06301
R14	2.06892	0.00002	-0.00003	-0.00035	-0.00038	2.06854
R15	2.06652	0.00005	-0.00018	0.00036	0.00018	2.06670
R16	2.68901	0.00065	0.00036	-0.00061	-0.00026	2.68876
R17	5.28942	0.00013	0.00141	-0.00489	-0.00348	5.28594
R18	2.50781	-0.00026	-0.00010	-0.00003	-0.00013	2.50769
R19	2.05125	-0.00014	-0.00030	0.00003	-0.00027	2.05097
R20	2.04395	-0.00010	-0.00012	0.00006	-0.00006	2.04389
R21	2.04800	-0.00010	-0.00009	0.00001	-0.00008	2.04792
R22	1.81827	-0.00074	-0.00023	0.00013	-0.00009	1.81818
A1	1.87525	-0.00008	-0.00004	-0.00001	-0.00006	1.87519
A2	2.27927	0.00003	-0.00001	-0.00008	-0.00008	2.27919
A3	2.12863	0.00005	0.00003	0.00008	0.00012	2.12875
A4	1.86894	-0.00013	-0.00007	-0.00003	-0.00012	1.86881
A5	2.28602	0.00005	-0.00003	-0.00029	-0.00028	2.28574
A6	2.12774	0.00007	0.00004	0.00032	0.00039	2.12812

A7	1.89199	0.00007	0.00001	-0.00005	0.00001	1.89200
A8	2.22830	0.00013	0.00028	0.00033	0.00074	2.22904
A9	2.15248	-0.00020	-0.00028	-0.00034	-0.00047	2.15201
A10	1.89214	0.00008	0.00011	-0.00001	0.00008	1.89221
A11	2.18939	-0.00004	-0.00010	-0.00013	-0.00016	2.18923
A12	2.19605	-0.00003	0.00016	0.00013	0.00036	2.19641
A13	1.89450	0.00007	-0.00006	0.00010	0.00006	1.89456
A14	2.19963	0.00006	0.00016	0.00013	0.00035	2.19998
A15	2.17322	-0.00014	-0.00056	-0.00043	-0.00094	2.17228
A16	1.94855	0.00030	-0.00011	-0.00073	-0.00084	1.94771
A17	1.87774	0.00002	-0.00018	-0.00078	-0.00095	1.87679
A18	1.89619	-0.00016	0.00042	0.00055	0.00096	1.89715
A19	1.91603	-0.00007	-0.00051	-0.00033	-0.00083	1.91520
A20	1.93298	-0.00015	0.00027	0.00116	0.00143	1.93441
A21	1.89061	0.00005	0.00009	0.00011	0.00020	1.89080
A22	1.91905	-0.00032	-0.00025	0.00016	-0.00014	1.91891
A23	1.90372	0.00123	0.00051	0.00017	0.00072	1.90444
A24	1.88981	-0.00024	0.00068	0.00192	0.00262	1.89242
A25	1.90335	-0.00047	-0.00035	-0.00019	-0.00051	1.90284
A26	1.88630	0.00026	-0.00047	-0.00216	-0.00262	1.88368
A27	1.96145	-0.00049	-0.00028	0.00010	-0.00009	1.96137
A28	2.56493	0.00201	-0.00072	0.00328	0.00256	2.56749
A29	2.15324	-0.00006	0.00025	0.00060	0.00085	2.15409
A30	1.95325	-0.00004	0.00039	0.00020	0.00058	1.95383
A31	2.17581	0.00011	-0.00064	-0.00077	-0.00142	2.17440
A32	2.08509	0.00009	0.00002	-0.00005	-0.00003	2.08506
A33	2.14557	-0.00006	0.00012	0.00030	0.00042	2.14599
A34	2.05252	-0.00003	-0.00014	-0.00026	-0.00039	2.05213
A35	1.89488	0.00034	0.00010	-0.00044	-0.00034	1.89454
D1	0.00361	-0.00002	0.00054	-0.00062	-0.00009	0.00352
D2	3.11131	-0.00010	-0.00023	-0.00057	-0.00080	3.11051
D3	-3.12857	0.00006	0.00155	0.00047	0.00201	-3.12656
D4	-0.02087	-0.00001	0.00079	0.00052	0.00130	-0.01957
D5	-0.03869	0.00005	-0.00079	0.00049	-0.00030	-0.03899
D6	-2.99608	0.00008	0.00118	0.00171	0.00287	-2.99321
D7	3.09448	-0.00003	-0.00170	-0.00048	-0.00218	3.09230
D8	0.13709	0.00000	0.00028	0.00073	0.00099	0.13808
D9	0.03243	-0.00001	-0.00010	0.00054	0.00044	0.03288
D10	3.02191	-0.00002	0.00231	0.00011	0.00240	3.02431
D11	-3.07902	0.00006	0.00058	0.00050	0.00109	-3.07793
D12	-0.08954	0.00005	0.00299	0.00007	0.00305	-0.08649
D13	-0.05694	0.00003	-0.00040	-0.00023	-0.00063	-0.05758
D14	-3.09013	-0.00002	-0.00332	-0.00009	-0.00342	-3.09355
D15	-3.05449	0.00001	-0.00270	0.00010	-0.00262	-3.05710

D16	0.19551	-0.00004	-0.00562	0.00025	-0.00540	0.19011
D17	0.63457	-0.00002	-0.00396	-0.00889	-0.01283	0.62174
D18	-2.46367	-0.00005	-0.00386	-0.00950	-0.01334	-2.47701
D19	-2.67996	-0.00001	-0.00119	-0.00934	-0.01054	-2.69051
D20	0.50498	-0.00004	-0.00109	-0.00995	-0.01106	0.49392
D21	0.05921	-0.00005	0.00074	-0.00015	0.00058	0.05979
D22	3.02005	-0.00005	-0.00106	-0.00128	-0.00236	3.01769
D23	3.09188	0.00001	0.00367	-0.00032	0.00334	3.09522
D24	-0.23047	0.00000	0.00187	-0.00144	0.00040	-0.23007
D25	1.23403	-0.00023	-0.00327	-0.00115	-0.00442	1.22960
D26	-2.94584	-0.00012	-0.00405	-0.00250	-0.00656	-2.95240
D27	-0.90267	-0.00013	-0.00383	-0.00250	-0.00634	-0.90901
D28	-1.69522	-0.00022	-0.00110	0.00019	-0.00091	-1.69613
D29	0.40809	-0.00011	-0.00188	-0.00116	-0.00305	0.40505
D30	2.45126	-0.00012	-0.00166	-0.00117	-0.00282	2.44844
D31	-1.09495	0.00016	0.00073	-0.01290	-0.01217	-1.10713
D32	0.99141	0.00016	0.00047	-0.01293	-0.01244	0.97897
D33	3.13091	0.00017	0.00106	-0.01151	-0.01047	3.12044
D34	3.10747	-0.00001	0.00134	-0.01124	-0.00991	3.09755
D35	-1.08936	-0.00001	0.00107	-0.01128	-0.01018	-1.09953
D36	1.05014	0.00000	0.00166	-0.00986	-0.00821	1.04193
D37	1.02051	0.00007	0.00138	-0.01190	-0.01052	1.00999
D38	3.10688	0.00006	0.00112	-0.01193	-0.01079	3.09609
D39	-1.03681	0.00007	0.00171	-0.01051	-0.00882	-1.04563
D40	-0.13938	0.00018	0.00108	0.03884	0.03994	-0.09944
D41	1.95668	0.00025	0.00088	0.03902	0.03989	1.99658
D42	-2.23527	-0.00004	-0.00003	0.03625	0.03622	-2.19905
D43	-1.91473	-0.00043	0.01269	0.01200	0.02476	-1.88997
D44	2.29032	-0.00006	0.01308	0.01194	0.02494	2.31526
D45	0.18920	0.00065	0.01380	0.01356	0.02738	0.21658
D46	-3.08938	0.00003	0.00048	-0.00039	0.00009	-3.08929
D47	0.05158	-0.00002	-0.00018	-0.00094	-0.00112	0.05046
D48	0.00331	0.00005	0.00040	0.00033	0.00073	0.00403
D49	-3.13892	0.00000	-0.00026	-0.00022	-0.00048	-3.13940

Item	Value	Threshold	Converged?
Maximum Force	0.002011	0.000450	NO
RMS Force	0.000298	0.000300	YES
Maximum Displacement	0.035759	0.001800	NO
RMS Displacement	0.009086	0.001200	NO

Predicted change in Energy=-1.346940D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.454366	-1.977039	-1.318398
2	6	0	-1.745184	-1.600460	-1.480658
3	7	0	-2.104501	-0.874328	-0.348685
4	6	0	-1.028361	-0.783881	0.458282
5	7	0	-0.028587	-1.486421	-0.089508
6	6	0	1.348949	-1.505556	0.418183
7	6	0	2.247730	-0.520845	-0.347127
8	1	0	0.197938	-2.537361	-1.965046
9	1	0	-2.426741	-1.754239	-2.297505
10	1	0	1.314346	-1.229419	1.472117
11	1	0	1.735758	-2.523617	0.342431
12	1	0	2.321007	-0.820950	-1.397253
13	1	0	1.810545	0.480109	-0.292074
14	35	0	-0.351043	2.057441	0.522708
15	1	0	-1.012679	-0.317195	1.424166
16	6	0	-3.314768	-0.163529	-0.118916
17	6	0	-4.498094	-0.574288	-0.557063
18	1	0	-3.144242	0.765832	0.415075
19	1	0	-5.371131	0.041271	-0.387630
20	1	0	-4.638610	-1.509427	-1.086408
21	8	0	3.553545	-0.573306	0.215488
22	1	0	3.708838	0.240328	0.704975

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.354382	0.000000			
3	N	2.208904	1.392028	0.000000		
4	C	2.215781	2.222639	1.348129	0.000000	
5	N	1.390024	2.212468	2.179736	1.339098	0.000000
6	C	2.547539	3.631565	3.593446	2.484759	1.468237
7	C	3.219502	4.288802	4.366562	3.383880	2.486025
8	H	1.075925	2.210913	3.267954	3.232803	2.161813
9	H	2.213267	1.074898	2.162402	3.239046	3.270799
10	H	3.387366	4.268170	3.889720	2.591263	2.075618
11	H	2.802453	4.036438	4.236199	3.268097	2.091712
12	H	3.007566	4.141074	4.548347	3.829183	2.770133
13	H	3.495817	4.287739	4.143101	3.196888	2.700125
14	Br	4.435919	4.397425	3.525509	2.921647	3.610781
15	H	3.253990	3.259039	2.155335	1.072835	2.150985
16	C	3.592975	2.526402	1.422243	2.438371	3.542583

17	C	4.347306	3.079703	2.421308	3.621312	4.585530
18	H	4.214700	3.339238	2.086747	2.623057	3.877442
19	H	5.395783	4.127649	3.392743	4.500677	5.564665
20	H	4.216679	2.921581	2.714645	3.993293	4.716637
21	O	4.515155	5.657605	5.694066	4.593164	3.709241
22	H	5.132545	6.157260	6.012284	4.852928	4.192995

		6	7	8	9	10
6	C	0.000000				
7	C	1.537258	0.000000			
8	H	2.840639	3.299341	0.000000		
9	H	4.657536	5.213052	2.759121	0.000000	
10	H	1.090058	2.164008	3.843328	5.336780	0.000000
11	H	1.091699	2.179152	2.773000	4.988748	1.768821
12	H	2.170112	1.094622	2.788526	4.921645	3.068142
13	H	2.158796	1.093649	3.808472	5.193135	2.506206
14	Br	3.949158	3.762684	5.253809	5.176005	3.805042
15	H	2.828691	3.716076	4.228651	4.232670	2.499900
16	C	4.882599	5.578633	4.624108	2.839930	5.009611
17	C	6.000523	6.749301	5.280983	2.951597	6.191222
18	H	5.034678	5.595520	5.267468	3.771426	4.997737
19	H	6.942729	7.639676	6.336569	3.942196	7.054709
20	H	6.173709	6.996107	5.022036	2.533585	6.485534
21	O	2.402170	1.422829	4.457841	6.593448	2.650211
22	H	2.949480	1.954773	5.212580	7.116074	2.912431

		11	12	13	14	15
11	H	0.000000				
12	H	2.503615	0.000000			
13	H	3.070922	1.781782	0.000000		
14	Br	5.037195	4.371640	2.797197	0.000000	
15	H	3.686782	4.396321	3.398790	2.624745	0.000000
16	C	5.593807	5.816211	5.168471	3.758731	2.775667
17	C	6.593169	6.875092	6.401633	5.028910	4.017397
18	H	5.885589	5.972550	5.013144	3.079253	2.595144
19	H	7.590752	7.805879	7.195706	5.485886	4.733624
20	H	6.610805	7.000492	6.795648	5.804743	4.568564
21	O	2.669116	2.044850	2.098893	4.718159	4.730423
22	H	3.415241	2.733450	2.157572	4.451714	4.808409

		16	17	18	19	20
16	C	0.000000				
17	C	1.327010	0.000000			
18	H	1.085328	2.138665	0.000000		
19	H	2.083933	1.081579	2.475552	0.000000	
20	H	2.121330	1.083714	3.108761	1.851902	0.000000
21	O	6.888648	8.088617	6.833263	8.966120	8.347615

```
    22    H       7.083286      8.343265      6.879309      9.147636      8.714964
                        21            22
    21    O       0.000000
    22    H       0.962140      0.000000
Stoichiometry       C7H11BrN2O
Framework group     C1[X(C7H11BrN2O)]
Deg. of freedom     60
Full point group                 C1          NOp     1
Largest Abelian subgroup         C1          NOp     1
Largest concise Abelian subgroup C1          NOp     1
                         Standard orientation:
---------------------------------------------------------------------
Center      Atomic      Atomic              Coordinates (Angstroms)
Number      Number       Type                X           Y           Z
---------------------------------------------------------------------
     1           6           0       -0.244933   -2.261327   -0.589171
     2           6           0       -1.529015   -1.854875   -0.731580
     3           7           0       -1.719777   -0.789035    0.143255
     4           6           0       -0.552059   -0.536995    0.768045
     5           7           0        0.344822   -1.449383    0.372650
     6           6           0        1.771155   -1.416959    0.719410
     7           6           0        2.612378   -0.789386   -0.403826
     8           1           0        0.301401   -3.042635   -1.087862
     9           1           0       -2.309155   -2.200456   -1.385309
    10           1           0        1.874355   -0.826857    1.630099
    11           1           0        2.103242   -2.435264    0.930553
    12           1           0        2.546993   -1.404017   -1.307237
    13           1           0        2.227131    0.210194   -0.624041
    14          35           0        0.246270    2.123990   -0.136308
    15           1           0       -0.401539    0.202644    1.530444
    16           6           0       -2.863126    0.049156    0.257117
    17           6           0       -4.106469   -0.384273    0.092214
    18           1           0       -2.591296    1.081966    0.450383
    19           1           0       -4.926495    0.318966    0.145363
    20           1           0       -4.348217   -1.423440   -0.097858
    21           8           0        3.972741   -0.766045    0.012478
    22           1           0        4.219303    0.144487    0.201824
---------------------------------------------------------------------
Rotational constants (GHZ):           0.8321645           0.5689459           0.3578851
Standard basis: 6-311++G(d,p) (5D, 7F)
There are     358 symmetry adapted cartesian basis functions of A     symmetry.
There are     345 symmetry adapted basis functions of A     symmetry.
   345 basis functions,     553 primitive gaussians,     358 cartesian basis functions
    55 alpha electrons        55 beta electrons
```

nuclear repulsion energy 867.6792376319 Hartrees.
NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 345 RedAO= T EigKep= 7.02D-06 NBF= 345
NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345
Initial guess from the checkpoint file: "."
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999997 0.000059 0.000045 0.002353 Ang= 0.27 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.33835081 A.U. after 10 cycles
NFock= 10 Conv=0.85D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000181225	0.000118685	0.000092167
2	6	-0.000254685	-0.000114010	0.000063915
3	7	0.000291254	0.000184962	-0.000065969
4	6	-0.000225722	-0.000426016	-0.000020542
5	7	-0.000339961	-0.000150713	-0.000343989
6	6	0.000116928	0.000014242	0.000376195

7	6	0.000064233	0.000054476	0.000177983
8	1	-0.000018697	-0.000008158	0.000002266
9	1	0.000046857	0.000095742	-0.000033058
10	1	0.000056878	0.000074084	-0.000157099
11	1	-0.000019726	-0.000019232	0.000069102
12	1	-0.000308170	0.000161699	-0.000175311
13	1	-0.000246218	-0.000421605	-0.000385911
14	35	0.000105270	0.000174258	0.000081210
15	1	0.000035429	0.000075446	-0.000057644
16	6	-0.000212488	0.000146629	0.000047988
17	6	0.000086894	0.000004815	0.000035993
18	1	0.000122688	-0.000119968	-0.000047915
19	1	0.000056147	-0.000054783	-0.000055230
20	1	0.000030476	0.000074073	0.000034226
21	8	0.000410372	0.000717518	0.000509920
22	1	0.000021017	-0.000582144	-0.000148297

Cartesian Forces: Max 0.000717518 RMS 0.000214074

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000840310 RMS 0.000152413
Search for a local minimum.
Step number 24 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 18 20 21 22 23 24
DE= -2.50D-05 DEPred=-1.35D-05 R= 1.85D+00
TightC=F SS= 1.41D+00 RLast= 9.12D-02 DXNew= 2.0938D+00 2.7358D-01
Trust test= 1.85D+00 RLast= 9.12D-02 DXMaxT set to 1.25D+00
ITU= 1 1 1 1 1 0 -1 1 1 1 1 1 1 1 1 1 1 1 1 0
ITU= 0 -1 0 0

Eigenvalues ---	0.00016	0.00152	0.00414	0.00710	0.00952
Eigenvalues ---	0.01240	0.01597	0.01776	0.01868	0.02070
Eigenvalues ---	0.02188	0.02413	0.03066	0.03096	0.03724
Eigenvalues ---	0.04358	0.04805	0.05460	0.06162	0.06677
Eigenvalues ---	0.09075	0.09314	0.13694	0.14173	0.15416
Eigenvalues ---	0.15820	0.15853	0.15992	0.15995	0.16536
Eigenvalues ---	0.16683	0.17207	0.20909	0.22716	0.22862
Eigenvalues ---	0.24019	0.24872	0.25378	0.29837	0.33215

Eigenvalues --- 0.33860 0.33880 0.33976 0.34139 0.34309
Eigenvalues --- 0.34514 0.34732 0.36263 0.36324 0.36585
Eigenvalues --- 0.37211 0.43171 0.43269 0.45769 0.48978
Eigenvalues --- 0.53358 0.54556 0.56004 0.60492 2.48259
En-DIIS/RFO-DIIS IScMMF= 0 using points: 24 23 22 21 20
RFO step: Lambda=-7.17142367D-06.
DidBck=F Rises=F RFO-DIIS coefs: 3.43141 0.27281 -6.28225 3.22473 0.35330
Iteration 1 RMS(Cart)= 0.05309575 RMS(Int)= 0.01906895
Iteration 2 RMS(Cart)= 0.02300374 RMS(Int)= 0.00070745
Iteration 3 RMS(Cart)= 0.00098116 RMS(Int)= 0.00002298
Iteration 4 RMS(Cart)= 0.00000136 RMS(Int)= 0.00002296
Iteration 5 RMS(Cart)= 0.00000000 RMS(Int)= 0.00002296

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55941	0.00013	-0.00013	0.00052	0.00038	2.55979
R2	2.62676	-0.00010	-0.00019	-0.00038	-0.00056	2.62620
R3	2.03320	-0.00001	0.00004	0.00001	0.00005	2.03325
R4	2.63055	-0.00006	-0.00005	-0.00037	-0.00043	2.63012
R5	2.03126	-0.00002	-0.00002	-0.00008	-0.00010	2.03117
R6	2.54760	-0.00028	0.00013	-0.00096	-0.00084	2.54676
R7	2.68765	-0.00006	-0.00179	-0.00074	-0.00253	2.68512
R8	2.53053	-0.00019	-0.00133	-0.00042	-0.00174	2.52879
R9	2.02736	-0.00002	0.00035	0.00044	0.00079	2.02815
R10	2.77457	0.00029	-0.00023	0.00117	0.00094	2.77550
R11	2.90500	0.00011	0.00475	0.00059	0.00534	2.91033
R12	2.05991	-0.00014	0.00014	-0.00019	-0.00005	2.05986
R13	2.06301	0.00000	0.00027	-0.00016	0.00011	2.06312
R14	2.06854	0.00011	-0.00266	0.00001	-0.00265	2.06589
R15	2.06670	-0.00017	0.00064	-0.00031	0.00033	2.06703
R16	2.68876	0.00052	-0.00197	-0.00091	-0.00288	2.68588
R17	5.28594	0.00005	-0.02469	-0.00936	-0.03405	5.25188
R18	2.50769	-0.00016	0.00004	-0.00019	-0.00015	2.50753
R19	2.05097	-0.00011	-0.00063	-0.00055	-0.00118	2.04979
R20	2.04389	-0.00009	0.00010	-0.00032	-0.00022	2.04367
R21	2.04792	-0.00008	-0.00002	-0.00020	-0.00022	2.04771
R22	1.81818	-0.00056	0.00095	-0.00006	0.00088	1.81906
A1	1.87519	-0.00005	0.00025	-0.00005	0.00018	1.87537
A2	2.27919	0.00001	-0.00030	-0.00033	-0.00063	2.27856
A3	2.12875	0.00004	-0.00001	0.00034	0.00032	2.12907
A4	1.86881	-0.00009	-0.00030	-0.00029	-0.00060	1.86821
A5	2.28574	0.00004	-0.00095	-0.00042	-0.00135	2.28439
A6	2.12812	0.00004	0.00130	0.00059	0.00192	2.13004
A7	1.89200	0.00005	-0.00025	0.00031	0.00009	1.89209

A8	2.22904	0.00008	0.00231	0.00162	0.00399	2.23303
A9	2.15201	-0.00013	-0.00126	-0.00070	-0.00190	2.15011
A10	1.89221	0.00008	0.00043	0.00037	0.00075	1.89297
A11	2.18923	-0.00003	-0.00087	0.00007	-0.00085	2.18838
A12	2.19641	-0.00005	0.00120	0.00105	0.00219	2.19861
A13	1.89456	0.00001	-0.00010	0.00000	-0.00007	1.89448
A14	2.19998	0.00012	0.00077	0.00108	0.00186	2.20184
A15	2.17228	-0.00014	-0.00216	-0.00209	-0.00423	2.16806
A16	1.94771	-0.00013	-0.00197	-0.00311	-0.00509	1.94262
A17	1.87679	0.00015	-0.00294	-0.00068	-0.00363	1.87316
A18	1.89715	-0.00003	0.00204	0.00110	0.00315	1.90030
A19	1.91520	-0.00004	-0.00113	-0.00067	-0.00181	1.91339
A20	1.93441	0.00006	0.00365	0.00255	0.00621	1.94062
A21	1.89080	0.00000	0.00020	0.00082	0.00102	1.89182
A22	1.91891	-0.00013	-0.00111	0.00123	0.00019	1.91910
A23	1.90444	0.00033	0.00119	-0.00273	-0.00154	1.90290
A24	1.89242	-0.00004	0.01728	0.00404	0.02134	1.91376
A25	1.90284	-0.00020	0.00293	-0.00037	0.00251	1.90535
A26	1.88368	0.00021	-0.01812	-0.00130	-0.01941	1.86427
A27	1.96137	-0.00017	-0.00240	-0.00077	-0.00324	1.95813
A28	2.56749	0.00084	0.00811	0.00514	0.01325	2.58074
A29	2.15409	-0.00009	0.00403	0.00065	0.00468	2.15877
A30	1.95383	-0.00010	0.00276	-0.00044	0.00232	1.95615
A31	2.17440	0.00019	-0.00675	-0.00020	-0.00695	2.16745
A32	2.08506	0.00007	-0.00109	0.00016	-0.00094	2.08413
A33	2.14599	-0.00005	0.00214	0.00041	0.00256	2.14855
A34	2.05213	-0.00001	-0.00106	-0.00057	-0.00163	2.05050
A35	1.89454	0.00030	-0.00281	-0.00065	-0.00345	1.89109
D1	0.00352	0.00002	-0.00039	0.00065	0.00026	0.00378
D2	3.11051	-0.00008	0.00256	-0.00348	-0.00091	3.10960
D3	-3.12656	0.00006	0.00559	0.00399	0.00957	-3.11700
D4	-0.01957	-0.00003	0.00854	-0.00015	0.00839	-0.01118
D5	-0.03899	0.00004	0.00061	0.00253	0.00314	-0.03585
D6	-2.99321	0.00010	0.00849	0.00852	0.01702	-2.97620
D7	3.09230	0.00000	-0.00474	-0.00046	-0.00521	3.08710
D8	0.13808	0.00005	0.00314	0.00553	0.00867	0.14675
D9	0.03288	-0.00007	0.00002	-0.00358	-0.00355	0.02932
D10	3.02431	-0.00006	0.00793	0.00537	0.01332	3.03763
D11	-3.07793	0.00002	-0.00256	0.00013	-0.00244	-3.08037
D12	-0.08649	0.00003	0.00535	0.00907	0.01444	-0.07205
D13	-0.05758	0.00009	0.00034	0.00517	0.00552	-0.05206
D14	-3.09355	-0.00003	-0.00825	-0.00964	-0.01789	-3.11144
D15	-3.05710	0.00006	-0.00748	-0.00353	-0.01099	-3.06809
D16	0.19011	-0.00006	-0.01607	-0.01834	-0.03439	0.15572

D17	0.62174	0.00000	-0.04414	-0.01665	-0.06078	0.56096
D18	-2.47701	-0.00001	-0.04507	-0.01669	-0.06176	-2.53878
D19	-2.69051	0.00003	-0.03501	-0.00637	-0.04138	-2.73188
D20	0.49392	0.00002	-0.03594	-0.00641	-0.04236	0.45157
D21	0.05979	-0.00008	-0.00059	-0.00477	-0.00537	0.05442
D22	3.01769	-0.00010	-0.00788	-0.01024	-0.01812	2.99957
D23	3.09522	0.00004	0.00791	0.01005	0.01798	3.11319
D24	-0.23007	0.00002	0.00062	0.00458	0.00523	-0.22484
D25	1.22960	-0.00007	-0.01682	-0.01000	-0.02683	1.20277
D26	-2.95240	-0.00010	-0.02125	-0.01312	-0.03437	-2.98677
D27	-0.90901	-0.00004	-0.02154	-0.01193	-0.03347	-0.94248
D28	-1.69613	-0.00003	-0.00807	-0.00338	-0.01145	-1.70758
D29	0.40505	-0.00006	-0.01250	-0.00650	-0.01899	0.38606
D30	2.44844	0.00000	-0.01279	-0.00531	-0.01809	2.43035
D31	-1.10713	0.00021	-0.06150	-0.01510	-0.07659	-1.18372
D32	0.97897	0.00008	-0.05785	-0.01649	-0.07435	0.90462
D33	3.12044	0.00005	-0.04917	-0.01660	-0.06576	3.05468
D34	3.09755	0.00013	-0.05588	-0.01186	-0.06774	3.02981
D35	-1.09953	0.00000	-0.05223	-0.01325	-0.06550	-1.16503
D36	1.04193	-0.00003	-0.04356	-0.01336	-0.05691	0.98503
D37	1.00999	0.00012	-0.05771	-0.01406	-0.07176	0.93823
D38	3.09609	0.00000	-0.05405	-0.01544	-0.06952	3.02657
D39	-1.04563	-0.00003	-0.04538	-0.01556	-0.06093	-1.10656
D40	-0.09944	0.00018	0.19845	0.08371	0.28214	0.18270
D41	1.99658	0.00010	0.19960	0.08334	0.28295	2.27953
D42	-2.19905	0.00012	0.17740	0.08098	0.25839	-1.94065
D43	-1.88997	-0.00005	0.23341	0.04502	0.27838	-1.61159
D44	2.31526	0.00001	0.23531	0.04204	0.27746	2.59272
D45	0.21658	0.00022	0.24518	0.04384	0.28896	0.50554
D46	-3.08929	0.00001	-0.00075	-0.00024	-0.00100	-3.09029
D47	0.05046	0.00000	-0.00297	-0.00034	-0.00331	0.04715
D48	0.00403	0.00001	0.00058	-0.00021	0.00038	0.00441
D49	-3.13940	0.00001	-0.00163	-0.00030	-0.00193	-3.14133

Item	Value	Threshold	Converged?
Maximum Force	0.000840	0.000450	NO
RMS Force	0.000152	0.000300	YES
Maximum Displacement	0.290753	0.001800	NO
RMS Displacement	0.060233	0.001200	NO

Predicted change in Energy=-8.697317D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-0.456354	-1.990923	-1.315186
2	6	0	-1.746686	-1.610163	-1.473184
3	7	0	-2.099020	-0.882926	-0.340006
4	6	0	-1.021120	-0.800052	0.464682
5	7	0	-0.024828	-1.501974	-0.087973
6	6	0	1.357229	-1.506369	0.409093
7	6	0	2.241985	-0.530568	-0.388949
8	1	0	0.193848	-2.546857	-1.967754
9	1	0	-2.430132	-1.761776	-2.288788
10	1	0	1.326928	-1.201330	1.455134
11	1	0	1.747655	-2.524666	0.358369
12	1	0	2.368885	-0.893655	-1.412274
13	1	0	1.758842	0.450469	-0.413255
14	35	0	-0.257451	2.105223	0.546005
15	1	0	-0.997499	-0.320404	1.424500
16	6	0	-3.308861	-0.179327	-0.094642
17	6	0	-4.489168	-0.557127	-0.568860
18	1	0	-3.145992	0.720870	0.488195
19	1	0	-5.359033	0.056728	-0.378909
20	1	0	-4.631951	-1.460863	-1.149429
21	8	0	3.538094	-0.476444	0.191806
22	1	0	3.554978	0.245255	0.828579

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.354584	0.000000			
3	N	2.208390	1.391799	0.000000		
4	C	2.214738	2.222172	1.347687	0.000000	
5	N	1.389726	2.212535	2.179224	1.338178	0.000000
6	C	2.548924	3.631532	3.591029	2.481636	1.468732
7	C	3.204931	4.272070	4.355557	3.383661	2.484483
8	H	1.075950	2.210806	3.267334	3.231751	2.161753
9	H	2.212738	1.074847	2.163276	3.239108	3.270562
10	H	3.387953	4.264890	3.880854	2.579796	2.073357
11	H	2.818390	4.049854	4.240277	3.263696	2.094472
12	H	3.032392	4.177921	4.594786	3.876063	2.802443
13	H	3.417743	4.202187	4.082451	3.172186	2.664454
14	Br	4.503555	4.483195	3.620142	3.005067	3.669865
15	H	3.254129	3.259038	2.154823	1.073253	2.151690
16	C	3.592827	2.527462	1.420905	2.435549	3.540383
17	C	4.344694	3.073743	2.423081	3.626924	4.588499

18	H	4.223762	3.352430	2.086679	2.613205	3.874877
19	H	5.394975	4.126138	3.392956	4.501468	5.564885
20	H	4.212369	2.907208	2.721197	4.010003	4.727998
21	O	4.529932	5.655653	5.676717	4.578823	3.718118
22	H	5.068235	6.070282	5.882693	4.708053	4.087528

		6	7	8	9	10
6	C	0.000000				
7	C	1.540082	0.000000			
8	H	2.843496	3.279163	0.000000		
9	H	4.657027	5.191718	2.757660	0.000000	
10	H	1.090031	2.165154	3.848438	5.333531	0.000000
11	H	1.091757	2.186154	2.797437	5.004333	1.769498
12	H	2.171692	1.093220	2.787907	4.955046	3.066328
13	H	2.160269	1.093824	3.721509	5.095012	2.530982
14	Br	3.958476	3.750828	5.307023	5.264055	3.777574
15	H	2.825298	3.718470	4.228922	4.233025	2.485946
16	C	4.877211	5.569729	4.624145	2.844396	4.993679
17	C	6.003150	6.733609	5.276984	2.940911	6.191810
18	H	5.024525	5.600516	5.278661	3.793102	4.963551
19	H	6.940634	7.623680	6.335422	3.941199	7.046169
20	H	6.188807	6.978164	5.013718	2.497337	6.508405
21	O	2.421597	1.421304	4.487125	6.589776	2.647775
22	H	2.841524	1.951468	5.187732	7.040433	2.729357

		11	12	13	14	15
11	H	0.000000				
12	H	2.486222	0.000000			
13	H	3.073590	1.782375	0.000000		
14	Br	5.048913	4.441370	2.779177	0.000000	
15	H	3.678488	4.439420	3.401323	2.683857	0.000000
16	C	5.592333	5.872242	5.116617	3.865320	2.769492
17	C	6.605219	6.917911	6.330646	5.122349	4.027564
18	H	5.873512	6.052466	4.994309	3.203661	2.564555
19	H	7.596854	7.854413	7.128840	5.574760	4.734712
20	H	6.641122	7.028693	6.710989	5.893023	4.597282
21	O	2.725551	2.028346	2.095473	4.603979	4.702710
22	H	3.340655	2.779452	2.193255	4.251346	4.626028

		16	17	18	19	20
16	C	0.000000				
17	C	1.326929	0.000000			
18	H	1.084702	2.134189	0.000000		
19	H	2.083204	1.081464	2.467895	0.000000	
20	H	2.122611	1.083599	3.106420	1.850792	0.000000
21	O	6.859382	8.063625	6.796942	8.931342	8.337723
22	H	6.938652	8.203958	6.726446	8.997398	8.593553

		21	22
21	O	0.000000	
22	H	0.962608	0.000000

Stoichiometry C7H11BrN2O

Framework group C1[X(C7H11BrN2O)]

Deg. of freedom 60

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.395844	-2.271810	-0.577804
2	6	0	-1.654208	-1.792553	-0.725226
3	7	0	-1.785750	-0.716590	0.147760
4	6	0	-0.609097	-0.534444	0.779085
5	7	0	0.236144	-1.494168	0.385110
6	6	0	1.664655	-1.527233	0.724872
7	6	0	2.525497	-0.963108	-0.420801
8	1	0	0.108497	-3.079032	-1.079502
9	1	0	-2.449425	-2.094175	-1.382455
10	1	0	1.799900	-0.918111	1.618655
11	1	0	1.947664	-2.554639	0.962098
12	1	0	2.483100	-1.632695	-1.283927
13	1	0	2.137685	0.018423	-0.708290
14	35	0	0.428333	2.133521	-0.135314
15	1	0	-0.415468	0.206351	1.531150
16	6	0	-2.881695	0.179288	0.271357
17	6	0	-4.144026	-0.167736	0.054945
18	1	0	-2.560285	1.184654	0.521387
19	1	0	-4.920087	0.582423	0.122439
20	1	0	-4.445649	-1.178367	-0.193725
21	8	0	3.885599	-0.904378	-0.012415
22	1	0	4.053182	-0.032180	0.358799

Rotational constants (GHZ): 0.8154138 0.5674660 0.3544595

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 863.6848723324 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 6.80D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Initial guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999558 0.000002 0.000936 0.029716 Ang= 3.41 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Keep R1 ints in memory in canonical form, NReq=1804729152.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3032.33819384 A.U. after 13 cycles

NFock= 13 Conv=0.11D-08 -V/T= 2.0017

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000497878	0.000325336	0.000247891
2	6	-0.000423230	0.000023074	0.000233989
3	7	0.001064672	0.000195732	0.000116912
4	6	-0.000389461	-0.000080856	-0.000839523
5	7	-0.000358412	0.000489352	-0.000223953
6	6	0.001241326	0.000203144	0.000200254
7	6	0.000891457	0.000149108	-0.000458188

8	1	-0.000125390	-0.000231080	0.000114533
9	1	0.000005780	0.000106342	-0.000000972
10	1	-0.000233438	0.000077500	0.000041327
11	1	-0.000168989	0.000058570	0.000067261
12	1	-0.000262492	-0.000002696	-0.000311940
13	1	-0.000197069	-0.000080017	-0.000053267
14	35	-0.000862802	-0.002806508	0.000610205
15	1	0.000542262	0.001244918	-0.000221138
16	6	-0.000845419	0.000719664	0.000161523
17	6	0.000061866	-0.000176732	-0.000126332
18	1	0.000223483	0.000030094	-0.000107260
19	1	0.000057631	-0.000039384	0.000032394
20	1	0.000093896	0.000050967	0.000053871
21	8	-0.000980043	-0.000951350	0.000636659
22	1	0.000166492	0.000694822	-0.000174244

Cartesian Forces: Max 0.002806508 RMS 0.000567584

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.014211654 RMS 0.002215306
Search for a local minimum.
Step number 25 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 18 20 21 22 23
25 24
DE= 1.57D-04 DEPred=-8.70D-05 R=-1.80D+00
Trust test=-1.80D+00 RLast= 7.26D-01 DXMaxT set to 6.23D-01
ITU= -1 1 1 1 1 1 0 -1 1 1 1 1 1 1 1 1 1 1 1 1
ITU= 0 0 -1 0 0
Use linear search instead of GDIIS.
Energy rises -- skip Quadratic/GDIIS search.
Quartic linear search produced a step of -0.54729.
Iteration 1 RMS(Cart)= 0.03326574 RMS(Int)= 0.00184485
Iteration 2 RMS(Cart)= 0.00325929 RMS(Int)= 0.00001485
Iteration 3 RMS(Cart)= 0.00001718 RMS(Int)= 0.00000752
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000752

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55979	0.00048	-0.00021	0.00000	-0.00020	2.55959
R2	2.62620	-0.00052	0.00031	0.00000	0.00031	2.62651

R3	2.03325	-0.00003	-0.00003	0.00000	-0.00003	2.03323
R4	2.63012	-0.00003	0.00024	0.00000	0.00024	2.63036
R5	2.03117	-0.00002	0.00005	0.00000	0.00005	2.03122
R6	2.54676	-0.00075	0.00046	0.00000	0.00045	2.54721
R7	2.68512	0.00063	0.00138	0.00000	0.00138	2.68650
R8	2.52879	-0.00001	0.00095	0.00000	0.00095	2.52974
R9	2.02815	0.00037	-0.00043	0.00000	-0.00043	2.02772
R10	2.77550	-0.00020	-0.00051	0.00000	-0.00051	2.77499
R11	2.91033	-0.00271	-0.00292	0.00000	-0.00292	2.90741
R12	2.05986	0.00007	0.00003	0.00000	0.00003	2.05989
R13	2.06312	-0.00012	-0.00006	0.00000	-0.00006	2.06306
R14	2.06589	0.00026	0.00145	0.00000	0.00145	2.06734
R15	2.06703	-0.00212	-0.00018	0.00000	-0.00018	2.06685
R16	2.68588	-0.00057	0.00158	0.00000	0.00158	2.68745
R17	5.25188	-0.00083	0.01864	0.00000	0.01864	5.27052
R18	2.50753	-0.00012	0.00008	0.00000	0.00008	2.50762
R19	2.04979	0.00000	0.00065	0.00000	0.00065	2.05044
R20	2.04367	-0.00007	0.00012	0.00000	0.00012	2.04379
R21	2.04771	-0.00008	0.00012	0.00000	0.00012	2.04782
R22	1.81906	0.00041	-0.00048	0.00000	-0.00048	1.81858
A1	1.87537	-0.00032	-0.00010	0.00000	-0.00010	1.87527
A2	2.27856	0.00012	0.00035	0.00000	0.00035	2.27891
A3	2.12907	0.00020	-0.00018	0.00000	-0.00017	2.12890
A4	1.86821	0.00007	0.00033	0.00000	0.00033	1.86854
A5	2.28439	0.00000	0.00074	0.00000	0.00074	2.28513
A6	2.13004	-0.00009	-0.00105	0.00000	-0.00105	2.12899
A7	1.89209	-0.00010	-0.00005	0.00000	-0.00005	1.89204
A8	2.23303	-0.00007	-0.00218	0.00000	-0.00217	2.23086
A9	2.15011	0.00016	0.00104	0.00000	0.00106	2.15117
A10	1.89297	0.00020	-0.00041	0.00000	-0.00041	1.89256
A11	2.18838	0.00007	0.00047	0.00000	0.00050	2.18888
A12	2.19861	-0.00021	-0.00120	0.00000	-0.00117	2.19744
A13	1.89448	0.00015	0.00004	0.00000	0.00004	1.89452
A14	2.20184	0.00174	-0.00102	0.00000	-0.00100	2.20084
A15	2.16806	-0.00204	0.00231	0.00000	0.00232	2.17038
A16	1.94262	-0.00665	0.00278	0.00000	0.00279	1.94541
A17	1.87316	0.00121	0.00198	0.00000	0.00199	1.87515
A18	1.90030	0.00272	-0.00173	0.00000	-0.00173	1.89857
A19	1.91339	0.00035	0.00099	0.00000	0.00100	1.91438
A20	1.94062	0.00328	-0.00340	0.00000	-0.00340	1.93722
A21	1.89182	-0.00084	-0.00056	0.00000	-0.00056	1.89126
A22	1.91910	0.00263	-0.00010	0.00000	-0.00012	1.91898
A23	1.90290	-0.01040	0.00084	0.00000	0.00085	1.90375
A24	1.91376	0.00238	-0.01168	0.00000	-0.01168	1.90208

A25	1.90535	0.00228	-0.00137	0.00000	-0.00136	1.90399
A26	1.86427	-0.00107	0.01062	0.00000	0.01063	1.87489
A27	1.95813	0.00449	0.00177	0.00000	0.00179	1.95992
A28	2.58074	-0.01421	-0.00725	0.00000	-0.00725	2.57349
A29	2.15877	-0.00038	-0.00256	0.00000	-0.00256	2.15621
A30	1.95615	-0.00002	-0.00127	0.00000	-0.00127	1.95488
A31	2.16745	0.00040	0.00380	0.00000	0.00380	2.17125
A32	2.08413	0.00004	0.00051	0.00000	0.00051	2.08464
A33	2.14855	-0.00011	-0.00140	0.00000	-0.00140	2.14715
A34	2.05050	0.00007	0.00089	0.00000	0.00089	2.05139
A35	1.89109	-0.00005	0.00189	0.00000	0.00189	1.89298
D1	0.00378	0.00036	-0.00014	0.00000	-0.00014	0.00364
D2	3.10960	-0.00006	0.00050	0.00000	0.00050	3.11009
D3	-3.11700	0.00031	-0.00524	0.00000	-0.00524	-3.12223
D4	-0.01118	-0.00011	-0.00459	0.00000	-0.00460	-0.01578
D5	-0.03585	-0.00023	-0.00172	0.00000	-0.00172	-0.03757
D6	-2.97620	0.00085	-0.00931	0.00000	-0.00932	-2.98552
D7	3.08710	-0.00018	0.00285	0.00000	0.00285	3.08995
D8	0.14675	0.00090	-0.00475	0.00000	-0.00475	0.14200
D9	0.02932	-0.00036	0.00195	0.00000	0.00194	0.03127
D10	3.03763	-0.00042	-0.00729	0.00000	-0.00730	3.03033
D11	-3.08037	0.00001	0.00133	0.00000	0.00133	-3.07903
D12	-0.07205	-0.00006	-0.00790	0.00000	-0.00791	-0.07996
D13	-0.05206	0.00022	-0.00302	0.00000	-0.00302	-0.05508
D14	-3.11144	-0.00057	0.00979	0.00000	0.00978	-3.10165
D15	-3.06809	0.00030	0.00601	0.00000	0.00600	-3.06209
D16	0.15572	-0.00049	0.01882	0.00000	0.01881	0.17452
D17	0.56096	0.00014	0.03327	0.00000	0.03327	0.59423
D18	-2.53878	0.00015	0.03380	0.00000	0.03380	-2.50497
D19	-2.73188	0.00005	0.02264	0.00000	0.02264	-2.70924
D20	0.45157	0.00006	0.02318	0.00000	0.02318	0.47475
D21	0.05442	0.00002	0.00294	0.00000	0.00294	0.05736
D22	2.99957	-0.00050	0.00991	0.00000	0.00991	3.00948
D23	3.11319	0.00083	-0.00984	0.00000	-0.00985	3.10335
D24	-0.22484	0.00031	-0.00286	0.00000	-0.00287	-0.22771
D25	1.20277	0.00225	0.01468	0.00000	0.01469	1.21746
D26	-2.98677	-0.00045	0.01881	0.00000	0.01881	-2.96797
D27	-0.94248	0.00064	0.01832	0.00000	0.01832	-0.92416
D28	-1.70758	0.00315	0.00627	0.00000	0.00627	-1.70131
D29	0.38606	0.00045	0.01039	0.00000	0.01039	0.39645
D30	2.43035	0.00154	0.00990	0.00000	0.00990	2.44025
D31	-1.18372	-0.00048	0.04192	0.00000	0.04191	-1.14180
D32	0.90462	-0.00248	0.04069	0.00000	0.04070	0.94532
D33	3.05468	-0.00214	0.03599	0.00000	0.03599	3.09067

D34	3.02981	0.00192	0.03707	0.00000	0.03707	3.06688
D35	-1.16503	-0.00008	0.03585	0.00000	0.03585	-1.12918
D36	0.98503	0.00026	0.03115	0.00000	0.03114	1.01617
D37	0.93823	0.00066	0.03927	0.00000	0.03927	0.97750
D38	3.02657	-0.00134	0.03805	0.00000	0.03805	3.06462
D39	-1.10656	-0.00100	0.03335	0.00000	0.03334	-1.07322
D40	0.18270	-0.00076	-0.15441	0.00000	-0.15440	0.02829
D41	2.27953	-0.00244	-0.15486	0.00000	-0.15486	2.12467
D42	-1.94065	0.00047	-0.14142	0.00000	-0.14142	-2.08207
D43	-1.61159	0.00376	-0.15235	0.00000	-0.15233	-1.76392
D44	2.59272	-0.00006	-0.15185	0.00000	-0.15188	2.44084
D45	0.50554	-0.00478	-0.15814	0.00000	-0.15813	0.34741
D46	-3.09029	-0.00003	0.00055	0.00000	0.00054	-3.08975
D47	0.04715	0.00003	0.00181	0.00000	0.00181	0.04896
D48	0.00441	-0.00005	-0.00021	0.00000	-0.00021	0.00420
D49	-3.14133	0.00000	0.00106	0.00000	0.00106	-3.14027

Item	Value	Threshold	Converged?
Maximum Force	0.014212	0.000450	NO
RMS Force	0.002215	0.000300	NO
Maximum Displacement	0.157129	0.001800	NO
RMS Displacement	0.033058	0.001200	NO

Predicted change in Energy=-1.912424D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.455525	-1.984147	-1.316513
2	6	0	-1.746023	-1.605359	-1.476945
3	7	0	-2.101716	-0.877601	-0.344996
4	6	0	-1.024598	-0.790258	0.460667
5	7	0	-0.026746	-1.493354	-0.088887
6	6	0	1.352950	-1.505868	0.413767
7	6	0	2.245639	-0.526114	-0.367438
8	1	0	0.195515	-2.543289	-1.965471
9	1	0	-2.428638	-1.758631	-2.292972
10	1	0	1.320645	-1.215676	1.463979
11	1	0	1.740965	-2.524330	0.350173
12	1	0	2.342643	-0.856354	-1.405869
13	1	0	1.787755	0.466988	-0.349179
14	35	0	-0.313348	2.071043	0.540266
15	1	0	-1.004985	-0.316849	1.423413

16	6	0	-3.311519	-0.169416	-0.108559
17	6	0	-4.493750	-0.565527	-0.562745
18	1	0	-3.144001	0.747484	0.446918
19	1	0	-5.365106	0.049820	-0.384454
20	1	0	-4.635765	-1.487241	-1.114648
21	8	0	3.547829	-0.530428	0.204191
22	1	0	3.638127	0.248228	0.762458

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.354476	0.000000			
3	N	2.208673	1.391925	0.000000		
4	C	2.215306	2.222427	1.347927	0.000000	
5	N	1.389890	2.212502	2.179506	1.338680	0.000000
6	C	2.548176	3.631574	3.592376	2.483351	1.468461
7	C	3.212925	4.281255	4.361599	3.383782	2.485332
8	H	1.075937	2.210869	3.267679	3.232327	2.161789
9	H	2.213031	1.074875	2.162799	3.239074	3.270695
10	H	3.387693	4.266771	3.885775	2.586074	2.074599
11	H	2.809663	4.042518	4.238062	3.266122	2.092961
12	H	3.018219	4.157313	4.569271	3.850537	2.784639
13	H	3.460651	4.249007	4.115328	3.185255	2.683861
14	Br	4.462333	4.431437	3.560401	2.949450	3.630827
15	H	3.254071	3.259059	2.155118	1.073024	2.151318
16	C	3.592924	2.526893	1.421637	2.437103	3.541601
17	C	4.346023	3.076852	2.422113	3.623933	4.586887
18	H	4.218934	3.345364	2.086717	2.618532	3.876303
19	H	5.395345	4.126853	3.392843	4.501108	5.564786
20	H	4.214507	2.914759	2.717614	4.000991	4.721788
21	O	4.522464	5.657435	5.686783	4.586980	3.713584
22	H	5.105252	6.118805	5.953129	4.786495	4.145985

		6	7	8	9	10
6	C	0.000000				
7	C	1.538536	0.000000			
8	H	2.841949	3.290245	0.000000		
9	H	4.657331	5.203426	2.758464	0.000000	
10	H	1.090046	2.164532	3.845725	5.335410	0.000000
11	H	1.091726	2.182323	2.784059	4.995808	1.769127
12	H	2.170815	1.093987	2.787304	4.936211	3.067511
13	H	2.159469	1.093729	3.769535	5.148755	2.517359
14	Br	3.948018	3.757335	5.275389	5.212302	3.784931
15	H	2.827191	3.717189	4.228802	4.232852	2.493610
16	C	4.880185	5.574609	4.624141	2.841961	5.002448

17	C	6.001810	6.742334	5.279052	2.946502	6.191728
18	H	5.030037	5.597629	5.272682	3.781449	4.982116
19	H	6.941874	7.632525	6.335956	3.941546	7.051061
20	H	6.180705	6.988262	5.018008	2.516647	6.496298
21	O	2.410996	1.422139	4.471807	6.592607	2.648959
22	H	2.901805	1.953277	5.204396	7.082991	2.829464

		11	12	13	14	15
11	H	0.000000				
12	H	2.495565	0.000000			
13	H	3.072340	1.782058	0.000000		
14	Br	5.037241	4.405836	2.789039	0.000000	
15	H	3.683077	4.416165	3.399394	2.638246	0.000000
16	C	5.593179	5.841614	5.144464	3.798640	2.772864
17	C	6.598636	6.894325	6.369380	5.063981	4.022206
18	H	5.880223	6.009025	5.003466	3.126200	2.581034
19	H	7.593561	7.827761	7.165103	5.519123	4.734288
20	H	6.624495	7.012917	6.757704	5.838101	4.581936
21	O	2.694758	2.037399	2.097360	4.667900	4.718075
22	H	3.384713	2.756814	2.169670	4.357313	4.723840

		16	17	18	19	20
16	C	0.000000				
17	C	1.326973	0.000000			
18	H	1.085045	2.136642	0.000000		
19	H	2.083603	1.081527	2.472088	0.000000	
20	H	2.121911	1.083662	3.107707	1.851400	0.000000
21	O	6.875959	8.078145	6.817080	8.951179	8.344222
22	H	7.016458	8.279238	6.807796	9.078160	8.659831

		21	22
21	O	0.000000	
22	H	0.962351	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.305181	-2.269001	-0.579259
2	6	0	-1.579448	-1.833562	-0.725012
3	7	0	-1.746081	-0.759824	0.144916

4	6	0	-0.574124	-0.533653	0.771230
5	7	0	0.302143	-1.466872	0.379667
6	6	0	1.729989	-1.458709	0.722552
7	6	0	2.578406	-0.861740	-0.413631
8	1	0	0.224293	-3.062757	-1.076499
9	1	0	-2.366111	-2.164079	-1.378675
10	1	0	1.846194	-0.855903	1.623286
11	1	0	2.042834	-2.479767	0.949337
12	1	0	2.525235	-1.505135	-1.296821
13	1	0	2.189168	0.128165	-0.668236
14	35	0	0.318628	2.127178	-0.135541
15	1	0	-0.405906	0.210246	1.526013
16	6	0	-2.870719	0.102095	0.260401
17	6	0	-4.122498	-0.296935	0.074168
18	1	0	-2.578807	1.124787	0.475367
19	1	0	-4.924956	0.425904	0.131321
20	1	0	-4.389012	-1.325581	-0.138391
21	8	0	3.938550	-0.816846	-0.000753
22	1	0	4.145709	0.083555	0.268474

Rotational constants (GHZ): 0.8262131 0.5689083 0.3567878

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 866.3535908782 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 6.93D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Lowest energy guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999931 0.000410 0.000344 0.011772 Ang= 1.35 deg.

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999839 0.000406 -0.000596 -0.017941 Ang= 2.06 deg.

Keep R1 ints in memory in canonical form, NReq=1804729152.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3032.33840028 A.U. after 11 cycles

NFock= 11 Conv=0.45D-08 -V/T= 2.0017

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000288229	0.000206643	0.000100245
2	6	-0.000294051	-0.000075213	0.000087462
3	7	0.000531762	0.000213552	-0.000007510
4	6	-0.000347753	-0.000381272	-0.000192882
5	7	-0.000307258	0.000073530	-0.000305980
6	6	0.000521386	0.000100995	0.000314591
7	6	0.000396817	0.000062675	-0.000033345
8	1	-0.000072196	-0.000110832	0.000050317
9	1	0.000030785	0.000098159	-0.000021977
10	1	-0.000051945	0.000081766	-0.000078877
11	1	-0.000072863	0.000024083	0.000060251
12	1	-0.000265722	0.000091669	-0.000205420
13	1	-0.000258510	-0.000340462	-0.000260918
14	35	-0.000159276	-0.000771895	0.000252414
15	1	0.000196654	0.000455609	-0.000111874
16	6	-0.000455987	0.000373857	0.000089452
17	6	0.000055238	-0.000082588	-0.000042729
18	1	0.000204324	-0.000055067	-0.000074395
19	1	0.000055849	-0.000047215	-0.000018258
20	1	0.000060846	0.000059336	0.000047055
21	8	-0.000133365	0.000151342	0.000473921
22	1	0.000077036	-0.000128670	-0.000121543

Cartesian Forces: Max 0.000771895 RMS 0.000237148

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.004166372 RMS 0.000673792

Search for a local minimum.

Step number 26 out of a maximum of 116

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 21 22 23 25 24
26

ITU= 0 -1 1 1 1 1 1 0 -1 1 1 1 1 1 1 1 1 1 1 1

ITU= 1 0 0 -1 0 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00060	0.00162	0.00412	0.00701	0.00939
Eigenvalues ---	0.01234	0.01600	0.01781	0.01883	0.02067
Eigenvalues ---	0.02184	0.02414	0.03066	0.03096	0.03695
Eigenvalues ---	0.04344	0.04824	0.05471	0.06029	0.06643
Eigenvalues ---	0.09092	0.09314	0.13684	0.14173	0.15488
Eigenvalues ---	0.15842	0.15880	0.15993	0.15996	0.16459
Eigenvalues ---	0.16732	0.17180	0.20938	0.22709	0.22879
Eigenvalues ---	0.24022	0.24864	0.25219	0.29820	0.33181
Eigenvalues ---	0.33851	0.33880	0.33911	0.34143	0.34281
Eigenvalues ---	0.34505	0.34726	0.36248	0.36320	0.36568
Eigenvalues ---	0.37211	0.43091	0.43192	0.45772	0.48899
Eigenvalues ---	0.53364	0.54520	0.55846	0.60479	3.23578

RFO step: Lambda=-2.65628531D-05 EMin= 5.99855409D-04

Quartic linear search produced a step of -0.10630.

Iteration 1 RMS(Cart)= 0.00760295 RMS(Int)= 0.00002779

Iteration 2 RMS(Cart)= 0.00003966 RMS(Int)= 0.00000458

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000458

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55959	0.00024	-0.00002	0.00040	0.00037	2.55996
R2	2.62651	-0.00020	0.00003	-0.00047	-0.00044	2.62607
R3	2.03323	-0.00002	0.00000	0.00001	0.00001	2.03323
R4	2.63036	-0.00003	0.00002	-0.00038	-0.00037	2.62999
R5	2.03122	-0.00002	0.00000	-0.00005	-0.00004	2.03118
R6	2.54721	-0.00041	0.00004	-0.00091	-0.00087	2.54635
R7	2.68650	0.00017	0.00012	-0.00012	0.00000	2.68650
R8	2.52974	-0.00007	0.00008	-0.00079	-0.00070	2.52904
R9	2.02772	0.00010	-0.00004	0.00032	0.00028	2.02800
R10	2.77499	0.00018	-0.00004	0.00068	0.00063	2.77562
R11	2.90741	-0.00080	-0.00026	0.00046	0.00021	2.90762
R12	2.05989	-0.00005	0.00000	-0.00043	-0.00043	2.05946
R13	2.06306	-0.00006	-0.00001	0.00014	0.00014	2.06320
R14	2.06734	0.00015	0.00013	0.00011	0.00024	2.06757
R15	2.06685	-0.00082	-0.00002	-0.00042	-0.00043	2.06642
R16	2.68745	0.00008	0.00014	0.00061	0.00075	2.68820
R17	5.27052	-0.00024	0.00164	-0.00703	-0.00539	5.26513
R18	2.50762	-0.00012	0.00001	-0.00032	-0.00032	2.50730
R19	2.05044	-0.00006	0.00006	-0.00036	-0.00030	2.05014
R20	2.04379	-0.00008	0.00001	-0.00016	-0.00015	2.04364

R21	2.04782	-0.00007	0.00001	-0.00015	-0.00014	2.04769
R22	1.81858	-0.00016	-0.00004	-0.00069	-0.00074	1.81784
A1	1.87527	-0.00012	-0.00001	-0.00008	-0.00009	1.87519
A2	2.27891	0.00003	0.00003	-0.00007	-0.00004	2.27887
A3	2.12890	0.00009	-0.00002	0.00011	0.00009	2.12899
A4	1.86854	-0.00003	0.00003	-0.00033	-0.00030	1.86824
A5	2.28513	0.00003	0.00006	-0.00022	-0.00015	2.28498
A6	2.12899	0.00000	-0.00009	0.00045	0.00036	2.12935
A7	1.89204	0.00001	0.00000	0.00019	0.00019	1.89223
A8	2.23086	0.00001	-0.00019	0.00107	0.00088	2.23174
A9	2.15117	-0.00002	0.00009	-0.00065	-0.00057	2.15060
A10	1.89256	0.00011	-0.00004	0.00035	0.00030	1.89286
A11	2.18888	0.00001	0.00004	0.00014	0.00015	2.18903
A12	2.19744	-0.00009	-0.00011	0.00075	0.00061	2.19805
A13	1.89452	0.00004	0.00000	0.00001	0.00002	1.89454
A14	2.20084	0.00059	-0.00009	0.00060	0.00050	2.20134
A15	2.17038	-0.00068	0.00020	-0.00167	-0.00147	2.16891
A16	1.94541	-0.00221	0.00024	-0.00261	-0.00236	1.94305
A17	1.87515	0.00050	0.00017	-0.00010	0.00008	1.87523
A18	1.89857	0.00083	-0.00015	0.00073	0.00058	1.89915
A19	1.91438	0.00011	0.00009	-0.00069	-0.00060	1.91378
A20	1.93722	0.00107	-0.00030	0.00221	0.00191	1.93913
A21	1.89126	-0.00027	-0.00005	0.00046	0.00042	1.89168
A22	1.91898	0.00070	-0.00001	0.00020	0.00019	1.91917
A23	1.90375	-0.00313	0.00007	-0.00114	-0.00107	1.90269
A24	1.90208	0.00082	-0.00103	0.00172	0.00069	1.90277
A25	1.90399	0.00062	-0.00012	-0.00107	-0.00119	1.90280
A26	1.87489	-0.00021	0.00093	0.00110	0.00203	1.87692
A27	1.95992	0.00126	0.00015	-0.00076	-0.00060	1.95932
A28	2.57349	-0.00417	-0.00064	0.00212	0.00148	2.57497
A29	2.15621	-0.00022	-0.00023	0.00034	0.00011	2.15632
A30	1.95488	-0.00010	-0.00011	0.00019	0.00008	1.95496
A31	2.17125	0.00032	0.00033	-0.00049	-0.00015	2.17110
A32	2.08464	0.00006	0.00005	0.00032	0.00036	2.08500
A33	2.14715	-0.00009	-0.00012	0.00023	0.00011	2.14726
A34	2.05139	0.00003	0.00008	-0.00055	-0.00047	2.05092
A35	1.89298	0.00013	0.00017	0.00064	0.00081	1.89379
D1	0.00364	0.00012	-0.00001	0.00132	0.00131	0.00495
D2	3.11009	-0.00007	0.00004	-0.00177	-0.00172	3.10837
D3	-3.12223	0.00013	-0.00046	0.00377	0.00331	-3.11892
D4	-0.01578	-0.00007	-0.00040	0.00068	0.00028	-0.01550
D5	-0.03757	-0.00003	-0.00015	0.00027	0.00012	-0.03745
D6	-2.98552	0.00033	-0.00082	0.00628	0.00546	-2.98005
D7	3.08995	-0.00003	0.00025	-0.00192	-0.00167	3.08828

D8	0.14200	0.00033	-0.00042	0.00409	0.00367	0.14567
D9	0.03127	-0.00017	0.00017	-0.00245	-0.00228	0.02899
D10	3.03033	-0.00017	-0.00064	0.00224	0.00160	3.03193
D11	-3.07903	0.00000	0.00012	0.00032	0.00043	-3.07860
D12	-0.07996	0.00000	-0.00069	0.00500	0.00431	-0.07565
D13	-0.05508	0.00015	-0.00027	0.00262	0.00236	-0.05272
D14	-3.10165	-0.00021	0.00086	-0.01101	-0.01015	-3.11180
D15	-3.06209	0.00015	0.00053	-0.00197	-0.00144	-3.06352
D16	0.17452	-0.00020	0.00166	-0.01560	-0.01395	0.16058
D17	0.59423	0.00006	0.00292	-0.01287	-0.00995	0.58428
D18	-2.50497	0.00006	0.00297	-0.01378	-0.01081	-2.51578
D19	-2.70924	0.00006	0.00199	-0.00746	-0.00547	-2.71471
D20	0.47475	0.00005	0.00204	-0.00836	-0.00633	0.46842
D21	0.05736	-0.00007	0.00026	-0.00180	-0.00154	0.05581
D22	3.00948	-0.00025	0.00087	-0.00737	-0.00650	3.00298
D23	3.10335	0.00030	-0.00086	0.01188	0.01101	3.11436
D24	-0.22771	0.00011	-0.00025	0.00630	0.00606	-0.22166
D25	1.21746	0.00065	0.00129	-0.00321	-0.00192	1.21554
D26	-2.96797	-0.00021	0.00165	-0.00566	-0.00401	-2.97197
D27	-0.92416	0.00019	0.00161	-0.00478	-0.00317	-0.92733
D28	-1.70131	0.00096	0.00055	0.00347	0.00402	-1.69729
D29	0.39645	0.00010	0.00091	0.00102	0.00193	0.39838
D30	2.44025	0.00049	0.00087	0.00190	0.00277	2.44302
D31	-1.14180	0.00002	0.00369	0.00018	0.00387	-1.13793
D32	0.94532	-0.00072	0.00358	-0.00171	0.00187	0.94719
D33	3.09067	-0.00062	0.00317	-0.00227	0.00089	3.09156
D34	3.06688	0.00071	0.00326	0.00238	0.00564	3.07252
D35	-1.12918	-0.00002	0.00315	0.00049	0.00364	-1.12554
D36	1.01617	0.00007	0.00274	-0.00008	0.00266	1.01883
D37	0.97750	0.00030	0.00345	0.00085	0.00430	0.98180
D38	3.06462	-0.00043	0.00334	-0.00104	0.00231	3.06693
D39	-1.07322	-0.00034	0.00293	-0.00160	0.00133	-1.07189
D40	0.02829	0.00007	-0.01358	0.02639	0.01281	0.04111
D41	2.12467	-0.00058	-0.01362	0.02531	0.01169	2.13637
D42	-2.08207	0.00036	-0.01243	0.02550	0.01306	-2.06901
D43	-1.76392	0.00120	-0.01340	0.01872	0.00533	-1.75860
D44	2.44084	0.00003	-0.01335	0.01691	0.00356	2.44440
D45	0.34741	-0.00136	-0.01391	0.01797	0.00407	0.35147
D46	-3.08975	-0.00001	0.00005	-0.00025	-0.00021	-3.08995
D47	0.04896	0.00002	0.00016	-0.00101	-0.00085	0.04811
D48	0.00420	-0.00002	-0.00002	0.00078	0.00077	0.00497
D49	-3.14027	0.00001	0.00009	0.00003	0.00012	-3.14016

Item	Value	Threshold	Converged?
Maximum Force	0.004166	0.000450	NO

RMS	Force	0.000674	0.000300	NO
Maximum	Displacement	0.036061	0.001800	NO
RMS	Displacement	0.007600	0.001200	NO

Predicted change in Energy=-1.268395D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.455491	-1.991098	-1.313190
2	6	0	-1.745516	-1.610481	-1.474774
3	7	0	-2.099670	-0.879369	-0.344744
4	6	0	-1.023590	-0.794354	0.461788
5	7	0	-0.026729	-1.499374	-0.086195
6	6	0	1.353782	-1.507146	0.415292
7	6	0	2.240134	-0.525043	-0.370384
8	1	0	0.195472	-2.550717	-1.961820
9	1	0	-2.427414	-1.762661	-2.291574
10	1	0	1.321938	-1.213407	1.464295
11	1	0	1.744803	-2.524696	0.354337
12	1	0	2.332753	-0.854775	-1.409510
13	1	0	1.778112	0.465862	-0.350727
14	35	0	-0.312396	2.067225	0.559349
15	1	0	-1.000991	-0.311461	1.419913
16	6	0	-3.308444	-0.169514	-0.108056
17	6	0	-4.490094	-0.559745	-0.568313
18	1	0	-3.140644	0.743099	0.454048
19	1	0	-5.360592	0.056434	-0.389195
20	1	0	-4.632724	-1.477321	-1.126774
21	8	0	3.544819	-0.522651	0.196538
22	1	0	3.632833	0.254314	0.756850

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.354674	0.000000			
3	N	2.208428	1.391732	0.000000		
4	C	2.214833	2.222052	1.347468	0.000000	
5	N	1.389657	2.212402	2.179068	1.338310	0.000000
6	C	2.548594	3.631622	3.591391	2.482365	1.468796
7	C	3.210077	4.275892	4.354320	3.378896	2.483697
8	H	1.075940	2.211039	3.267417	3.231842	2.161635

9	H	2.213120	1.074852	2.162815	3.238726	3.270520
10	H	3.387991	4.266739	3.884792	2.584982	2.074777
11	H	2.811880	4.045214	4.239786	3.266440	2.093724
12	H	3.012443	4.148208	4.558586	3.843234	2.780976
13	H	3.457163	4.241537	4.104495	3.177713	2.681339
14	Br	4.471786	4.440384	3.562885	2.950245	3.635789
15	H	3.254014	3.258985	2.154909	1.073173	2.151439
16	C	3.593029	2.527261	1.421637	2.436330	3.540997
17	C	4.345301	3.075456	2.422039	3.623921	4.586608
18	H	4.220073	3.347548	2.086648	2.616436	3.875179
19	H	5.395013	4.126240	3.392833	4.500843	5.564390
20	H	4.212837	2.911152	2.717624	4.001977	4.722127
21	O	4.520851	5.653697	5.681592	4.584162	3.713473
22	H	5.103071	6.114265	5.946456	4.782159	4.144700

		6	7	8	9	10
6	C	0.000000				
7	C	1.538647	0.000000			
8	H	2.842778	3.288870	0.000000		
9	H	4.657237	5.196987	2.758496	0.000000	
10	H	1.089818	2.164019	3.846503	5.335342	0.000000
11	H	1.091797	2.183847	2.786698	4.998894	1.769266
12	H	2.171146	1.094113	2.783745	4.925595	3.067429
13	H	2.158611	1.093500	3.768304	5.140005	2.514427
14	Br	3.946268	3.754952	5.285793	5.221981	3.775251
15	H	2.825577	3.708864	4.228701	4.232706	2.492283
16	C	4.878474	5.566142	4.624284	2.842900	5.000244
17	C	6.001329	6.733228	5.278292	2.944704	6.191809
18	H	5.026428	5.589333	5.274023	3.784966	4.976259
19	H	6.940807	7.622958	6.335632	3.941025	7.050115
20	H	6.182000	6.979623	5.016070	2.510293	6.499330
21	O	2.411996	1.422536	4.470982	6.587556	2.650575
22	H	2.900599	1.953884	5.203346	7.077264	2.827529

		11	12	13	14	15
11	H	0.000000				
12	H	2.499096	0.000000			
13	H	3.072729	1.781216	0.000000		
14	Br	5.035855	4.405826	2.786185	0.000000	
15	H	3.684189	4.406209	3.385677	2.621618	0.000000
16	C	5.594282	5.829792	5.131827	3.797991	2.771133
17	C	6.601989	6.880836	6.355284	5.062189	4.023498
18	H	5.878437	5.998677	4.991862	3.124642	2.573540
19	H	7.596164	7.814019	7.150539	5.516094	4.734378
20	H	6.630501	6.998955	6.743666	5.837127	4.586321
21	O	2.696877	2.039313	2.097119	4.660171	4.712285

22	H	3.383722	2.759239	2.170591	4.346318	4.715090
		16	17	18	19	20
16	C	0.000000				
17	C	1.326806	0.000000			
18	H	1.084887	2.136268	0.000000		
19	H	2.083603	1.081446	2.471990	0.000000	
20	H	2.121760	1.083590	3.107341	1.851005	0.000000
21	O	6.869112	8.071320	6.809100	8.943420	8.338750
22	H	7.007783	8.270471	6.797837	9.068310	8.652516
		21	22			
21	O	0.000000				
22	H	0.961962	0.000000			

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.311584	-2.277023	-0.567614
2	6	0	-1.584433	-1.838078	-0.717028
3	7	0	-1.746825	-0.756997	0.144255
4	6	0	-0.575239	-0.532085	0.770730
5	7	0	0.297838	-1.470603	0.386031
6	6	0	1.726763	-1.459933	0.725769
7	6	0	2.569562	-0.869456	-0.418111
8	1	0	0.215839	-3.074944	-1.060354
9	1	0	-2.371364	-2.169475	-1.369886
10	1	0	1.845156	-0.849759	1.620964
11	1	0	2.040664	-2.479126	0.959721
12	1	0	2.510252	-1.516646	-1.298287
13	1	0	2.178490	0.118786	-0.675371
14	35	0	0.325640	2.127780	-0.133417
15	1	0	-0.402089	0.222569	1.513842
16	6	0	-2.868268	0.109679	0.255114
17	6	0	-4.120827	-0.283829	0.063641
18	1	0	-2.573090	1.130811	0.472228
19	1	0	-4.920580	0.442122	0.117641
20	1	0	-4.390950	-1.311046	-0.150895
21	8	0	3.932238	-0.820959	-0.012685

```
      22                1                   0             4.139450       0.079636       0.254450
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.8249621           0.5700118           0.3568296
 Standard basis: 6-311++G(d,p) (5D, 7F)
 There are     358 symmetry adapted cartesian basis functions of A      symmetry.
 There are     345 symmetry adapted basis functions of A      symmetry.
    345 basis functions,      553 primitive gaussians,      358 cartesian basis functions
     55 alpha electrons              55 beta electrons
          nuclear repulsion energy              866.4505856144 Hartrees.
 NAtoms=       22 NActive=       22 NUniq=       22 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      345 RedAO= T EigKep=    6.89D-06    NBF=      345
 NBsUse=      345 1.00D-06 EigRej= -1.00D+00 NBFU=      345
 Initial guess from the checkpoint file:    "."
 B after Tr=          0.000000        0.000000        0.000000
             Rot=        0.999999        0.000484       -0.000107        0.001212 Ang=      0.15 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn=                5 AccDes=
0.00D+00
 Harris functional with IExCor=     402 and IRadAn=              5 diagonalized for initial guess.
 HarFok:    IExCor=     402 AccDes= 0.00D+00 IRadAn=                5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=    3500011 ScaDFX=    1.000000    1.000000    1.000000    1.000000
 FoFCou: FMM=F IPFlag=                  0 FMFlag=           100000 FMFlg1=                  0
             NFxFlg=                    0 DoJE=T BraDBF=F KetDBF=T FulRan=T
             wScrn=      0.000000  ICntrl=             500  IOpCl=      0  I1Cent=        200000004  NGrid=
0
             NMat0=         1 NMatS0=            1 NMatT0=         0 NMatD0=         1 NMtDS0=         0
NMtDT0=         0
 Petite list used in FoFCou.
 Keep R1 ints in memory in canonical form, NReq=1804729152.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                      energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3032.33842115          A.U. after      10 cycles
                  NFock= 10    Conv=0.71D-08         -V/T= 2.0017
 Calling FoFJK, ICntrl=              2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 ---------------------------------------------------------------------
 Center          Atomic                                Forces (Hartrees/Bohr)
```

Number	Number	X	Y	Z
1	6	0.000152535	0.000134979	-0.000098533
2	6	-0.000077734	-0.000009901	-0.000064152
3	7	0.000181735	0.000137310	0.000049080
4	6	-0.000388470	-0.000248864	0.000049237
5	7	0.000028784	0.000155996	-0.000145670
6	6	0.000514428	0.000116533	0.000024552
7	6	0.000623643	0.000020131	0.000187997
8	1	-0.000106724	-0.000190338	0.000082876
9	1	0.000007498	0.000033996	-0.000005130
10	1	-0.000109776	0.000050218	0.000073687
11	1	-0.000059622	0.000113404	-0.000020768
12	1	0.000006412	0.000007127	-0.000047548
13	1	-0.000304825	-0.000173484	-0.000220610
14	35	-0.000054940	-0.000464111	0.000227278
15	1	0.000132194	0.000261608	-0.000007002
16	6	-0.000371616	0.000286899	0.000098115
17	6	-0.000085862	-0.000134643	-0.000150243
18	1	0.000245548	0.000030206	-0.000071439
19	1	0.000035251	-0.000001803	0.000023689
20	1	0.000054339	0.000011240	0.000032404
21	8	-0.000420718	-0.000397293	-0.000076879
22	1	-0.000002080	0.000260790	0.000059060

Cartesian Forces: Max 0.000623643 RMS 0.000193303

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.002616835 RMS 0.000410843
Search for a local minimum.
Step number 27 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 21 22 23 25 24
26 27
DE= -2.09D-05 DEPred=-1.27D-05 R= 1.65D+00
TightC=F SS= 1.41D+00 RLast= 4.03D-02 DXNew= 1.0469D+00 1.2094D-01
Trust test= 1.65D+00 RLast= 4.03D-02 DXMaxT set to 6.23D-01
ITU= 1 0 -1 1 1 1 1 1 0 -1 1 1 1 1 1 1 1 1 1 1
ITU= 1 1 0 0 -1 0 0

Eigenvalues --- 0.00045 0.00132 0.00429 0.00673 0.00826
Eigenvalues --- 0.01164 0.01614 0.01763 0.02005 0.02066
Eigenvalues --- 0.02277 0.02446 0.03066 0.03104 0.03683
Eigenvalues --- 0.04439 0.04835 0.05459 0.05988 0.06774
Eigenvalues --- 0.09039 0.09279 0.13768 0.14152 0.15345
Eigenvalues --- 0.15701 0.15910 0.15981 0.16002 0.16158
Eigenvalues --- 0.16694 0.17510 0.20770 0.22789 0.22856
Eigenvalues --- 0.24018 0.24851 0.26253 0.29751 0.33209
Eigenvalues --- 0.33875 0.33880 0.33965 0.34134 0.34221
Eigenvalues --- 0.34492 0.34782 0.36196 0.36316 0.36554
Eigenvalues --- 0.37204 0.43104 0.45039 0.46037 0.49674
Eigenvalues --- 0.53307 0.54650 0.58049 0.60960 2.14742
En-DIIS/RFO-DIIS IScMMF= 0 using points: 27 26
RFO step: Lambda=-1.45118871D-05.
DidBck=F Rises=F RFO-DIIS coefs: 1.74236 -0.74236
Iteration 1 RMS(Cart)= 0.01571792 RMS(Int)= 0.00019488
Iteration 2 RMS(Cart)= 0.00040363 RMS(Int)= 0.00002211
Iteration 3 RMS(Cart)= 0.00000022 RMS(Int)= 0.00002211

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55996	0.00013	0.00028	0.00028	0.00053	2.56050
R2	2.62607	0.00003	-0.00033	-0.00010	-0.00043	2.62564
R3	2.03323	-0.00001	0.00001	0.00000	0.00001	2.03324
R4	2.62999	0.00009	-0.00027	0.00006	-0.00021	2.62978
R5	2.03118	-0.00001	-0.00003	-0.00002	-0.00005	2.03113
R6	2.54635	-0.00007	-0.00064	-0.00036	-0.00099	2.54536
R7	2.68650	0.00017	0.00000	-0.00009	-0.00009	2.68641
R8	2.52904	0.00024	-0.00052	-0.00022	-0.00072	2.52832
R9	2.02800	0.00011	0.00021	0.00061	0.00082	2.02882
R10	2.77562	0.00024	0.00047	0.00103	0.00150	2.77712
R11	2.90762	-0.00059	0.00015	-0.00026	-0.00011	2.90751
R12	2.05946	0.00009	-0.00032	0.00008	-0.00024	2.05922
R13	2.06320	-0.00013	0.00010	-0.00028	-0.00018	2.06301
R14	2.06757	0.00005	0.00018	-0.00001	0.00017	2.06774
R15	2.06642	-0.00041	-0.00032	0.00014	-0.00018	2.06624
R16	2.68820	-0.00040	0.00056	-0.00110	-0.00055	2.68766
R17	5.26513	-0.00014	-0.00400	-0.01113	-0.01513	5.25000
R18	2.50730	0.00007	-0.00023	0.00009	-0.00014	2.50716
R19	2.05014	0.00002	-0.00022	-0.00012	-0.00034	2.04980
R20	2.04364	-0.00003	-0.00011	-0.00006	-0.00018	2.04346
R21	2.04769	-0.00003	-0.00010	-0.00007	-0.00017	2.04752
R22	1.81784	0.00025	-0.00055	0.00020	-0.00034	1.81750
A1	1.87519	-0.00003	-0.00006	0.00000	-0.00007	1.87512
A2	2.27887	-0.00003	-0.00003	-0.00026	-0.00028	2.27859

A3	2.12899	0.00005	0.00007	0.00027	0.00034	2.12933
A4	1.86824	0.00004	-0.00022	-0.00011	-0.00034	1.86790
A5	2.28498	-0.00002	-0.00011	-0.00049	-0.00060	2.28438
A6	2.12935	-0.00003	0.00027	0.00062	0.00088	2.13023
A7	1.89223	-0.00002	0.00014	0.00007	0.00023	1.89246
A8	2.23174	-0.00006	0.00065	0.00116	0.00178	2.23352
A9	2.15060	0.00008	-0.00042	-0.00037	-0.00083	2.14978
A10	1.89286	0.00005	0.00022	0.00030	0.00047	1.89333
A11	2.18903	0.00004	0.00011	0.00033	0.00030	2.18932
A12	2.19805	-0.00007	0.00045	0.00058	0.00089	2.19893
A13	1.89454	-0.00004	0.00001	0.00006	0.00009	1.89463
A14	2.20134	0.00025	0.00037	0.00067	0.00102	2.20236
A15	2.16891	-0.00023	-0.00109	-0.00081	-0.00192	2.16698
A16	1.94305	-0.00110	-0.00175	-0.00151	-0.00326	1.93979
A17	1.87523	0.00020	0.00006	-0.00072	-0.00066	1.87456
A18	1.89915	0.00042	0.00043	0.00025	0.00068	1.89983
A19	1.91378	0.00008	-0.00045	0.00000	-0.00046	1.91332
A20	1.93913	0.00052	0.00142	0.00117	0.00259	1.94172
A21	1.89168	-0.00011	0.00031	0.00081	0.00112	1.89280
A22	1.91917	0.00045	0.00014	0.00080	0.00094	1.92011
A23	1.90269	-0.00198	-0.00079	-0.00180	-0.00259	1.90009
A24	1.90277	0.00051	0.00051	0.00000	0.00051	1.90328
A25	1.90280	0.00048	-0.00089	0.00087	-0.00002	1.90278
A26	1.87692	-0.00022	0.00151	0.00019	0.00170	1.87862
A27	1.95932	0.00080	-0.00045	0.00000	-0.00044	1.95888
A28	2.57497	-0.00262	0.00110	0.00343	0.00453	2.57950
A29	2.15632	-0.00017	0.00008	0.00068	0.00077	2.15709
A30	1.95496	-0.00015	0.00006	-0.00057	-0.00051	1.95445
A31	2.17110	0.00032	-0.00011	-0.00014	-0.00026	2.17084
A32	2.08500	0.00001	0.00027	-0.00020	0.00007	2.08507
A33	2.14726	-0.00006	0.00008	0.00041	0.00049	2.14775
A34	2.05092	0.00005	-0.00035	-0.00021	-0.00056	2.05036
A35	1.89379	-0.00012	0.00060	-0.00142	-0.00082	1.89297
D1	0.00495	0.00004	0.00097	-0.00082	0.00015	0.00510
D2	3.10837	-0.00002	-0.00128	-0.00028	-0.00156	3.10681
D3	-3.11892	-0.00002	0.00246	-0.00123	0.00123	-3.11770
D4	-0.01550	-0.00008	0.00020	-0.00069	-0.00048	-0.01598
D5	-0.03745	0.00003	0.00009	0.00371	0.00379	-0.03365
D6	-2.98005	0.00016	0.00406	0.00424	0.00831	-2.97175
D7	3.08828	0.00008	-0.00124	0.00407	0.00282	3.09110
D8	0.14567	0.00021	0.00273	0.00460	0.00734	0.15300
D9	0.02899	-0.00009	-0.00169	-0.00232	-0.00401	0.02498
D10	3.03193	-0.00008	0.00119	0.00451	0.00571	3.03764
D11	-3.07860	-0.00004	0.00032	-0.00277	-0.00245	-3.08105

D12	-0.07565	-0.00003	0.00320	0.00406	0.00727	-0.06838
D13	-0.05272	0.00011	0.00175	0.00466	0.00641	-0.04631
D14	-3.11180	-0.00011	-0.00753	-0.01070	-0.01823	-3.13003
D15	-3.06352	0.00012	-0.00107	-0.00194	-0.00299	-3.06652
D16	0.16058	-0.00010	-0.01035	-0.01729	-0.02763	0.13295
D17	0.58428	0.00007	-0.00739	-0.01281	-0.02020	0.56407
D18	-2.51578	0.00008	-0.00802	-0.01222	-0.02025	-2.53602
D19	-2.71471	0.00007	-0.00406	-0.00500	-0.00905	-2.72376
D20	0.46842	0.00008	-0.00470	-0.00441	-0.00910	0.45932
D21	0.05581	-0.00008	-0.00115	-0.00517	-0.00632	0.04950
D22	3.00298	-0.00014	-0.00483	-0.00549	-0.01031	2.99267
D23	3.11436	0.00014	0.00818	0.01027	0.01846	3.13282
D24	-0.22166	0.00008	0.00450	0.00996	0.01447	-0.20719
D25	1.21554	0.00039	-0.00143	0.00209	0.00066	1.21620
D26	-2.97197	-0.00004	-0.00298	0.00074	-0.00223	-2.97421
D27	-0.92733	0.00016	-0.00235	0.00144	-0.00091	-0.92824
D28	-1.69729	0.00050	0.00298	0.00257	0.00556	-1.69174
D29	0.39838	0.00008	0.00143	0.00123	0.00266	0.40104
D30	2.44302	0.00027	0.00206	0.00193	0.00398	2.44701
D31	-1.13793	-0.00001	0.00287	-0.00653	-0.00365	-1.14159
D32	0.94719	-0.00036	0.00139	-0.00609	-0.00470	0.94249
D33	3.09156	-0.00031	0.00066	-0.00722	-0.00656	3.08500
D34	3.07252	0.00037	0.00418	-0.00470	-0.00052	3.07201
D35	-1.12554	0.00002	0.00270	-0.00426	-0.00156	-1.12711
D36	1.01883	0.00007	0.00197	-0.00540	-0.00342	1.01541
D37	0.98180	0.00013	0.00319	-0.00645	-0.00325	0.97855
D38	3.06693	-0.00022	0.00171	-0.00601	-0.00430	3.06262
D39	-1.07189	-0.00017	0.00099	-0.00714	-0.00616	-1.07805
D40	0.04111	0.00009	0.00951	0.04555	0.05507	0.09617
D41	2.13637	-0.00026	0.00868	0.04596	0.05465	2.19101
D42	-2.06901	0.00029	0.00970	0.04678	0.05647	-2.01254
D43	-1.75860	0.00072	0.00395	-0.01182	-0.00787	-1.76646
D44	2.44440	0.00002	0.00264	-0.01289	-0.01024	2.43416
D45	0.35147	-0.00092	0.00302	-0.01409	-0.01107	0.34041
D46	-3.08995	-0.00001	-0.00015	-0.00028	-0.00044	-3.09039
D47	0.04811	0.00004	-0.00063	0.00040	-0.00023	0.04788
D48	0.00497	-0.00004	0.00057	-0.00096	-0.00039	0.00458
D49	-3.14016	0.00001	0.00009	-0.00027	-0.00018	-3.14034

Item	Value	Threshold	Converged?
Maximum Force	0.002617	0.000450	NO
RMS Force	0.000411	0.000300	NO
Maximum Displacement	0.086906	0.001800	NO
RMS Displacement	0.015648	0.001200	NO

Predicted change in Energy=-1.579826D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.457037	-2.004512	-1.308246
2	6	0	-1.745766	-1.619536	-1.472183
3	7	0	-2.097078	-0.881966	-0.345607
4	6	0	-1.022800	-0.801854	0.462956
5	7	0	-0.027098	-1.509016	-0.083441
6	6	0	1.354929	-1.510359	0.416251
7	6	0	2.232056	-0.524539	-0.374989
8	1	0	0.192099	-2.568826	-1.954642
9	1	0	-2.427009	-1.771954	-2.289452
10	1	0	1.323022	-1.212311	1.463903
11	1	0	1.750122	-2.526349	0.357975
12	1	0	2.326368	-0.857204	-1.413121
13	1	0	1.759409	0.461292	-0.358227
14	35	0	-0.291217	2.069008	0.605337
15	1	0	-0.994379	-0.302032	1.412691
16	6	0	-3.304678	-0.170710	-0.107420
17	6	0	-4.485367	-0.550396	-0.578614
18	1	0	-3.136446	0.734253	0.466453
19	1	0	-5.354304	0.066922	-0.396428
20	1	0	-4.629248	-1.460290	-1.149022
21	8	0	3.536403	-0.505748	0.191681
22	1	0	3.618368	0.279249	0.741300

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.354956	0.000000			
3	N	2.208283	1.391618	0.000000		
4	C	2.214414	2.221721	1.346946	0.000000	
5	N	1.389428	2.212384	2.178702	1.337928	0.000000
6	C	2.549764	3.632136	3.590495	2.481483	1.469589
7	C	3.208194	4.269183	4.343964	3.372409	2.481526
8	H	1.075944	2.211163	3.267234	3.231555	2.161628
9	H	2.213060	1.074826	2.163207	3.238618	3.270351
10	H	3.388362	4.266602	3.883366	2.583263	2.074881
11	H	2.814277	4.048830	4.242637	3.267109	2.094832
12	H	3.012417	4.143298	4.550502	3.839226	2.780595

13	H	3.448965	4.225755	4.083748	3.163948	2.673804
14	Br	4.503650	4.476289	3.587991	2.966031	3.653277
15	H	3.254331	3.259279	2.154967	1.073605	2.151942
16	C	3.593587	2.528217	1.421589	2.435290	3.540363
17	C	4.344452	3.073587	2.422428	3.624565	4.586973
18	H	4.222514	3.351510	2.086119	2.612879	3.873330
19	H	5.394948	4.125885	3.393006	4.500582	5.564231
20	H	4.210567	2.905901	2.718790	4.004807	4.724153
21	O	4.521464	5.648918	5.671536	4.576855	3.712247
22	H	5.101483	6.105639	5.932631	4.773541	4.143369

		6	7	8	9	10
6	C	0.000000				
7	C	1.538588	0.000000			
8	H	2.844935	3.291784	0.000000		
9	H	4.657501	5.189229	2.758048	0.000000	
10	H	1.089691	2.163538	3.847801	5.335129	0.000000
11	H	1.091700	2.185576	2.788805	5.002639	1.769799
12	H	2.171844	1.094203	2.788906	4.919279	3.067584
13	H	2.156578	1.093407	3.766513	5.122803	2.512278
14	Br	3.944290	3.748925	5.319455	5.262547	3.756322
15	H	2.823508	3.695294	4.229068	4.233080	2.490296
16	C	4.876559	5.554477	4.625001	2.845268	4.996958
17	C	6.001696	6.720559	5.276950	2.942110	6.192527
18	H	5.021280	5.577939	5.277428	3.792016	4.966978
19	H	6.939890	7.609411	6.335438	3.941327	7.048683
20	H	6.185706	6.967945	5.012311	2.499515	6.505258
21	O	2.412157	1.422247	4.477428	6.581913	2.648931
22	H	2.903706	1.952955	5.207586	7.066786	2.831169

		11	12	13	14	15
11	H	0.000000				
12	H	2.500977	0.000000			
13	H	3.072301	1.781201	0.000000		
14	Br	5.034438	4.414595	2.778179	0.000000	
15	H	3.686773	4.395542	3.361869	2.601555	0.000000
16	C	5.596126	5.821065	5.109531	3.821689	2.768657
17	C	6.607792	6.869518	6.330033	5.084675	4.026659
18	H	5.875529	5.992318	4.972324	3.145821	2.560801
19	H	7.600463	7.802588	7.124739	5.535949	4.734763
20	H	6.641075	6.986705	6.718093	5.861078	4.595238
21	O	2.702089	2.040367	2.096490	4.631539	4.696845
22	H	3.392442	2.757230	2.167447	4.301928	4.697455

		16	17	18	19	20
16	C	0.000000				
17	C	1.326731	0.000000			

18	H	1.084707	2.135902	0.000000		
19	H	2.083497	1.081352	2.471596	0.000000	
20	H	2.121895	1.083501	3.107127	1.850535	0.000000
21	O	6.855807	8.058793	6.792644	8.928521	8.329855
22	H	6.989374	8.252334	6.775698	9.047007	8.638430

		21	22
21	O	0.000000	
22	H	0.961779	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.356525	-2.292534	-0.545360
2	6	0	-1.621397	-1.832781	-0.702299
3	7	0	-1.763603	-0.735333	0.141495
4	6	0	-0.589996	-0.525118	0.768169
5	7	0	0.267225	-1.482335	0.395397
6	6	0	1.698262	-1.484369	0.729793
7	6	0	2.539210	-0.916608	-0.426799
8	1	0	0.156331	-3.107226	-1.025895
9	1	0	-2.413369	-2.159791	-1.351217
10	1	0	1.826925	-0.862638	1.615414
11	1	0	2.001481	-2.503740	0.976269
12	1	0	2.470748	-1.575094	-1.297998
13	1	0	2.151653	0.070122	-0.694575
14	35	0	0.376986	2.131436	-0.129050
15	1	0	-0.398656	0.247454	1.488689
16	6	0	-2.870172	0.151117	0.244586
17	6	0	-4.128410	-0.219127	0.044659
18	1	0	-2.557933	1.166532	0.463739
19	1	0	-4.914956	0.521322	0.093692
20	1	0	-4.416517	-1.240911	-0.171966
21	8	0	3.903800	-0.869012	-0.028783
22	1	0	4.118196	0.036016	0.216122

Rotational constants (GHZ): 0.8192036 0.5708585 0.3557306
Standard basis: 6-311++G(d,p) (5D, 7F)

```
 There are     358 symmetry adapted cartesian basis functions of A     symmetry.
 There are     345 symmetry adapted basis functions of A     symmetry.
   345 basis functions,     553 primitive gaussians,     358 cartesian basis functions
    55 alpha electrons        55 beta electrons
         nuclear repulsion energy        865.6040445847 Hartrees.
 NAtoms=     22 NActive=     22 NUniq=     22 SFac= 1.00D+00 NAtFMM=     60 NAOKFM=F
Big=F
 Integral buffers will be     131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=    345 RedAO= T EigKep=  6.80D-06  NBF=    345
 NBsUse=    345 1.00D-06 EigRej= -1.00D+00 NBFU=    345
 Initial guess from the checkpoint file:  "."
 B after Tr=      0.000000     0.000000     0.000000
          Rot=     0.999963     0.000857     0.000024     0.008567 Ang=    0.99 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn=        5 AccDes=
0.00D+00
 Harris functional with IExCor=  402 and IRadAn=        5 diagonalized for initial guess.
 HarFok:  IExCor=  402 AccDes= 0.00D+00 IRadAn=        5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=  3500011 ScaDFX=  1.000000  1.000000  1.000000  1.000000
 FoFCou: FMM=F IPFlag=           0 FMFlag=      100000 FMFlg1=           0
          NFxFlg=           0 DoJE=T BraDBF=F KetDBF=T FulRan=T
          wScrn=     0.000000 ICntrl=        500 IOpCl=     0 I1Cent=  200000004 NGrid=
0
          NMat0=     1 NMatS0=     1 NMatT0=     0 NMatD0=     1 NMtDS0=     0
NMtDT0=     0
 Petite list used in FoFCou.
 Keep R1 ints in memory in canonical form, NReq=1804729152.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                 energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:  E(RB3LYP) =  -3032.33845724     A.U. after    11 cycles
             NFock= 11  Conv=0.98D-08     -V/T= 2.0017
 Calling FoFJK, ICntrl=        2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center     Atomic                     Forces (Hartrees/Bohr)
 Number     Number              X              Y              Z
 -------------------------------------------------------------------
      1          6          0.000063868    0.000222337   -0.000198165
      2          6          0.000058977    0.000009523   -0.000134159
```

3	7	0.000067847	-0.000132226	0.000140174
4	6	-0.000233580	-0.000077381	-0.000023303
5	7	0.000199483	0.000126896	0.000079523
6	6	0.000297608	0.000131845	-0.000182709
7	6	0.000603216	-0.000019802	0.000213783
8	1	-0.000102932	-0.000202231	0.000095851
9	1	-0.000042600	-0.000018617	0.000026803
10	1	-0.000090153	0.000022554	0.000128137
11	1	-0.000061328	0.000088778	-0.000059422
12	1	0.000078013	-0.000121774	-0.000007151
13	1	-0.000222296	-0.000000976	-0.000224943
14	35	-0.000097966	-0.000444929	0.000220689
15	1	0.000135611	0.000233227	0.000073451
16	6	-0.000316503	0.000327583	-0.000008620
17	6	-0.000111519	-0.000155566	-0.000147352
18	1	0.000149668	0.000109432	-0.000017590
19	1	0.000011105	0.000046055	0.000058145
20	1	0.000065850	-0.000022852	0.000010665
21	8	-0.000462102	-0.000573456	-0.000286365
22	1	0.000009733	0.000451580	0.000242559

Cartesian Forces: Max 0.000603216 RMS 0.000197957

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.002607516 RMS 0.000388746
Search for a local minimum.
Step number 28 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 21 22 23 25 24
26 27 28
DE= -3.61D-05 DEPred=-1.58D-05 R= 2.28D+00
TightC=F SS= 1.41D+00 RLast= 1.14D-01 DXNew= 1.0469D+00 3.4335D-01
Trust test= 2.28D+00 RLast= 1.14D-01 DXMaxT set to 6.23D-01
ITU= 1 1 0 -1 1 1 1 1 1 0 -1 1 1 1 1 1 1 1 1 1
ITU= 1 1 1 0 0 -1 0 0
Eigenvalues --- 0.00045 0.00125 0.00468 0.00627 0.00726
Eigenvalues --- 0.01112 0.01632 0.01744 0.02002 0.02070
Eigenvalues --- 0.02304 0.02440 0.03066 0.03109 0.03667
Eigenvalues --- 0.04417 0.04857 0.05437 0.05895 0.06891

Eigenvalues --- 0.08989 0.09231 0.13667 0.14153 0.14926
Eigenvalues --- 0.15505 0.15961 0.15977 0.16000 0.16064
Eigenvalues --- 0.16532 0.17582 0.20667 0.22842 0.22904
Eigenvalues --- 0.24109 0.24829 0.26977 0.29711 0.33440
Eigenvalues --- 0.33860 0.33878 0.34010 0.34044 0.34273
Eigenvalues --- 0.34495 0.34834 0.35991 0.36313 0.36417
Eigenvalues --- 0.37245 0.43074 0.45092 0.46079 0.50223
Eigenvalues --- 0.53320 0.54617 0.59512 0.62180 1.55100
En-DIIS/RFO-DIIS IScMMF= 0 using points: 28 27 26
RFO step: Lambda=-1.56152575D-05.
DidBck=F Rises=F RFO-DIIS coefs: 1.44368 0.14589 -0.58957
Iteration 1 RMS(Cart)= 0.01359454 RMS(Int)= 0.00013736
Iteration 2 RMS(Cart)= 0.00025468 RMS(Int)= 0.00003910
Iteration 3 RMS(Cart)= 0.00000009 RMS(Int)= 0.00003910

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56050	0.00005	0.00046	-0.00003	0.00038	2.56088
R2	2.62564	0.00010	-0.00045	0.00022	-0.00025	2.62539
R3	2.03324	-0.00001	0.00001	-0.00001	0.00000	2.03324
R4	2.62978	0.00012	-0.00031	0.00025	-0.00007	2.62971
R5	2.03113	0.00001	-0.00005	0.00003	-0.00002	2.03111
R6	2.54536	0.00008	-0.00095	0.00020	-0.00072	2.54464
R7	2.68641	0.00029	-0.00004	0.00084	0.00080	2.68722
R8	2.52832	0.00026	-0.00073	0.00019	-0.00051	2.52781
R9	2.02882	0.00018	0.00053	0.00057	0.00109	2.02991
R10	2.77712	0.00006	0.00104	0.00027	0.00131	2.77843
R11	2.90751	-0.00056	0.00007	-0.00021	-0.00013	2.90738
R12	2.05922	0.00013	-0.00036	0.00031	-0.00005	2.05917
R13	2.06301	-0.00011	0.00000	-0.00020	-0.00020	2.06281
R14	2.06774	0.00005	0.00022	-0.00005	0.00016	2.06791
R15	2.06624	-0.00025	-0.00033	0.00051	0.00018	2.06642
R16	2.68766	-0.00044	0.00020	-0.00088	-0.00068	2.68698
R17	5.25000	-0.00010	-0.00989	-0.00483	-0.01473	5.23527
R18	2.50716	0.00010	-0.00025	0.00012	-0.00013	2.50703
R19	2.04980	0.00010	-0.00033	0.00030	-0.00002	2.04978
R20	2.04346	0.00002	-0.00017	0.00010	-0.00006	2.04339
R21	2.04752	0.00001	-0.00016	0.00004	-0.00012	2.04740
R22	1.81750	0.00051	-0.00059	0.00083	0.00024	1.81774
A1	1.87512	0.00001	-0.00008	0.00005	-0.00005	1.87507
A2	2.27859	-0.00003	-0.00015	-0.00008	-0.00022	2.27837
A3	2.12933	0.00002	0.00020	0.00010	0.00031	2.12964
A4	1.86790	0.00006	-0.00033	0.00006	-0.00028	1.86762
A5	2.28438	0.00000	-0.00036	0.00005	-0.00031	2.28407
A6	2.13023	-0.00006	0.00060	0.00001	0.00061	2.13084

A7	1.89246	-0.00004	0.00021	-0.00005	0.00020	1.89266
A8	2.23352	-0.00013	0.00131	-0.00035	0.00091	2.23443
A9	2.14978	0.00017	-0.00070	0.00032	-0.00043	2.14935
A10	1.89333	0.00002	0.00038	0.00003	0.00031	1.89364
A11	2.18932	0.00007	0.00022	0.00044	0.00040	2.18972
A12	2.19893	-0.00008	0.00075	-0.00016	0.00034	2.19927
A13	1.89463	-0.00005	0.00005	-0.00002	0.00008	1.89472
A14	2.20236	0.00023	0.00075	0.00010	0.00081	2.20317
A15	2.16698	-0.00020	-0.00172	0.00041	-0.00135	2.16563
A16	1.93979	-0.00080	-0.00284	0.00074	-0.00210	1.93768
A17	1.87456	0.00009	-0.00025	-0.00074	-0.00100	1.87357
A18	1.89983	0.00034	0.00064	-0.00068	-0.00004	1.89979
A19	1.91332	0.00003	-0.00056	0.00051	-0.00006	1.91326
A20	1.94172	0.00042	0.00227	-0.00004	0.00223	1.94395
A21	1.89280	-0.00008	0.00074	0.00018	0.00092	1.89372
A22	1.92011	0.00039	0.00053	-0.00013	0.00039	1.92050
A23	1.90009	-0.00184	-0.00178	-0.00102	-0.00281	1.89729
A24	1.90328	0.00045	0.00063	-0.00050	0.00013	1.90341
A25	1.90278	0.00051	-0.00071	0.00206	0.00135	1.90413
A26	1.87862	-0.00022	0.00195	-0.00019	0.00176	1.88038
A27	1.95888	0.00075	-0.00055	-0.00020	-0.00075	1.95813
A28	2.57950	-0.00261	0.00288	0.00055	0.00344	2.58294
A29	2.15709	-0.00018	0.00041	-0.00045	-0.00004	2.15705
A30	1.95445	-0.00003	-0.00018	-0.00012	-0.00030	1.95415
A31	2.17084	0.00021	-0.00021	0.00059	0.00039	2.17123
A32	2.08507	-0.00003	0.00024	-0.00026	-0.00002	2.08505
A33	2.14775	-0.00006	0.00028	-0.00011	0.00017	2.14792
A34	2.05036	0.00009	-0.00052	0.00038	-0.00015	2.05022
A35	1.89297	-0.00011	0.00012	-0.00074	-0.00063	1.89234
D1	0.00510	0.00006	0.00084	-0.00049	0.00035	0.00545
D2	3.10681	0.00004	-0.00171	0.00276	0.00106	3.10787
D3	-3.11770	-0.00006	0.00250	-0.00501	-0.00251	-3.12021
D4	-0.01598	-0.00008	-0.00005	-0.00176	-0.00180	-0.01778
D5	-0.03365	-0.00002	0.00175	0.00113	0.00288	-0.03077
D6	-2.97175	0.00008	0.00691	-0.00149	0.00543	-2.96631
D7	3.09110	0.00008	0.00027	0.00518	0.00544	3.09653
D8	0.15300	0.00018	0.00542	0.00256	0.00799	0.16100
D9	0.02498	-0.00007	-0.00312	-0.00031	-0.00343	0.02154
D10	3.03764	-0.00008	0.00348	-0.00091	0.00258	3.04022
D11	-3.08105	-0.00005	-0.00083	-0.00321	-0.00404	-3.08509
D12	-0.06838	-0.00007	0.00577	-0.00381	0.00197	-0.06641
D13	-0.04631	0.00005	0.00424	0.00102	0.00526	-0.04105
D14	-3.13003	-0.00008	-0.01407	-0.00453	-0.01860	3.13455
D15	-3.06652	0.00009	-0.00218	0.00165	-0.00051	-3.06703

D16	0.13295	-0.00004	-0.02048	-0.00391	-0.02437	0.10857
D17	0.56407	0.00009	-0.01483	0.00301	-0.01182	0.55225
D18	-2.53602	0.00009	-0.01535	0.00237	-0.01299	-2.54901
D19	-2.72376	0.00005	-0.00724	0.00230	-0.00494	-2.72870
D20	0.45932	0.00005	-0.00777	0.00165	-0.00611	0.45322
D21	0.04950	-0.00002	-0.00371	-0.00133	-0.00504	0.04446
D22	2.99267	-0.00006	-0.00841	0.00118	-0.00722	2.98545
D23	3.13282	0.00012	0.01468	0.00429	0.01898	-3.13138
D24	-0.20719	0.00009	0.00999	0.00680	0.01680	-0.19039
D25	1.21620	0.00037	-0.00084	0.00679	0.00596	1.22216
D26	-2.97421	0.00000	-0.00335	0.00738	0.00404	-2.97017
D27	-0.92824	0.00014	-0.00227	0.00683	0.00456	-0.92369
D28	-1.69174	0.00047	0.00484	0.00384	0.00868	-1.68306
D29	0.40104	0.00010	0.00232	0.00443	0.00676	0.40780
D30	2.44701	0.00023	0.00340	0.00388	0.00728	2.45428
D31	-1.14159	-0.00009	0.00066	-0.00586	-0.00520	-1.14678
D32	0.94249	-0.00036	-0.00098	-0.00405	-0.00503	0.93746
D33	3.08500	-0.00032	-0.00238	-0.00526	-0.00764	3.07737
D34	3.07201	0.00027	0.00309	-0.00573	-0.00263	3.06937
D35	-1.12711	0.00000	0.00145	-0.00391	-0.00246	-1.12957
D36	1.01541	0.00004	0.00005	-0.00512	-0.00507	1.01034
D37	0.97855	0.00008	0.00109	-0.00625	-0.00516	0.97339
D38	3.06262	-0.00019	-0.00055	-0.00444	-0.00499	3.05763
D39	-1.07805	-0.00015	-0.00195	-0.00564	-0.00760	-1.08565
D40	0.09617	0.00003	0.03199	0.01315	0.04514	0.14132
D41	2.19101	-0.00029	0.03114	0.01361	0.04475	2.23576
D42	-2.01254	0.00024	0.03276	0.01461	0.04736	-1.96517
D43	-1.76646	0.00068	-0.00035	-0.00217	-0.00252	-1.76898
D44	2.43416	0.00008	-0.00245	-0.00162	-0.00407	2.43009
D45	0.34041	-0.00085	-0.00251	-0.00393	-0.00644	0.33397
D46	-3.09039	-0.00003	-0.00031	-0.00105	-0.00137	-3.09175
D47	0.04788	0.00002	-0.00060	-0.00006	-0.00067	0.04721
D48	0.00458	-0.00004	0.00028	-0.00035	-0.00007	0.00451
D49	-3.14034	0.00001	-0.00001	0.00064	0.00063	-3.13971

Item	Value	Threshold	Converged?
Maximum Force	0.002608	0.000450	NO
RMS Force	0.000389	0.000300	NO
Maximum Displacement	0.079248	0.001800	NO
RMS Displacement	0.013519	0.001200	NO

Predicted change in Energy=-1.624585D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.459155	-2.017098	-1.304949
2	6	0	-1.746931	-1.628741	-1.470066
3	7	0	-2.094623	-0.883991	-0.347145
4	6	0	-1.021001	-0.806755	0.461939
5	7	0	-0.026931	-1.516773	-0.083063
6	6	0	1.356650	-1.513701	0.414348
7	6	0	2.225852	-0.522067	-0.378235
8	1	0	0.186839	-2.588790	-1.948002
9	1	0	-2.429216	-1.784021	-2.285913
10	1	0	1.324590	-1.215929	1.462047
11	1	0	1.755173	-2.528187	0.354596
12	1	0	2.323063	-0.855098	-1.416074
13	1	0	1.743117	0.458962	-0.361005
14	35	0	-0.275273	2.066602	0.647274
15	1	0	-0.985376	-0.289013	1.402441
16	6	0	-3.300642	-0.169139	-0.109173
17	6	0	-4.481284	-0.542426	-0.585378
18	1	0	-3.130577	0.731983	0.470155
19	1	0	-5.348684	0.076596	-0.401864
20	1	0	-4.626892	-1.448879	-1.160685
21	8	0	3.528799	-0.489559	0.190131
22	1	0	3.602849	0.299144	0.735773

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.355158	0.000000			
3	N	2.208184	1.391580	0.000000		
4	C	2.214157	2.221548	1.346568	0.000000	
5	N	1.389298	2.212401	2.178418	1.337658	0.000000
6	C	2.550792	3.632694	3.589943	2.480980	1.470280
7	C	3.209856	4.266125	4.335719	3.365857	2.480241
8	H	1.075945	2.211240	3.267132	3.231461	2.161693
9	H	2.213087	1.074816	2.163522	3.238642	3.270312
10	H	3.388198	4.266374	3.882574	2.582526	2.074724
11	H	2.813992	4.050077	4.244614	3.268332	2.095327
12	H	3.017172	4.143222	4.545260	3.835627	2.781583
13	H	3.445563	4.215324	4.065952	3.149544	2.667180
14	Br	4.530076	4.506048	3.606231	2.974331	3.665467
15	H	3.254712	3.259775	2.155337	1.074184	2.152379
16	C	3.594285	2.529128	1.422015	2.435054	3.540337

17	C	4.343957	3.072367	2.422720	3.624955	4.587258
18	H	4.224326	3.354393	2.086276	2.611147	3.872412
19	H	5.395055	4.125755	3.393322	4.500589	5.564307
20	H	4.208767	2.902110	2.719068	4.005955	4.724989
21	O	4.524645	5.646886	5.662784	4.568936	3.711202
22	H	5.101902	6.099395	5.918928	4.762142	4.140453

		6	7	8	9	10
6	C	0.000000				
7	C	1.538517	0.000000			
8	H	2.846923	3.300467	0.000000		
9	H	4.658032	5.186657	2.757822	0.000000	
10	H	1.089665	2.163412	3.848072	5.334884	0.000000
11	H	1.091592	2.187030	2.786629	5.003516	1.770275
12	H	2.172132	1.094290	2.802158	4.919722	3.067691
13	H	2.154513	1.093502	3.772181	5.113179	2.510766
14	Br	3.941573	3.742793	5.349923	5.298146	3.741447
15	H	2.821573	3.679280	4.229483	4.233636	2.489712
16	C	4.875684	5.544284	4.625854	2.847002	4.995726
17	C	6.002025	6.710364	5.275957	2.940129	6.193039
18	H	5.018108	5.566303	5.280176	3.797116	4.962532
19	H	6.939507	7.598193	6.335364	3.941425	7.048218
20	H	6.187706	6.959260	5.009119	2.491634	6.507928
21	O	2.411922	1.421889	4.488550	6.580605	2.646492
22	H	2.904330	1.952313	5.216506	7.060876	2.830792

		11	12	13	14	15
11	H	0.000000				
12	H	2.501400	0.000000			
13	H	3.071692	1.782206	0.000000		
14	Br	5.031944	4.420982	2.770385	0.000000	
15	H	3.690865	4.382949	3.333749	2.573606	0.000000
16	C	5.598344	5.814171	5.088953	3.837135	2.767636
17	C	6.612125	6.861993	6.308431	5.100685	4.029518
18	H	5.874743	5.984886	4.951592	3.156793	2.552151
19	H	7.604072	7.794381	7.102219	5.549803	4.735784
20	H	6.647686	6.979947	6.697489	5.879108	4.601689
21	O	2.707177	2.041400	2.095734	4.605855	4.678428
22	H	3.398972	2.756914	2.164964	4.262813	4.673562

		16	17	18	19	20
16	C	0.000000				
17	C	1.326661	0.000000			
18	H	1.084695	2.136043	0.000000		
19	H	2.083394	1.081318	2.471831	0.000000	
20	H	2.121874	1.083437	3.107210	1.850369	0.000000
21	O	6.843502	8.047710	6.776272	8.915195	8.322277

22 H 6.970754 8.234494 6.752550 9.026278 8.624429

21 22

21 O 0.000000

22 H 0.961905 0.000000

Stoichiometry C7H11BrN2O

Framework group C1[X(C7H11BrN2O)]

Deg. of freedom 60

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.395994	-2.306170	-0.524701
2	6	0	-1.653902	-1.829022	-0.687336
3	7	0	-1.777006	-0.716005	0.138818
4	6	0	-0.600785	-0.516952	0.763419
5	7	0	0.241755	-1.491091	0.402160
6	6	0	1.674701	-1.505072	0.731086
7	6	0	2.513972	-0.954429	-0.434870
8	1	0	0.102288	-3.137836	-0.991287
9	1	0	-2.451998	-2.154550	-1.329445
10	1	0	1.812423	-0.876042	1.610133
11	1	0	1.968186	-2.525182	0.985676
12	1	0	2.438686	-1.621690	-1.298910
13	1	0	2.128603	0.031388	-0.709467
14	35	0	0.419500	2.131928	-0.124891
15	1	0	-0.391008	0.273324	1.460074
16	6	0	-2.869968	0.188883	0.232298
17	6	0	-4.133229	-0.162716	0.030855
18	1	0	-2.542065	1.200365	0.446652
19	1	0	-4.908168	0.590209	0.073533
20	1	0	-4.436937	-1.181056	-0.180287
21	8	0	3.879672	-0.906860	-0.041972
22	1	0	4.098119	0.001005	0.188948

Rotational constants (GHZ): 0.8156148 0.5716112 0.3549472

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 865.1222467899 Hartrees.
NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 345 RedAO= T EigKep= 6.73D-06 NBF= 345
NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345
Initial guess from the checkpoint file: "."
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999974 0.000816 -0.000069 0.007217 Ang= 0.83 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.33848429 A.U. after 11 cycles
NFock= 11 Conv=0.38D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000037882	0.000149954	-0.000207613
2	6	0.000135688	-0.000011973	-0.000156639
3	7	-0.000130436	-0.000182400	0.000161488
4	6	-0.000125390	0.000000218	-0.000023104
5	7	0.000310402	0.000074158	0.000139081
6	6	-0.000036724	0.000085161	-0.000252727

7	6	0.000417097	-0.000001484	0.000399817
8	1	-0.000060123	-0.000142068	0.000068875
9	1	-0.000054061	-0.000025536	0.000030650
10	1	-0.000021307	-0.000005374	0.000130165
11	1	-0.000029845	0.000062571	-0.000060932
12	1	0.000164877	-0.000115004	0.000037277
13	1	-0.000065990	0.000059754	-0.000376516
14	35	-0.000085683	-0.000115814	0.000205150
15	1	0.000091696	0.000092684	0.000127165
16	6	-0.000097821	0.000191316	-0.000026280
17	6	-0.000134531	-0.000122302	-0.000106811
18	1	0.000062552	0.000103095	-0.000006226
19	1	0.000003674	0.000070975	0.000046535
20	1	0.000054572	-0.000040789	-0.000006134
21	8	-0.000351887	-0.000524009	-0.000348123
22	1	-0.000008878	0.000396868	0.000224904

Cartesian Forces: Max 0.000524009 RMS 0.000170662

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.001218819 RMS 0.000171497
Search for a local minimum.
Step number 29 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 23 25 24 26 27
28 29
DE= -2.71D-05 DEPred=-1.62D-05 R= 1.67D+00
TightC=F SS= 1.41D+00 RLast= 9.67D-02 DXNew= 1.0469D+00 2.9021D-01
Trust test= 1.67D+00 RLast= 9.67D-02 DXMaxT set to 6.23D-01
ITU= 1 1 1 0 -1 1 1 1 1 1 0 -1 1 1 1 1 1 1 1 1
ITU= 1 1 1 1 0 0 -1 0 0
Eigenvalues --- 0.00026 0.00120 0.00487 0.00606 0.00723
Eigenvalues --- 0.01098 0.01614 0.01848 0.02068 0.02071
Eigenvalues --- 0.02319 0.02400 0.03066 0.03106 0.03670
Eigenvalues --- 0.04434 0.04854 0.05490 0.05982 0.07006
Eigenvalues --- 0.08950 0.09232 0.13646 0.14201 0.15018
Eigenvalues --- 0.15686 0.15971 0.15998 0.16014 0.16238
Eigenvalues --- 0.16633 0.17726 0.20698 0.22847 0.23042
Eigenvalues --- 0.24199 0.24822 0.26925 0.29801 0.33372

Eigenvalues --- 0.33873 0.33879 0.34012 0.34116 0.34308
Eigenvalues --- 0.34489 0.34831 0.35956 0.36313 0.36385
Eigenvalues --- 0.37253 0.43074 0.44936 0.45928 0.50276
Eigenvalues --- 0.53351 0.54612 0.59212 0.61830 1.50065
En-DIIS/RFO-DIIS IScMMF= 0 using points: 29 28 27 26
RFO step: Lambda=-4.38875784D-06.
DidBck=F Rises=F RFO-DIIS coefs: 1.40068 0.09487 -0.53266 0.03711
Iteration 1 RMS(Cart)= 0.01868854 RMS(Int)= 0.00032235
Iteration 2 RMS(Cart)= 0.00084464 RMS(Int)= 0.00005746
Iteration 3 RMS(Cart)= 0.00000082 RMS(Int)= 0.00005746

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56088	-0.00001	0.00040	0.00003	0.00037	2.56125
R2	2.62539	0.00016	-0.00030	0.00008	-0.00024	2.62516
R3	2.03324	0.00000	0.00000	0.00002	0.00003	2.03327
R4	2.62971	0.00013	-0.00012	0.00016	0.00003	2.62973
R5	2.03111	0.00001	-0.00003	0.00002	-0.00001	2.03109
R6	2.54464	0.00016	-0.00074	-0.00004	-0.00073	2.54392
R7	2.68722	0.00017	0.00028	0.00038	0.00065	2.68787
R8	2.52781	0.00021	-0.00054	-0.00024	-0.00073	2.52708
R9	2.02991	0.00016	0.00083	0.00072	0.00156	2.03147
R10	2.77843	-0.00004	0.00124	0.00006	0.00130	2.77973
R11	2.90738	-0.00021	-0.00012	0.00056	0.00045	2.90782
R12	2.05917	0.00012	-0.00012	0.00016	0.00004	2.05921
R13	2.06281	-0.00007	-0.00018	-0.00005	-0.00023	2.06258
R14	2.06791	0.00001	0.00014	-0.00017	-0.00003	2.06788
R15	2.06642	0.00002	0.00000	0.00046	0.00047	2.06688
R16	2.68698	-0.00039	-0.00057	-0.00071	-0.00128	2.68571
R17	5.23527	0.00007	-0.01320	-0.00190	-0.01510	5.22017
R18	2.50703	0.00012	-0.00011	0.00002	-0.00010	2.50693
R19	2.04978	0.00009	-0.00017	0.00006	-0.00010	2.04967
R20	2.04339	0.00004	-0.00011	0.00007	-0.00004	2.04335
R21	2.04740	0.00003	-0.00013	0.00000	-0.00012	2.04728
R22	1.81774	0.00046	-0.00005	0.00066	0.00061	1.81835
A1	1.87507	0.00004	-0.00005	-0.00001	-0.00008	1.87499
A2	2.27837	-0.00003	-0.00023	-0.00002	-0.00024	2.27813
A3	2.12964	-0.00001	0.00029	0.00006	0.00036	2.13000
A4	1.86762	0.00005	-0.00027	-0.00006	-0.00034	1.86727
A5	2.28407	0.00001	-0.00041	0.00003	-0.00038	2.28369
A6	2.13084	-0.00006	0.00067	0.00011	0.00078	2.13162
A7	1.89266	-0.00004	0.00019	-0.00004	0.00021	1.89287
A8	2.23443	-0.00012	0.00122	0.00008	0.00123	2.23566
A9	2.14935	0.00015	-0.00056	-0.00002	-0.00065	2.14870
A10	1.89364	0.00000	0.00034	0.00011	0.00030	1.89393

A11	2.18972	0.00008	0.00030	0.00037	0.00029	2.19002
A12	2.19927	-0.00008	0.00055	-0.00022	-0.00005	2.19923
A13	1.89472	-0.00006	0.00008	0.00002	0.00018	1.89490
A14	2.20317	0.00008	0.00081	0.00055	0.00131	2.20448
A15	2.16563	-0.00002	-0.00144	-0.00044	-0.00192	2.16372
A16	1.93768	0.00001	-0.00237	0.00051	-0.00187	1.93582
A17	1.87357	-0.00005	-0.00073	-0.00068	-0.00142	1.87214
A18	1.89979	0.00002	0.00030	-0.00037	-0.00006	1.89973
A19	1.91326	-0.00004	-0.00023	-0.00017	-0.00041	1.91285
A20	1.94395	0.00004	0.00210	0.00071	0.00282	1.94677
A21	1.89372	0.00001	0.00091	-0.00007	0.00083	1.89455
A22	1.92050	0.00013	0.00061	-0.00019	0.00042	1.92092
A23	1.89729	-0.00064	-0.00237	-0.00052	-0.00290	1.89439
A24	1.90341	0.00014	0.00028	0.00134	0.00162	1.90502
A25	1.90413	0.00024	0.00058	0.00171	0.00229	1.90642
A26	1.88038	-0.00013	0.00147	-0.00176	-0.00030	1.88008
A27	1.95813	0.00028	-0.00050	-0.00057	-0.00107	1.95706
A28	2.58294	-0.00122	0.00357	0.00072	0.00429	2.58723
A29	2.15705	-0.00011	0.00036	0.00005	0.00041	2.15746
A30	1.95415	0.00001	-0.00037	0.00048	0.00011	1.95426
A31	2.17123	0.00009	0.00003	-0.00051	-0.00048	2.17075
A32	2.08505	-0.00005	0.00001	-0.00037	-0.00036	2.08469
A33	2.14792	-0.00004	0.00031	0.00014	0.00045	2.14837
A34	2.05022	0.00009	-0.00032	0.00023	-0.00009	2.05013
A35	1.89234	-0.00011	-0.00069	-0.00047	-0.00116	1.89119
D1	0.00545	0.00002	0.00017	0.00002	0.00018	0.00563
D2	3.10787	0.00005	-0.00028	0.00216	0.00189	3.10976
D3	-3.12021	-0.00008	-0.00052	-0.00273	-0.00325	-3.12346
D4	-0.01778	-0.00006	-0.00097	-0.00058	-0.00155	-0.01934
D5	-0.03077	-0.00002	0.00303	0.00040	0.00342	-0.02736
D6	-2.96631	-0.00003	0.00609	-0.00022	0.00587	-2.96044
D7	3.09653	0.00007	0.00364	0.00286	0.00649	3.10303
D8	0.16100	0.00006	0.00670	0.00224	0.00895	0.16994
D9	0.02154	-0.00002	-0.00328	-0.00042	-0.00370	0.01785
D10	3.04022	-0.00004	0.00381	-0.00020	0.00362	3.04385
D11	-3.08509	-0.00004	-0.00285	-0.00234	-0.00519	-3.09028
D12	-0.06641	-0.00006	0.00423	-0.00212	0.00213	-0.06428
D13	-0.04105	0.00000	0.00520	0.00067	0.00587	-0.03518
D14	3.13455	-0.00001	-0.01611	-0.00744	-0.02355	3.11101
D15	-3.06703	0.00005	-0.00164	0.00045	-0.00116	-3.06819
D16	0.10857	0.00003	-0.02294	-0.00765	-0.03058	0.07800
D17	0.55225	0.00007	-0.01438	-0.00441	-0.01879	0.53347
D18	-2.54901	0.00007	-0.01484	-0.00500	-0.01984	-2.56885
D19	-2.72870	0.00002	-0.00626	-0.00416	-0.01042	-2.73912

D20	0.45322	0.00003	-0.00672	-0.00475	-0.01147	0.44175
D21	0.04446	0.00001	-0.00509	-0.00066	-0.00575	0.03871
D22	2.98545	0.00004	-0.00776	0.00009	-0.00767	2.97777
D23	-3.13138	0.00003	0.01635	0.00752	0.02387	-3.10751
D24	-0.19039	0.00006	0.01368	0.00826	0.02194	-0.16845
D25	1.22216	0.00014	0.00279	0.00403	0.00682	1.22898
D26	-2.97017	0.00007	0.00066	0.00370	0.00437	-2.96580
D27	-0.92369	0.00007	0.00149	0.00305	0.00455	-0.91914
D28	-1.68306	0.00012	0.00608	0.00325	0.00932	-1.67374
D29	0.40780	0.00005	0.00395	0.00292	0.00687	0.41467
D30	2.45428	0.00005	0.00479	0.00227	0.00705	2.46133
D31	-1.14678	-0.00007	-0.00404	-0.01311	-0.01715	-1.16393
D32	0.93746	-0.00010	-0.00441	-0.01146	-0.01587	0.92159
D33	3.07737	-0.00007	-0.00634	-0.01166	-0.01800	3.05937
D34	3.06937	0.00001	-0.00152	-0.01248	-0.01400	3.05538
D35	-1.12957	-0.00002	-0.00190	-0.01082	-0.01272	-1.14229
D36	1.01034	0.00001	-0.00383	-0.01102	-0.01485	0.99549
D37	0.97339	-0.00001	-0.00384	-0.01274	-0.01658	0.95681
D38	3.05763	-0.00003	-0.00422	-0.01108	-0.01530	3.04233
D39	-1.08565	-0.00001	-0.00615	-0.01128	-0.01743	-1.10307
D40	0.14132	0.00007	0.04490	0.03960	0.08451	0.22582
D41	2.23576	-0.00002	0.04457	0.04007	0.08464	2.32040
D42	-1.96517	0.00015	0.04648	0.03864	0.08511	-1.88006
D43	-1.76898	0.00021	-0.00510	0.02499	0.01988	-1.74910
D44	2.43009	0.00006	-0.00684	0.02548	0.01864	2.44873
D45	0.33397	-0.00032	-0.00822	0.02487	0.01665	0.35062
D46	-3.09175	0.00000	-0.00076	-0.00028	-0.00103	-3.09279
D47	0.04721	0.00002	-0.00035	-0.00056	-0.00091	0.04631
D48	0.00451	-0.00002	-0.00025	0.00041	0.00016	0.00467
D49	-3.13971	0.00000	0.00016	0.00013	0.00029	-3.13942

Item	Value	Threshold	Converged?
Maximum Force	0.001219	0.000450	NO
RMS Force	0.000171	0.000300	YES
Maximum Displacement	0.084570	0.001800	NO
RMS Displacement	0.018547	0.001200	NO

Predicted change in Energy=-1.215288D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.462521	-2.032304	-1.302232

2	6	0	-1.749419	-1.640315	-1.467239
3	7	0	-2.091914	-0.887802	-0.347885
4	6	0	-1.018096	-0.813655	0.460586
5	7	0	-0.026428	-1.526532	-0.084110
6	6	0	1.359139	-1.518332	0.409741
7	6	0	2.219505	-0.520080	-0.384628
8	1	0	0.179219	-2.612313	-1.942111
9	1	0	-2.433933	-1.799359	-2.280479
10	1	0	1.327301	-1.220566	1.457470
11	1	0	1.761213	-2.531210	0.348686
12	1	0	2.329122	-0.859257	-1.419217
13	1	0	1.720610	0.453217	-0.375559
14	35	0	-0.243691	2.075751	0.692026
15	1	0	-0.972420	-0.274279	1.389364
16	6	0	-3.296079	-0.169744	-0.108116
17	6	0	-4.476458	-0.532663	-0.592772
18	1	0	-3.124834	0.724358	0.481545
19	1	0	-5.341595	0.088429	-0.405734
20	1	0	-4.624305	-1.432148	-1.178231
21	8	0	3.517476	-0.461797	0.191327
22	1	0	3.568458	0.323723	0.744721

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.355356	0.000000			
3	N	2.208073	1.391594	0.000000		
4	C	2.213887	2.221421	1.346183	0.000000	
5	N	1.389173	2.212394	2.178023	1.337271	0.000000
6	C	2.552148	3.633327	3.589057	2.480000	1.470970
7	C	3.212800	4.263723	4.327229	3.358964	2.479410
8	H	1.075959	2.211318	3.267039	3.231360	2.161800
9	H	2.213074	1.074809	2.163986	3.238772	3.270252
10	H	3.387969	4.265714	3.880860	2.580744	2.074287
11	H	2.814148	4.051643	4.246480	3.269109	2.095794
12	H	3.030346	4.152933	4.549081	3.839221	2.788617
13	H	3.435491	4.197111	4.041589	3.131232	2.656406
14	Br	4.571768	4.553986	3.644172	3.000323	3.691346
15	H	3.255048	3.260362	2.155855	1.075007	2.152711
16	C	3.595010	2.530208	1.422360	2.434594	3.540066
17	C	4.343264	3.070558	2.423250	3.626125	4.587949
18	H	4.227169	3.358751	2.086609	2.608499	3.871252
19	H	5.395051	4.125418	3.393640	4.500767	5.564399
20	H	4.206663	2.896866	2.720072	4.009115	4.727206

21	O	4.531842	5.646232	5.651327	4.557162	3.710632
22	H	5.098007	6.085231	5.890789	4.734009	4.127180

		6	7	8	9	10
6	C	0.000000				
7	C	1.538753	0.000000			
8	H	2.849599	3.311490	0.000000		
9	H	4.658718	5.185103	2.757527	0.000000	
10	H	1.089685	2.163339	3.848663	5.334243	0.000000
11	H	1.091472	2.189161	2.785145	5.004734	1.770725
12	H	2.172634	1.094273	2.822890	4.930747	3.067494
13	H	2.152758	1.093748	3.771929	5.095395	2.513212
14	Br	3.945400	3.736958	5.394023	5.352516	3.730902
15	H	2.818421	3.660035	4.229823	4.234340	2.487733
16	C	4.874209	5.533612	4.626811	2.849229	4.993088
17	C	6.002563	6.699209	5.274561	2.936798	6.193571
18	H	5.014063	5.555254	5.284341	3.804638	4.955469
19	H	6.938768	7.585576	6.335128	3.941181	7.046926
20	H	6.191178	6.949778	5.005012	2.479420	6.512550
21	O	2.412964	1.421214	4.507798	6.581654	2.641158
22	H	2.895941	1.951181	5.227458	7.048973	2.813472

		11	12	13	14	15
11	H	0.000000				
12	H	2.498685	0.000000			
13	H	3.071316	1.783844	0.000000		
14	Br	5.036031	4.437453	2.762396	0.000000	
15	H	3.694523	4.373844	3.301002	2.557336	0.000000
16	C	5.600124	5.816984	5.062289	3.872925	2.766362
17	C	6.617331	6.863352	6.278757	5.135255	4.034092
18	H	5.872804	5.988854	4.928131	3.189287	2.540531
19	H	7.607991	7.795201	7.071684	5.580605	4.737470
20	H	6.656895	6.981149	6.667596	5.915488	4.611883
21	O	2.718767	2.040591	2.094598	4.564672	4.650766
22	H	3.402002	2.760077	2.164795	4.195815	4.625230

		16	17	18	19	20
16	C	0.000000				
17	C	1.326611	0.000000			
18	H	1.084640	2.135684	0.000000		
19	H	2.083114	1.081295	2.470971	0.000000	
20	H	2.122027	1.083373	3.107055	1.850246	0.000000
21	O	6.826382	8.032609	6.753627	8.896200	8.312995
22	H	6.934891	8.200180	6.710435	8.987099	8.596639

		21	22
21	O	0.000000	
22	H	0.962230	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.467513	-2.319004	-0.504813
2	6	0	-1.712540	-1.810211	-0.672225
3	7	0	-1.802718	-0.681626	0.136908
4	6	0	-0.621686	-0.507964	0.759173
5	7	0	0.194336	-1.507503	0.407998
6	6	0	1.628885	-1.549365	0.730596
7	6	0	2.471686	-1.023035	-0.444318
8	1	0	0.005630	-3.172701	-0.957610
9	1	0	-2.521073	-2.124888	-1.306627
10	1	0	1.782708	-0.915575	1.603558
11	1	0	1.901656	-2.573248	0.992460
12	1	0	2.391582	-1.702971	-1.297959
13	1	0	2.091763	-0.038336	-0.731217
14	35	0	0.497356	2.133229	-0.120476
15	1	0	-0.381773	0.298197	1.428640
16	6	0	-2.871211	0.253259	0.223054
17	6	0	-4.142517	-0.063185	0.014388
18	1	0	-2.517153	1.255362	0.439558
19	1	0	-4.896237	0.711169	0.052890
20	1	0	-4.473570	-1.072516	-0.198569
21	8	0	3.837630	-0.977149	-0.054520
22	1	0	4.056025	-0.069389	0.178206

Rotational constants (GHZ): 0.8086216 0.5713875 0.3531634
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 358 symmetry adapted cartesian basis functions of A symmetry.
There are 345 symmetry adapted basis functions of A symmetry.
345 basis functions, 553 primitive gaussians, 358 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 863.6710678604 Hartrees.
NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.

Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 345 RedAO= T EigKep= 6.62D-06 NBF= 345
NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345
Initial guess from the checkpoint file: "."
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999913 0.000558 0.000044 0.013193 Ang= 1.51 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.33849663 A.U. after 12 cycles
NFock= 12 Conv=0.19D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000050463	0.000058801	-0.000084737
2	6	0.000090340	-0.000010983	-0.000070568
3	7	-0.000138691	-0.000205718	0.000173105
4	6	-0.000007990	0.000200598	-0.000299081
5	7	0.000328129	0.000116020	0.000158399
6	6	-0.000224325	0.000025963	-0.000226690
7	6	0.000217582	0.000011327	0.000468724
8	1	0.000000040	-0.000062763	0.000036800
9	1	-0.000059554	-0.000017741	0.000036821
10	1	0.000027804	-0.000028552	0.000109164

11	1	-0.000005712	0.000034435	-0.000049494
12	1	0.000180026	-0.000080635	0.000055755
13	1	0.000196908	0.000123609	-0.000516554
14	35	-0.000321777	-0.000462683	0.000289301
15	1	0.000169414	0.000245292	0.000144900
16	6	0.000013459	0.000134210	-0.000055257
17	6	-0.000112458	-0.000067811	-0.000061956
18	1	-0.000025886	0.000090045	0.000004732
19	1	-0.000006960	0.000062634	0.000046956
20	1	0.000039180	-0.000049127	-0.000020496
21	8	-0.000277493	-0.000461729	-0.000291442
22	1	-0.000031575	0.000344808	0.000151618

Cartesian Forces: Max 0.000516554 RMS 0.000184430

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.003174698 RMS 0.000432227
Search for a local minimum.
Step number 30 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 25 26 27 28 29
30
DE= -1.23D-05 DEPred=-1.22D-05 R= 1.02D+00
TightC=F SS= 1.41D+00 RLast= 1.71D-01 DXNew= 1.0469D+00 5.1350D-01
Trust test= 1.02D+00 RLast= 1.71D-01 DXMaxT set to 6.23D-01
ITU= 1 1 1 1 0 -1 1 1 1 1 1 0 -1 1 1 1 1 1 1 1
ITU= 1 1 1 1 1 0 0 -1 0 0

Eigenvalues ---	0.00052	0.00152	0.00478	0.00584	0.00846
Eigenvalues ---	0.01083	0.01642	0.01917	0.02069	0.02077
Eigenvalues ---	0.02305	0.02361	0.03066	0.03105	0.03692
Eigenvalues ---	0.04498	0.04989	0.05496	0.05957	0.06979
Eigenvalues ---	0.08962	0.09232	0.13671	0.14216	0.14990
Eigenvalues ---	0.15794	0.15975	0.16003	0.16042	0.16248
Eigenvalues ---	0.16628	0.17633	0.20727	0.22849	0.23079
Eigenvalues ---	0.24204	0.24850	0.26707	0.29871	0.33441
Eigenvalues ---	0.33869	0.33881	0.34037	0.34090	0.34262
Eigenvalues ---	0.34487	0.34799	0.35891	0.36312	0.36379
Eigenvalues ---	0.37393	0.43073	0.44885	0.45959	0.50015
Eigenvalues ---	0.53348	0.54613	0.58661	0.61224	1.82805

En-DIIS/RFO-DIIS IScMMF= 0 using points: 30 29 28 27 26

RFO step: Lambda=-1.65447058D-05.

DidBck=T Rises=F RFO-DIIS coefs: 0.62707 1.52226 -1.55518 0.23840 0.16744

Iteration 1 RMS(Cart)= 0.00723908 RMS(Int)= 0.00002295

Iteration 2 RMS(Cart)= 0.00002351 RMS(Int)= 0.00001179

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001179

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56125	0.00006	0.00002	0.00007	0.00008	2.56133
R2	2.62516	0.00005	0.00005	0.00008	0.00014	2.62529
R3	2.03327	0.00001	-0.00001	0.00005	0.00004	2.03331
R4	2.62973	0.00009	0.00006	0.00021	0.00027	2.63000
R5	2.03109	0.00001	0.00001	0.00001	0.00002	2.03112
R6	2.54392	0.00009	-0.00001	-0.00001	-0.00001	2.54391
R7	2.68787	0.00015	0.00072	-0.00020	0.00051	2.68838
R8	2.52708	0.00014	0.00010	-0.00023	-0.00012	2.52696
R9	2.03147	0.00026	0.00030	0.00061	0.00091	2.03238
R10	2.77973	-0.00023	0.00030	-0.00018	0.00012	2.77985
R11	2.90782	-0.00044	-0.00031	0.00031	0.00000	2.90782
R12	2.05921	0.00010	0.00010	0.00004	0.00014	2.05935
R13	2.06258	-0.00003	-0.00010	-0.00002	-0.00012	2.06247
R14	2.06788	-0.00001	0.00009	0.00003	0.00012	2.06800
R15	2.06688	-0.00025	0.00018	0.00020	0.00038	2.06726
R16	2.68571	-0.00034	-0.00021	-0.00028	-0.00048	2.68522
R17	5.22017	0.00007	-0.00425	0.00885	0.00460	5.22477
R18	2.50693	0.00010	0.00000	0.00008	0.00008	2.50701
R19	2.04967	0.00007	0.00020	-0.00005	0.00015	2.04982
R20	2.04335	0.00005	0.00004	0.00004	0.00008	2.04343
R21	2.04728	0.00004	0.00000	0.00003	0.00003	2.04730
R22	1.81835	0.00036	0.00031	0.00013	0.00044	1.81879
A1	1.87499	-0.00001	0.00002	-0.00008	-0.00007	1.87492
A2	2.27813	0.00002	-0.00004	0.00015	0.00010	2.27824
A3	2.13000	-0.00001	0.00007	-0.00006	0.00000	2.13000
A4	1.86727	0.00006	-0.00001	0.00001	0.00000	1.86727
A5	2.28369	0.00002	0.00006	0.00007	0.00012	2.28381
A6	2.13162	-0.00008	-0.00001	-0.00004	-0.00005	2.13157
A7	1.89287	-0.00007	0.00003	-0.00010	-0.00005	1.89283
A8	2.23566	-0.00007	-0.00028	0.00024	-0.00004	2.23562
A9	2.14870	0.00014	0.00018	-0.00016	0.00002	2.14872
A10	1.89393	0.00003	0.00001	0.00011	0.00008	1.89401
A11	2.19002	0.00009	0.00020	0.00043	0.00056	2.19058
A12	2.19923	-0.00012	-0.00006	-0.00051	-0.00064	2.19858
A13	1.89490	-0.00002	-0.00001	0.00008	0.00009	1.89499

A14	2.20448	0.00038	-0.00006	0.00078	0.00072	2.20521
A15	2.16372	-0.00038	0.00019	-0.00045	-0.00027	2.16345
A16	1.93582	-0.00078	0.00000	0.00113	0.00113	1.93695
A17	1.87214	0.00011	-0.00036	0.00028	-0.00008	1.87207
A18	1.89973	0.00038	-0.00039	-0.00034	-0.00073	1.89900
A19	1.91285	-0.00006	0.00037	-0.00047	-0.00009	1.91276
A20	1.94677	0.00045	0.00015	-0.00021	-0.00007	1.94670
A21	1.89455	-0.00010	0.00022	-0.00040	-0.00019	1.89436
A22	1.92092	0.00049	-0.00012	0.00018	0.00006	1.92098
A23	1.89439	-0.00189	-0.00091	0.00064	-0.00028	1.89411
A24	1.90502	0.00048	-0.00078	-0.00051	-0.00129	1.90373
A25	1.90642	0.00047	0.00091	0.00034	0.00125	1.90766
A26	1.88008	-0.00033	0.00110	-0.00070	0.00041	1.88049
A27	1.95706	0.00082	-0.00018	0.00005	-0.00014	1.95692
A28	2.58723	-0.00317	0.00027	-0.00140	-0.00114	2.58609
A29	2.15746	-0.00003	-0.00053	0.00030	-0.00023	2.15723
A30	1.95426	0.00006	-0.00019	0.00019	0.00000	1.95426
A31	2.17075	-0.00003	0.00075	-0.00052	0.00023	2.17098
A32	2.08469	-0.00005	0.00002	-0.00038	-0.00036	2.08432
A33	2.14837	-0.00002	-0.00019	0.00013	-0.00006	2.14831
A34	2.05013	0.00007	0.00017	0.00025	0.00042	2.05055
A35	1.89119	-0.00013	-0.00009	-0.00031	-0.00040	1.89078
D1	0.00563	0.00008	0.00005	-0.00015	-0.00009	0.00554
D2	3.10976	0.00005	0.00143	0.00067	0.00210	3.11186
D3	-3.12346	0.00000	-0.00273	-0.00096	-0.00369	-3.12715
D4	-0.01934	-0.00003	-0.00135	-0.00014	-0.00149	-0.02082
D5	-0.02736	-0.00010	0.00047	0.00030	0.00077	-0.02659
D6	-2.96044	0.00004	-0.00023	-0.00174	-0.00198	-2.96242
D7	3.10303	-0.00003	0.00296	0.00103	0.00399	3.10702
D8	0.16994	0.00012	0.00226	-0.00101	0.00124	0.17119
D9	0.01785	-0.00004	-0.00056	-0.00005	-0.00061	0.01724
D10	3.04385	-0.00009	-0.00097	-0.00021	-0.00120	3.04265
D11	-3.09028	-0.00001	-0.00179	-0.00079	-0.00258	-3.09286
D12	-0.06428	-0.00006	-0.00220	-0.00095	-0.00316	-0.06745
D13	-0.03518	-0.00002	0.00086	0.00024	0.00110	-0.03409
D14	3.11101	-0.00007	-0.00350	-0.00509	-0.00860	3.10240
D15	-3.06819	0.00004	0.00130	0.00036	0.00165	-3.06654
D16	0.07800	-0.00001	-0.00306	-0.00497	-0.00805	0.06995
D17	0.53347	0.00006	0.00329	-0.00312	0.00017	0.53363
D18	-2.56885	0.00007	0.00250	-0.00237	0.00013	-2.56872
D19	-2.73912	-0.00001	0.00280	-0.00329	-0.00050	-2.73962
D20	0.44175	-0.00001	0.00201	-0.00254	-0.00054	0.44121
D21	0.03871	0.00007	-0.00083	-0.00033	-0.00115	0.03755
D22	2.97777	0.00005	-0.00017	0.00183	0.00166	2.97943

D23	-3.10751	0.00013	0.00358	0.00504	0.00861	-3.09891
D24	-0.16845	0.00010	0.00424	0.00720	0.01142	-0.15703
D25	1.22898	0.00047	0.00435	0.00573	0.01009	1.23906
D26	-2.96580	0.00002	0.00459	0.00599	0.01057	-2.95523
D27	-0.91914	0.00016	0.00444	0.00548	0.00993	-0.90921
D28	-1.67374	0.00058	0.00357	0.00330	0.00687	-1.66687
D29	0.41467	0.00012	0.00380	0.00356	0.00736	0.42203
D30	2.46133	0.00026	0.00365	0.00306	0.00671	2.46804
D31	-1.16393	-0.00018	0.00125	-0.00481	-0.00356	-1.16749
D32	0.92159	-0.00046	0.00173	-0.00390	-0.00217	0.91942
D33	3.05937	-0.00035	0.00045	-0.00376	-0.00331	3.05606
D34	3.05538	0.00020	0.00146	-0.00555	-0.00409	3.05128
D35	-1.14229	-0.00009	0.00194	-0.00464	-0.00271	-1.14500
D36	0.99549	0.00002	0.00065	-0.00450	-0.00385	0.99164
D37	0.95681	0.00008	0.00085	-0.00460	-0.00375	0.95306
D38	3.04233	-0.00021	0.00133	-0.00369	-0.00236	3.03997
D39	-1.10307	-0.00010	0.00005	-0.00355	-0.00350	-1.10658
D40	0.22582	-0.00011	-0.00413	0.01521	0.01109	0.23691
D41	2.32040	-0.00037	-0.00427	0.01600	0.01173	2.33213
D42	-1.88006	0.00005	-0.00241	0.01539	0.01298	-1.86708
D43	-1.74910	0.00070	-0.00801	-0.00210	-0.01011	-1.75920
D44	2.44873	0.00003	-0.00807	-0.00162	-0.00969	2.43904
D45	0.35062	-0.00083	-0.00980	-0.00161	-0.01141	0.33921
D46	-3.09279	0.00000	-0.00097	0.00108	0.00011	-3.09268
D47	0.04631	0.00000	-0.00019	0.00034	0.00015	0.04646
D48	0.00467	-0.00001	-0.00011	0.00025	0.00014	0.00481
D49	-3.13942	0.00000	0.00067	-0.00049	0.00018	-3.13924

Item	Value	Threshold	Converged?
Maximum Force	0.003175	0.000450	NO
RMS Force	0.000432	0.000300	NO
Maximum Displacement	0.039428	0.001800	NO
RMS Displacement	0.007235	0.001200	NO

Predicted change in Energy=-1.059671D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.464868	-2.038194	-1.302382
2	6	0	-1.751873	-1.646064	-1.466568
3	7	0	-2.091790	-0.888616	-0.349584
4	6	0	-1.016583	-0.812481	0.456847

5	7	0	-0.026160	-1.527475	-0.087185
6	6	0	1.359730	-1.519631	0.405948
7	6	0	2.219686	-0.517074	-0.383427
8	1	0	0.174440	-2.623784	-1.939644
9	1	0	-2.438699	-1.809493	-2.277002
10	1	0	1.327951	-1.227094	1.455228
11	1	0	1.762362	-2.531910	0.339961
12	1	0	2.332826	-0.853064	-1.418746
13	1	0	1.718776	0.455381	-0.371557
14	35	0	-0.242582	2.074430	0.712891
15	1	0	-0.965829	-0.263290	1.380149
16	6	0	-3.294754	-0.167596	-0.111075
17	6	0	-4.476238	-0.530879	-0.592870
18	1	0	-3.121340	0.728644	0.474838
19	1	0	-5.340098	0.092469	-0.407202
20	1	0	-4.625970	-1.432622	-1.174391
21	8	0	3.515391	-0.458729	0.196975
22	1	0	3.565971	0.330194	0.745949

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.355399	0.000000			
3	N	2.208219	1.391734	0.000000		
4	C	2.213967	2.221495	1.346180	0.000000	
5	N	1.389245	2.212430	2.178031	1.337207	0.000000
6	C	2.552734	3.633783	3.589150	2.479821	1.471031
7	C	3.219489	4.268618	4.327588	3.356599	2.480422
8	H	1.075980	2.211429	3.267246	3.231490	2.161883
9	H	2.213188	1.074822	2.164093	3.238886	3.270348
10	H	3.387697	4.265882	3.881565	2.581764	2.074339
11	H	2.810978	4.049460	4.246219	3.269960	2.095270
12	H	3.040586	4.161238	4.552098	3.839015	2.791541
13	H	3.442768	4.202444	4.040697	3.126646	2.656575
14	Br	4.585239	4.568379	3.650763	2.999815	3.696036
15	H	3.255336	3.260940	2.156571	1.075487	2.152721
16	C	3.595359	2.530556	1.422631	2.434847	3.540275
17	C	4.343558	3.070692	2.423376	3.626350	4.588257
18	H	4.227381	3.359128	2.086906	2.608715	3.871186
19	H	5.395270	4.125543	3.393722	4.500922	5.564580
20	H	4.206884	2.896783	2.719984	4.009138	4.727500
21	O	4.537096	5.649886	5.650134	4.553181	3.710196
22	H	5.104173	6.089359	5.890327	4.731710	4.128977

	6	7	8	9	10

6	C	0.000000				
7	C	1.538752	0.000000			
8	H	2.850590	3.323112	0.000000		
9	H	4.659431	5.191967	2.757784	0.000000	
10	H	1.089760	2.163324	3.847919	5.334452	0.000000
11	H	1.091410	2.189064	2.779665	5.001929	1.770615
12	H	2.172725	1.094338	2.839967	4.941539	3.067474
13	H	2.152696	1.093947	3.784855	5.103428	2.514082
14	Br	3.947011	3.739060	5.411383	5.370964	3.730644
15	H	2.817034	3.649946	4.230032	4.234955	2.489173
16	C	4.874375	5.532211	4.627292	2.849544	4.994522
17	C	6.002815	6.699212	5.274737	2.936447	6.194193
18	H	5.013928	5.551125	5.284947	3.805360	4.958051
19	H	6.938859	7.584355	6.335340	3.941031	7.047891
20	H	6.191417	6.951752	5.004839	2.478293	6.512013
21	O	2.411651	1.420958	4.518247	6.587588	2.637893
22	H	2.899130	1.950855	5.238404	7.054967	2.817261

		11	12	13	14	15
11	H	0.000000				
12	H	2.497399	0.000000			
13	H	3.071167	1.784850	0.000000		
14	Br	5.037584	4.443740	2.764829	0.000000	
15	H	3.697520	4.366093	3.285128	2.536387	0.000000
16	C	5.600700	5.818035	5.058798	3.875739	2.767093
17	C	6.617736	6.866529	6.276933	5.139697	4.035762
18	H	5.873667	5.986267	4.921157	3.186700	2.539636
19	H	7.608584	7.796859	7.068287	5.582781	4.738715
20	H	6.656762	6.987162	6.668201	5.922443	4.614070
21	O	2.718756	2.040714	2.094433	4.561297	4.638904
22	H	3.407268	2.758016	2.162549	4.189096	4.614286

		16	17	18	19	20
16	C	0.000000				
17	C	1.326651	0.000000			
18	H	1.084718	2.135918	0.000000		
19	H	2.082968	1.081337	2.470951	0.000000	
20	H	2.122043	1.083387	3.107240	1.850530	0.000000
21	O	6.823323	8.030890	6.747834	8.893173	8.313295
22	H	6.931943	8.198231	6.704655	8.983559	8.596692

		21	22
21	O	0.000000	
22	H	0.962461	0.000000

Stoichiometry C7H11BrN2O

Framework group C1[X(C7H11BrN2O)]

Deg. of freedom 60

Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.481820	-2.326374	-0.495659
2	6	0	-1.724891	-1.812858	-0.663538
3	7	0	-1.806622	-0.676295	0.135504
4	6	0	-0.622821	-0.503350	0.752679
5	7	0	0.187230	-1.509660	0.407309
6	6	0	1.622157	-1.556426	0.727826
7	6	0	2.466532	-1.034075	-0.447733
8	1	0	-0.015441	-3.188307	-0.939839
9	1	0	-2.537868	-2.130244	-1.290894
10	1	0	1.779370	-0.923006	1.600545
11	1	0	1.890875	-2.581254	0.989923
12	1	0	2.386272	-1.716031	-1.299831
13	1	0	2.088698	-0.048833	-0.736280
14	35	0	0.509068	2.134601	-0.118490
15	1	0	-0.373416	0.311745	1.408492
16	6	0	-2.869771	0.265602	0.215645
17	6	0	-4.143343	-0.045821	0.013081
18	1	0	-2.509452	1.267708	0.421964
19	1	0	-4.892471	0.733281	0.046190
20	1	0	-4.480389	-1.055322	-0.189490
21	8	0	3.831568	-0.989893	-0.055501
22	1	0	4.053374	-0.080122	0.166875

Rotational constants (GHZ): 0.8066993 0.5715010 0.3525333
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 358 symmetry adapted cartesian basis functions of A symmetry.
There are 345 symmetry adapted basis functions of A symmetry.
345 basis functions, 553 primitive gaussians, 358 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 863.3705849070 Hartrees.
NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 6.60D-06 NBF= 345
NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345
Initial guess from the checkpoint file: "."
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999998 0.000369 -0.000111 0.002138 Ang= 0.25 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.33851074 A.U. after 10 cycles
NFock= 10 Conv=0.62D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000061191	-0.000041121	0.000006006
2	6	0.000033895	-0.000059764	-0.000008452
3	7	-0.000025899	-0.000089994	0.000070640
4	6	-0.000050409	-0.000009409	-0.000144430
5	7	0.000261612	0.000133210	0.000010310
6	6	-0.000304605	-0.000013783	-0.000131362
7	6	-0.000023373	-0.000033015	0.000484138
8	1	0.000031011	0.000016581	-0.000007069
9	1	-0.000031152	0.000004973	0.000016907
10	1	0.000044238	-0.000022501	0.000045382
11	1	0.000023453	0.000007917	-0.000029254
12	1	0.000085453	-0.000009449	0.000037512
13	1	0.000272656	0.000016113	-0.000595476

14	35	-0.000219135	-0.000126729	0.000237643
15	1	0.000074379	0.000155246	0.000129587
16	6	0.000050674	0.000071312	-0.000090286
17	6	-0.000046753	-0.000006582	-0.000016275
18	1	-0.000035828	0.000040472	0.000031706
19	1	-0.000008675	0.000017594	0.000028049
20	1	0.000014903	-0.000035220	-0.000014326
21	8	-0.000076325	-0.000121119	-0.000123273
22	1	-0.000008928	0.000105269	0.000062323

Cartesian Forces: Max 0.000595476 RMS 0.000133109

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.001566053 RMS 0.000187426
Search for a local minimum.
Step number 31 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 25 26 27 28 29
30 31
DE= -1.41D-05 DEPred=-1.06D-05 R= 1.33D+00
TightC=F SS= 1.41D+00 RLast= 4.19D-02 DXNew= 1.0469D+00 1.2574D-01
Trust test= 1.33D+00 RLast= 4.19D-02 DXMaxT set to 6.23D-01
ITU= 1 1 1 1 1 0 -1 1 1 1 1 1 0 -1 1 1 1 1 1 1
ITU= 1 1 1 1 1 1 0 0 -1 0 0
Eigenvalues --- 0.00033 0.00142 0.00482 0.00558 0.00823
Eigenvalues --- 0.01064 0.01516 0.01844 0.02070 0.02088
Eigenvalues --- 0.02309 0.02519 0.03066 0.03103 0.03689
Eigenvalues --- 0.04483 0.04998 0.05516 0.06049 0.06632
Eigenvalues --- 0.09093 0.09313 0.13682 0.14211 0.15075
Eigenvalues --- 0.15959 0.15964 0.16003 0.16036 0.16260
Eigenvalues --- 0.17370 0.17928 0.20815 0.22613 0.22887
Eigenvalues --- 0.24131 0.24954 0.25519 0.29868 0.33230
Eigenvalues --- 0.33871 0.33905 0.33958 0.34147 0.34240
Eigenvalues --- 0.34480 0.34799 0.36098 0.36320 0.36387
Eigenvalues --- 0.37215 0.43066 0.44924 0.45878 0.49839
Eigenvalues --- 0.53357 0.54610 0.58343 0.60987 1.74893
En-DIIS/RFO-DIIS IScMMF= 0 using points: 31 30 29 28 27
RFO step: Lambda=-4.81852294D-06.
DidBck=F Rises=F RFO-DIIS coefs: 1.65486 -0.35235 0.35944 -0.83691

0.17496

Iteration 1 RMS(Cart)= 0.02099632 RMS(Int)= 0.00030029

Iteration 2 RMS(Cart)= 0.00061934 RMS(Int)= 0.00008303

Iteration 3 RMS(Cart)= 0.00000040 RMS(Int)= 0.00008303

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56133	0.00001	0.00033	0.00006	0.00030	2.56163
R2	2.62529	0.00002	-0.00007	0.00000	-0.00009	2.62520
R3	2.03331	0.00001	0.00003	0.00007	0.00011	2.03341
R4	2.63000	0.00003	0.00017	0.00011	0.00025	2.63025
R5	2.03112	0.00001	0.00001	0.00001	0.00002	2.03114
R6	2.54391	0.00002	-0.00053	-0.00011	-0.00056	2.54335
R7	2.68838	0.00006	0.00108	0.00002	0.00110	2.68949
R8	2.52696	0.00006	-0.00051	-0.00026	-0.00070	2.52626
R9	2.03238	0.00019	0.00165	0.00104	0.00269	2.03507
R10	2.77985	-0.00020	0.00107	-0.00037	0.00070	2.78055
R11	2.90782	-0.00015	0.00006	0.00025	0.00032	2.90814
R12	2.05935	0.00004	0.00011	0.00005	0.00017	2.05951
R13	2.06247	0.00000	-0.00025	0.00002	-0.00023	2.06224
R14	2.06800	-0.00002	0.00015	-0.00007	0.00008	2.06808
R15	2.06726	-0.00013	0.00054	0.00005	0.00058	2.06784
R16	2.68522	-0.00010	-0.00106	-0.00035	-0.00141	2.68381
R17	5.22477	0.00017	-0.00866	0.01424	0.00558	5.23035
R18	2.50701	0.00004	-0.00004	0.00006	0.00002	2.50703
R19	2.04982	0.00005	0.00011	0.00003	0.00014	2.04996
R20	2.04343	0.00002	0.00003	0.00007	0.00009	2.04352
R21	2.04730	0.00003	-0.00007	0.00009	0.00002	2.04733
R22	1.81879	0.00012	0.00069	0.00018	0.00087	1.81966
A1	1.87492	-0.00001	-0.00009	-0.00011	-0.00023	1.87469
A2	2.27824	0.00002	-0.00010	0.00021	0.00011	2.27835
A3	2.13000	-0.00002	0.00025	-0.00010	0.00015	2.13015
A4	1.86727	0.00002	-0.00023	-0.00005	-0.00030	1.86697
A5	2.28381	0.00002	-0.00013	0.00005	-0.00007	2.28374
A6	2.13157	-0.00005	0.00045	0.00002	0.00047	2.13205
A7	1.89283	-0.00001	0.00013	0.00005	0.00029	1.89312
A8	2.23562	-0.00003	0.00064	0.00028	0.00085	2.23647
A9	2.14872	0.00004	-0.00032	-0.00023	-0.00063	2.14809
A10	1.89401	0.00000	0.00026	-0.00001	0.00002	1.89403
A11	2.19058	0.00004	0.00067	0.00027	0.00039	2.19097
A12	2.19858	-0.00004	-0.00037	-0.00031	-0.00123	2.19736
A13	1.89499	0.00000	0.00015	0.00019	0.00046	1.89545
A14	2.20521	0.00015	0.00123	0.00075	0.00192	2.20712
A15	2.16345	-0.00015	-0.00132	-0.00026	-0.00164	2.16180
A16	1.93695	-0.00024	-0.00065	0.00103	0.00038	1.93733

A17	1.87207	0.00005	-0.00102	0.00038	-0.00065	1.87142
A18	1.89900	0.00014	-0.00064	-0.00041	-0.00105	1.89795
A19	1.91276	-0.00004	-0.00014	-0.00016	-0.00031	1.91245
A20	1.94670	0.00013	0.00183	-0.00044	0.00139	1.94809
A21	1.89436	-0.00003	0.00054	-0.00039	0.00014	1.89451
A22	1.92098	0.00016	0.00026	0.00012	0.00039	1.92137
A23	1.89411	-0.00065	-0.00246	0.00085	-0.00161	1.89250
A24	1.90373	0.00021	-0.00036	0.00008	-0.00029	1.90344
A25	1.90766	0.00015	0.00241	0.00050	0.00290	1.91057
A26	1.88049	-0.00013	0.00104	-0.00108	-0.00004	1.88045
A27	1.95692	0.00028	-0.00083	-0.00048	-0.00132	1.95560
A28	2.58609	-0.00157	0.00204	-0.00321	-0.00117	2.58492
A29	2.15723	-0.00001	-0.00019	0.00044	0.00025	2.15748
A30	1.95426	0.00005	-0.00008	0.00038	0.00030	1.95456
A31	2.17098	-0.00004	0.00031	-0.00078	-0.00048	2.17050
A32	2.08432	-0.00002	-0.00037	-0.00033	-0.00070	2.08363
A33	2.14831	-0.00001	0.00012	0.00028	0.00041	2.14872
A34	2.05055	0.00003	0.00025	0.00004	0.00029	2.05084
A35	1.89078	-0.00003	-0.00089	-0.00047	-0.00136	1.88942
D1	0.00554	0.00004	0.00020	0.00005	0.00025	0.00579
D2	3.11186	0.00000	0.00292	0.00084	0.00376	3.11563
D3	-3.12715	0.00003	-0.00528	-0.00008	-0.00535	-3.13251
D4	-0.02082	-0.00001	-0.00255	0.00072	-0.00184	-0.02267
D5	-0.02659	-0.00004	0.00278	0.00097	0.00374	-0.02285
D6	-2.96242	0.00000	0.00262	-0.00248	0.00013	-2.96230
D7	3.10702	-0.00003	0.00768	0.00108	0.00876	3.11578
D8	0.17119	0.00001	0.00753	-0.00237	0.00515	0.17634
D9	0.01724	-0.00003	-0.00309	-0.00104	-0.00413	0.01311
D10	3.04265	-0.00005	0.00102	-0.00012	0.00090	3.04355
D11	-3.09286	0.00000	-0.00550	-0.00175	-0.00726	-3.10011
D12	-0.06745	-0.00002	-0.00140	-0.00082	-0.00222	-0.06967
D13	-0.03409	0.00001	0.00485	0.00167	0.00651	-0.02757
D14	3.10240	-0.00003	-0.02188	-0.00810	-0.03002	3.07239
D15	-3.06654	0.00004	0.00091	0.00075	0.00168	-3.06486
D16	0.06995	0.00000	-0.02582	-0.00901	-0.03485	0.03509
D17	0.53363	0.00003	-0.00986	-0.00603	-0.01590	0.51774
D18	-2.56872	0.00001	-0.01097	-0.00703	-0.01800	-2.58672
D19	-2.73962	0.00000	-0.00517	-0.00496	-0.01012	-2.74974
D20	0.44121	-0.00002	-0.00627	-0.00596	-0.01223	0.42898
D21	0.03755	0.00001	-0.00473	-0.00163	-0.00635	0.03120
D22	2.97943	0.00002	-0.00421	0.00186	-0.00235	2.97708
D23	-3.09891	0.00005	0.02219	0.00819	0.03034	-3.06856
D24	-0.15703	0.00006	0.02271	0.01168	0.03434	-0.12269
D25	1.23906	0.00018	0.01250	0.00676	0.01926	1.25832

D26	-2.95523	0.00002	0.01131	0.00739	0.01870	-2.93652
D27	-0.90921	0.00008	0.01105	0.00691	0.01797	-0.89124
D28	-1.66687	0.00019	0.01209	0.00273	0.01481	-1.65206
D29	0.42203	0.00004	0.01090	0.00336	0.01425	0.43628
D30	2.46804	0.00009	0.01065	0.00288	0.01352	2.48156
D31	-1.16749	-0.00006	-0.01032	-0.00480	-0.01512	-1.18260
D32	0.91942	-0.00018	-0.00873	-0.00360	-0.01233	0.90709
D33	3.05606	-0.00012	-0.01152	-0.00361	-0.01513	3.04093
D34	3.05128	0.00005	-0.00857	-0.00579	-0.01436	3.03693
D35	-1.14500	-0.00007	-0.00698	-0.00459	-0.01157	-1.15657
D36	0.99164	-0.00001	-0.00977	-0.00460	-0.01437	0.97727
D37	0.95306	0.00004	-0.01032	-0.00491	-0.01523	0.93784
D38	3.03997	-0.00008	-0.00873	-0.00371	-0.01244	3.02753
D39	-1.10658	-0.00002	-0.01152	-0.00372	-0.01524	-1.12181
D40	0.23691	0.00002	0.05307	0.02080	0.07388	0.31079
D41	2.33213	-0.00009	0.05334	0.02176	0.07510	2.40723
D42	-1.86708	0.00002	0.05572	0.02043	0.07614	-1.79094
D43	-1.75920	0.00024	-0.00089	0.00678	0.00588	-1.75332
D44	2.43904	0.00001	-0.00161	0.00721	0.00560	2.44465
D45	0.33921	-0.00026	-0.00476	0.00760	0.00283	0.34204
D46	-3.09268	-0.00003	-0.00107	-0.00088	-0.00195	-3.09463
D47	0.04646	-0.00001	-0.00058	-0.00061	-0.00119	0.04527
D48	0.00481	0.00000	0.00016	0.00028	0.00044	0.00525
D49	-3.13924	0.00001	0.00065	0.00055	0.00120	-3.13804

Item	Value	Threshold	Converged?
Maximum Force	0.001566	0.000450	NO
RMS Force	0.000187	0.000300	YES
Maximum Displacement	0.116596	0.001800	NO
RMS Displacement	0.020868	0.001200	NO

Predicted change in Energy=-1.502852D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.470580	-2.057215	-1.300017
2	6	0	-1.757438	-1.663443	-1.462731
3	7	0	-2.090034	-0.893045	-0.352251
4	6	0	-1.012835	-0.815398	0.450875
5	7	0	-0.025523	-1.534697	-0.092225
6	6	0	1.361980	-1.523625	0.397402
7	6	0	2.215468	-0.511198	-0.386708

8	1	0	0.163103	-2.654993	-1.931650
9	1	0	-2.449151	-1.836251	-2.267053
10	1	0	1.330932	-1.238228	1.448759
11	1	0	1.767903	-2.533933	0.323812
12	1	0	2.340765	-0.846491	-1.420898
13	1	0	1.702429	0.455279	-0.376294
14	35	0	-0.215739	2.085224	0.774591
15	1	0	-0.947690	-0.236046	1.356327
16	6	0	-3.290347	-0.166311	-0.114239
17	6	0	-4.472742	-0.521982	-0.599494
18	1	0	-3.114312	0.726410	0.476384
19	1	0	-5.333641	0.104951	-0.411874
20	1	0	-4.626251	-1.420619	-1.184848
21	8	0	3.505163	-0.436534	0.203305
22	1	0	3.538892	0.351266	0.755979

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.355557	0.000000			
3	N	2.208208	1.391869	0.000000		
4	C	2.213995	2.221599	1.345882	0.000000	
5	N	1.389195	2.212327	2.177506	1.336837	0.000000
6	C	2.554257	3.634614	3.588316	2.478748	1.471402
7	C	3.230968	4.274281	4.322538	3.349033	2.481191
8	H	1.076036	2.211682	3.267352	3.231620	2.161973
9	H	2.213307	1.074831	2.164502	3.239178	3.270288
10	H	3.387028	4.265632	3.881468	2.582208	2.074246
11	H	2.806223	4.046914	4.246557	3.271393	2.094740
12	H	3.063352	4.179047	4.558087	3.840721	2.799700
13	H	3.447878	4.200002	4.025088	3.109902	2.650758
14	Br	4.639908	4.629790	3.694975	3.025519	3.727114
15	H	3.255834	3.261939	2.157739	1.076910	2.152949
16	C	3.596203	2.531728	1.423216	2.434693	3.540062
17	C	4.343383	3.069362	2.424070	3.627717	4.589190
18	H	4.230070	3.363432	2.087683	2.606536	3.869954
19	H	5.395658	4.125621	3.394192	4.501194	5.564776
20	H	4.205725	2.892450	2.721021	4.012314	4.730067
21	O	4.548969	5.654729	5.641212	4.540610	3.709319
22	H	5.109184	6.085462	5.870374	4.708759	4.120845

		6	7	8	9	10
6	C	0.000000				
7	C	1.538921	0.000000			
8	H	2.853381	3.345878	0.000000		

9	H	4.660662	5.200974	2.758026	0.000000	
10	H	1.089847	2.163311	3.846845	5.334221	0.000000
11	H	1.091289	2.190116	2.770766	4.998288	1.770679
12	H	2.173188	1.094381	2.876415	4.963759	3.067271
13	H	2.151876	1.094256	3.802953	5.105066	2.517298
14	Br	3.956673	3.741763	5.471464	5.442213	3.727201
15	H	2.812823	3.622077	4.230362	4.236026	2.490990
16	C	4.873215	5.523330	4.628481	2.851476	4.994816
17	C	6.003422	6.691603	5.274034	2.933082	6.196046
18	H	5.010598	5.539238	5.289043	3.812626	4.956361
19	H	6.938194	7.574253	6.335709	3.940842	7.048590
20	H	6.194598	6.947891	5.001930	2.466512	6.515918
21	O	2.410949	1.420213	4.544113	6.596646	2.630808
22	H	2.895296	1.949623	5.258982	7.055537	2.807404

		11	12	13	14	15
11	H	0.000000				
12	H	2.493922	0.000000			
13	H	3.070802	1.786974	0.000000		
14	Br	5.047242	4.466637	2.767784	0.000000	
15	H	3.704162	4.347363	3.240839	2.502492	0.000000
16	C	5.602090	5.820604	5.038141	3.913137	2.766852
17	C	6.621638	6.870509	6.256005	5.177616	4.041410
18	H	5.872746	5.985948	4.899140	3.215125	2.528809
19	H	7.611627	7.798711	7.044876	5.614454	4.741243
20	H	6.663387	6.994617	6.650184	5.965145	4.625213
21	O	2.726110	2.040079	2.093112	4.531087	4.604081
22	H	3.412850	2.758428	2.159967	4.135724	4.564512

		16	17	18	19	20
16	C	0.000000				
17	C	1.326663	0.000000			
18	H	1.084793	2.135727	0.000000		
19	H	2.082600	1.081385	2.469946	0.000000	
20	H	2.122295	1.083399	3.107312	1.850745	0.000000
21	O	6.808290	8.018651	6.726401	8.876718	8.307545
22	H	6.903888	8.172280	6.669635	8.952452	8.577643

		21	22
21	O	0.000000	
22	H	0.962920	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.562953	-2.342200	-0.469042
2	6	0	-1.791839	-1.796258	-0.640284
3	7	0	-1.833626	-0.639297	0.132370
4	6	0	-0.642513	-0.489762	0.740882
5	7	0	0.136337	-1.524620	0.409832
6	6	0	1.571789	-1.603650	0.723287
7	6	0	2.422630	-1.107150	-0.459014
8	1	0	-0.126897	-3.230085	-0.892560
9	1	0	-2.619578	-2.105810	-1.252075
10	1	0	1.747883	-0.969186	1.591741
11	1	0	1.816289	-2.633155	0.990217
12	1	0	2.334442	-1.799105	-1.302277
13	1	0	2.057306	-0.119859	-0.757662
14	35	0	0.591680	2.137557	-0.112187
15	1	0	-0.354617	0.345765	1.356305
16	6	0	-2.868028	0.335919	0.199527
17	6	0	-4.150257	0.061592	-0.002130
18	1	0	-2.478048	1.328690	0.397257
19	1	0	-4.874767	0.864010	0.022496
20	1	0	-4.518207	-0.938993	-0.194989
21	8	0	3.787246	-1.074461	-0.066893
22	1	0	4.017502	-0.164617	0.148475

Rotational constants (GHZ): 0.7975489 0.5705304 0.3497608
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 358 symmetry adapted cartesian basis functions of A symmetry.
There are 345 symmetry adapted basis functions of A symmetry.
345 basis functions, 553 primitive gaussians, 358 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 861.4071365728 Hartrees.
NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 345 RedAO= T EigKep= 6.48D-06 NBF= 345
NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345
Initial guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999898 0.000731 -0.000085 0.014289 Ang= 1.64 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.33851885 A.U. after 11 cycles
NFock= 11 Conv=0.56D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000008298	-0.000213848	0.000231885
2	6	-0.000129337	-0.000045673	0.000114180
3	7	-0.000021541	0.000023141	-0.000048283
4	6	0.000048991	0.000006138	-0.000461877
5	7	0.000097759	0.000161229	-0.000083589
6	6	-0.000377546	-0.000158086	0.000014554
7	6	-0.000344609	-0.000065315	0.000534957
8	1	0.000090714	0.000132749	-0.000069413
9	1	0.000007485	0.000033766	-0.000007708
10	1	0.000083521	-0.000012614	-0.000050445
11	1	0.000065915	-0.000022709	-0.000000781
12	1	-0.000023154	0.000089197	0.000028435
13	1	0.000440641	-0.000045143	-0.000770475
14	35	-0.000270330	-0.000249468	0.000296386
15	1	0.000052876	0.000329863	0.000261821
16	6	0.000117913	-0.000065398	-0.000050988

17	6	0.000038783	0.000069087	0.000069233
18	1	-0.000043235	-0.000033684	0.000002972
19	1	-0.000000706	-0.000030385	-0.000017630
20	1	-0.000013236	-0.000004336	-0.000009342
21	8	0.000146902	0.000252205	0.000081056
22	1	0.000023896	-0.000150715	-0.000064949

Cartesian Forces: Max 0.000770475 RMS 0.000189679

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.002269752 RMS 0.000292354
Search for a local minimum.
Step number 32 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 25 26 27 28 29
30 31 32
DE= -8.11D-06 DEPred=-1.50D-05 R= 5.40D-01
TightC=F SS= 1.41D+00 RLast= 1.61D-01 DXNew= 1.0469D+00 4.8234D-01
Trust test= 5.40D-01 RLast= 1.61D-01 DXMaxT set to 6.23D-01
ITU= 1 1 1 1 1 1 0 -1 1 1 1 1 1 0 -1 1 1 1 1 1
ITU= 1 1 1 1 1 1 1 0 0 -1 0 0
Eigenvalues --- 0.00006 0.00147 0.00497 0.00546 0.00798
Eigenvalues --- 0.01134 0.01311 0.01744 0.02056 0.02095
Eigenvalues --- 0.02315 0.02751 0.03066 0.03122 0.03725
Eigenvalues --- 0.04480 0.04972 0.05463 0.06079 0.06484
Eigenvalues --- 0.09135 0.09362 0.13901 0.14456 0.15097
Eigenvalues --- 0.15717 0.15979 0.16015 0.16075 0.16184
Eigenvalues --- 0.16872 0.17850 0.20769 0.22427 0.23048
Eigenvalues --- 0.24671 0.25108 0.25281 0.29801 0.33495
Eigenvalues --- 0.33867 0.33901 0.33971 0.34078 0.34310
Eigenvalues --- 0.34487 0.34879 0.36039 0.36316 0.36384
Eigenvalues --- 0.38385 0.43063 0.45759 0.46044 0.50679
Eigenvalues --- 0.53399 0.54758 0.59791 0.63363 1.88232
Eigenvalue 1 is 5.52D-05 Eigenvector:

	D42	D41	D40	D16	D24
1	-0.46911	-0.46295	-0.45562	0.23046	-0.22018
	D23	D14	D25	D26	D27
1	-0.19761	0.19577	-0.12705	-0.12260	-0.11952

En-DIIS/RFO-DIIS IScMMF= 0 using points: 32 31 30 29 28

RFO step: Lambda=-1.01926674D-05.

DidBck=T Rises=F RFO-DIIS coefs: 0.69173 1.69428 -0.79041 -0.21860 -0.37699

Iteration 1 RMS(Cart)= 0.02604790 RMS(Int)= 0.00049828

Iteration 2 RMS(Cart)= 0.00098557 RMS(Int)= 0.00018918

Iteration 3 RMS(Cart)= 0.00000112 RMS(Int)= 0.00018918

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00018918

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56163	0.00009	0.00039	0.00003	0.00022	2.56186
R2	2.62520	-0.00013	-0.00002	0.00002	-0.00006	2.62514
R3	2.03341	0.00002	0.00004	0.00011	0.00015	2.03356
R4	2.63025	-0.00007	0.00028	0.00016	0.00038	2.63063
R5	2.03114	0.00000	0.00001	0.00002	0.00004	2.03117
R6	2.54335	-0.00006	-0.00054	-0.00009	-0.00047	2.54288
R7	2.68949	-0.00011	0.00106	0.00027	0.00133	2.69082
R8	2.52626	-0.00002	-0.00058	-0.00033	-0.00075	2.52551
R9	2.03507	0.00040	0.00177	0.00183	0.00360	2.03867
R10	2.78055	-0.00022	0.00121	-0.00066	0.00055	2.78110
R11	2.90814	-0.00019	0.00011	0.00046	0.00057	2.90871
R12	2.05951	-0.00006	0.00015	0.00013	0.00028	2.05979
R13	2.06224	0.00005	-0.00030	0.00004	-0.00026	2.06197
R14	2.06808	-0.00006	0.00019	-0.00021	-0.00002	2.06806
R15	2.06784	-0.00035	0.00068	0.00011	0.00079	2.06864
R16	2.68381	0.00017	-0.00125	-0.00061	-0.00186	2.68195
R17	5.23035	0.00016	-0.00989	0.02279	0.01289	5.24324
R18	2.50703	-0.00005	-0.00001	0.00009	0.00008	2.50711
R19	2.04996	-0.00003	0.00009	0.00015	0.00024	2.05020
R20	2.04352	-0.00002	0.00003	0.00013	0.00016	2.04368
R21	2.04733	0.00001	-0.00009	0.00017	0.00008	2.04740
R22	1.81966	-0.00016	0.00079	0.00045	0.00125	1.82090
A1	1.87469	-0.00003	-0.00009	-0.00016	-0.00032	1.87436
A2	2.27835	0.00005	-0.00012	0.00034	0.00021	2.27856
A3	2.13015	-0.00002	0.00028	-0.00017	0.00011	2.13025
A4	1.86697	-0.00001	-0.00022	-0.00009	-0.00037	1.86660
A5	2.28374	0.00002	-0.00015	0.00013	-0.00001	2.28373
A6	2.13205	-0.00001	0.00048	0.00001	0.00050	2.13255
A7	1.89312	0.00001	0.00005	0.00016	0.00047	1.89359
A8	2.23647	0.00005	0.00076	0.00024	0.00083	2.23730
A9	2.14809	-0.00006	-0.00033	-0.00031	-0.00080	2.14730
A10	1.89403	0.00000	0.00040	-0.00015	-0.00029	1.89374
A11	2.19097	-0.00001	0.00098	0.00015	-0.00012	2.19084
A12	2.19736	0.00001	-0.00041	-0.00061	-0.00226	2.19510
A13	1.89545	0.00003	0.00012	0.00034	0.00074	1.89619

A14	2.20712	0.00014	0.00150	0.00095	0.00231	2.20943
A15	2.16180	-0.00018	-0.00152	-0.00018	-0.00186	2.15994
A16	1.93733	-0.00073	-0.00046	0.00169	0.00123	1.93856
A17	1.87142	0.00023	-0.00113	0.00047	-0.00066	1.87076
A18	1.89795	0.00031	-0.00074	-0.00073	-0.00147	1.89648
A19	1.91245	-0.00006	-0.00030	-0.00002	-0.00033	1.91212
A20	1.94809	0.00036	0.00200	-0.00081	0.00118	1.94927
A21	1.89451	-0.00010	0.00054	-0.00059	-0.00006	1.89445
A22	1.92137	0.00027	0.00036	-0.00001	0.00035	1.92172
A23	1.89250	-0.00105	-0.00267	0.00136	-0.00132	1.89119
A24	1.90344	0.00041	-0.00069	0.00071	0.00000	1.90344
A25	1.91057	0.00019	0.00271	0.00114	0.00385	1.91442
A26	1.88045	-0.00018	0.00106	-0.00219	-0.00113	1.87932
A27	1.95560	0.00038	-0.00071	-0.00102	-0.00174	1.95386
A28	2.58492	-0.00227	0.00264	-0.00569	-0.00305	2.58187
A29	2.15748	0.00005	-0.00017	0.00054	0.00037	2.15784
A30	1.95456	0.00001	-0.00014	0.00066	0.00051	1.95507
A31	2.17050	-0.00006	0.00033	-0.00112	-0.00079	2.16972
A32	2.08363	0.00002	-0.00051	-0.00048	-0.00099	2.08263
A33	2.14872	0.00000	0.00012	0.00040	0.00053	2.14924
A34	2.05084	-0.00003	0.00039	0.00008	0.00046	2.05131
A35	1.88942	0.00008	-0.00106	-0.00070	-0.00177	1.88766
D1	0.00579	0.00006	0.00003	0.00013	0.00018	0.00597
D2	3.11563	-0.00003	0.00328	0.00192	0.00521	3.12083
D3	-3.13251	0.00011	-0.00634	-0.00056	-0.00691	-3.13942
D4	-0.02267	0.00003	-0.00310	0.00122	-0.00189	-0.02456
D5	-0.02285	-0.00007	0.00303	0.00147	0.00447	-0.01839
D6	-2.96230	0.00003	0.00276	-0.00442	-0.00171	-2.96400
D7	3.11578	-0.00011	0.00875	0.00209	0.01083	3.12661
D8	0.17634	-0.00002	0.00847	-0.00380	0.00466	0.18100
D9	0.01311	-0.00003	-0.00307	-0.00168	-0.00474	0.00836
D10	3.04355	-0.00006	0.00119	-0.00081	0.00039	3.04394
D11	-3.10011	0.00004	-0.00595	-0.00328	-0.00923	-3.10934
D12	-0.06967	0.00002	-0.00169	-0.00240	-0.00410	-0.07377
D13	-0.02757	-0.00001	0.00499	0.00262	0.00760	-0.01997
D14	3.07239	-0.00005	-0.02371	-0.01274	-0.03652	3.03586
D15	-3.06486	0.00001	0.00089	0.00176	0.00267	-3.06220
D16	0.03509	-0.00004	-0.02781	-0.01360	-0.04145	-0.00636
D17	0.51774	0.00000	-0.01051	-0.00791	-0.01842	0.49932
D18	-2.58672	-0.00001	-0.01098	-0.01007	-0.02105	-2.60777
D19	-2.74974	-0.00002	-0.00564	-0.00688	-0.01252	-2.76227
D20	0.42898	-0.00003	-0.00610	-0.00905	-0.01515	0.41383
D21	0.03120	0.00005	-0.00497	-0.00254	-0.00748	0.02373
D22	2.97708	0.00000	-0.00427	0.00332	-0.00094	2.97614

D23	-3.06856	0.00009	0.02395	0.01287	0.03671	-3.03185
D24	-0.12269	0.00005	0.02465	0.01873	0.04325	-0.07943
D25	1.25832	0.00033	0.01435	0.01099	0.02536	1.28368
D26	-2.93652	-0.00002	0.01301	0.01223	0.02526	-2.91126
D27	-0.89124	0.00014	0.01264	0.01140	0.02407	-0.86717
D28	-1.65206	0.00041	0.01378	0.00417	0.01793	-1.63413
D29	0.43628	0.00006	0.01244	0.00541	0.01783	0.45411
D30	2.48156	0.00022	0.01207	0.00458	0.01664	2.49820
D31	-1.18260	-0.00001	-0.01244	-0.00802	-0.02046	-1.20306
D32	0.90709	-0.00025	-0.01055	-0.00580	-0.01635	0.89074
D33	3.04093	-0.00019	-0.01352	-0.00577	-0.01929	3.02164
D34	3.03693	0.00019	-0.01058	-0.00961	-0.02019	3.01674
D35	-1.15657	-0.00005	-0.00869	-0.00740	-0.01609	-1.17265
D36	0.97727	0.00001	-0.01166	-0.00737	-0.01902	0.95825
D37	0.93784	0.00012	-0.01232	-0.00834	-0.02066	0.91718
D38	3.02753	-0.00013	-0.01044	-0.00612	-0.01656	3.01097
D39	-1.12181	-0.00006	-0.01340	-0.00609	-0.01949	-1.14131
D40	0.31079	0.00000	0.05994	0.03349	0.09344	0.40423
D41	2.40723	-0.00019	0.06039	0.03497	0.09535	2.50258
D42	-1.79094	-0.00005	0.06306	0.03234	0.09539	-1.69555
D43	-1.75332	0.00043	-0.00493	0.02091	0.01598	-1.73734
D44	2.44465	-0.00002	-0.00558	0.02179	0.01620	2.46085
D45	0.34204	-0.00037	-0.00920	0.02244	0.01323	0.35527
D46	-3.09463	0.00000	-0.00038	-0.00198	-0.00236	-3.09699
D47	0.04527	-0.00001	-0.00022	-0.00123	-0.00145	0.04382
D48	0.00525	0.00001	0.00013	0.00050	0.00063	0.00588
D49	-3.13804	0.00000	0.00029	0.00124	0.00153	-3.13651

Item	Value	Threshold	Converged?
Maximum Force	0.002270	0.000450	NO
RMS Force	0.000292	0.000300	YES
Maximum Displacement	0.136530	0.001800	NO
RMS Displacement	0.025909	0.001200	NO

Predicted change in Energy=-2.146692D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.478029	-2.079719	-1.297806
2	6	0	-1.765036	-1.684952	-1.457896
3	7	0	-2.088533	-0.898950	-0.355439
4	6	0	-1.008320	-0.818134	0.442898

5	7	0	-0.024793	-1.542257	-0.099686
6	6	0	1.364543	-1.528020	0.385520
7	6	0	2.211292	-0.503395	-0.390602
8	1	0	0.148792	-2.692068	-1.922424
9	1	0	-2.463377	-1.870160	-2.253711
10	1	0	1.334701	-1.252887	1.439795
11	1	0	1.774079	-2.535892	0.301357
12	1	0	2.353342	-0.837613	-1.422961
13	1	0	1.684223	0.456007	-0.382771
14	35	0	-0.176608	2.106401	0.846839
15	1	0	-0.925393	-0.202622	1.325004
16	6	0	-3.285756	-0.165577	-0.118013
17	6	0	-4.469374	-0.512858	-0.606469
18	1	0	-3.106799	0.723462	0.477495
19	1	0	-5.326714	0.118358	-0.416440
20	1	0	-4.627477	-1.408263	-1.195618
21	8	0	3.492722	-0.409578	0.212182
22	1	0	3.502866	0.371837	0.775898

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.355676	0.000000			
3	N	2.208165	1.392071	0.000000		
4	C	2.214239	2.221938	1.345634	0.000000	
5	N	1.389165	2.212136	2.176758	1.336442	0.000000
6	C	2.555979	3.635530	3.587267	2.477440	1.471693
7	C	3.246578	4.283268	4.318124	3.340611	2.482729
8	H	1.076115	2.211969	3.267466	3.231916	2.162075
9	H	2.213431	1.074850	2.164993	3.239699	3.270174
10	H	3.385868	4.265169	3.881581	2.583131	2.074117
11	H	2.799538	4.042822	4.246261	3.272991	2.093821
12	H	3.094375	4.204788	4.568765	3.844812	2.811246
13	H	3.455796	4.199642	4.008783	3.091108	2.644604
14	Br	4.713168	4.712671	3.759397	3.067216	3.772488
15	H	3.256187	3.262949	2.159086	1.078815	2.153008
16	C	3.597107	2.533056	1.423921	2.434577	3.539698
17	C	4.343251	3.067927	2.424972	3.629498	4.590293
18	H	4.233196	3.368460	2.088748	2.604099	3.868512
19	H	5.396118	4.125786	3.394769	4.501556	5.564921
20	H	4.204666	2.887718	2.722414	4.016377	4.733258
21	O	4.564679	5.662134	5.631348	4.525431	3.708522
22	H	5.114480	6.080379	5.844533	4.677363	4.107893

	6	7	8	9	10

6	C	0.000000				
7	C	1.539223	0.000000			
8	H	2.856512	3.375007	0.000000		
9	H	4.662143	5.214572	2.758389	0.000000	
10	H	1.089993	2.163447	3.844755	5.333705	0.000000
11	H	1.091150	2.191120	2.758832	4.992756	1.770648
12	H	2.173704	1.094370	2.923783	4.995707	3.066831
13	H	2.151471	1.094675	3.826023	5.110192	2.522742
14	Br	3.974541	3.747581	5.549776	5.536765	3.731014
15	H	2.807689	3.587835	4.230484	4.237131	2.494847
16	C	4.871866	5.514160	4.629813	2.853614	4.995762
17	C	6.004097	6.684159	5.273343	2.929112	6.198559
18	H	5.007048	5.526379	5.293801	3.821041	4.955694
19	H	6.937335	7.563649	6.336217	3.940617	7.049850
20	H	6.198278	6.945186	4.998915	2.452802	6.520515
21	O	2.410416	1.419229	4.576917	6.609769	2.622071
22	H	2.886915	1.948054	5.283774	7.056992	2.789521

		11	12	13	14	15
11	H	0.000000				
12	H	2.488567	0.000000			
13	H	3.070433	1.789739	0.000000		
14	Br	5.064940	4.496650	2.774606	0.000000	
15	H	3.712028	4.324885	3.187536	2.474047	0.000000
16	C	5.603231	5.827001	5.015691	3.969839	2.766764
17	C	6.625521	6.879068	6.233418	5.234545	4.048041
18	H	5.871745	5.988475	4.874986	3.261128	2.516830
19	H	7.614561	7.804501	7.019144	5.663196	4.744184
20	H	6.670263	7.007793	6.631273	6.027830	4.638160
21	O	2.735488	2.038404	2.091381	4.494099	4.560805
22	H	3.415959	2.760281	2.158022	4.068449	4.499000

		16	17	18	19	20
16	C	0.000000				
17	C	1.326705	0.000000			
18	H	1.084917	2.135433	0.000000		
19	H	2.082112	1.081470	2.468460	0.000000	
20	H	2.122667	1.083440	3.107414	1.851113	0.000000
21	O	6.790900	8.004738	6.701332	8.857558	8.301621
22	H	6.868281	8.139425	6.625735	8.913328	8.553252

		21	22
21	O	0.000000	
22	H	0.963580	0.000000

Stoichiometry C7H11BrN2O

Framework group C1[X(C7H11BrN2O)]

Deg. of freedom 60

Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.681197	-2.353073	-0.439911
2	6	0	-1.887987	-1.760325	-0.613583
3	7	0	-1.872393	-0.582912	0.128923
4	6	0	-0.671919	-0.470966	0.726469
5	7	0	0.060766	-1.543068	0.410480
6	6	0	1.494555	-1.672627	0.715999
7	6	0	2.357458	-1.210344	-0.471814
8	1	0	-0.289158	-3.272111	-0.839533
9	1	0	-2.736040	-2.052549	-1.205796
10	1	0	1.697645	-1.042217	1.581691
11	1	0	1.701790	-2.709467	0.985490
12	1	0	2.256691	-1.911985	-1.305595
13	1	0	2.014558	-0.217938	-0.781434
14	35	0	0.712476	2.136827	-0.104603
15	1	0	-0.330532	0.381570	1.292578
16	6	0	-2.863912	0.437698	0.181804
17	6	0	-4.156710	0.217415	-0.018928
18	1	0	-2.432055	1.414910	0.370490
19	1	0	-4.844839	1.051570	-0.003347
20	1	0	-4.568350	-0.768037	-0.201353
21	8	0	3.721030	-1.201561	-0.078362
22	1	0	3.965037	-0.295025	0.138756

Rotational constants (GHZ): 0.7859740 0.5675375 0.3456806
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 358 symmetry adapted cartesian basis functions of A symmetry.
There are 345 symmetry adapted basis functions of A symmetry.
345 basis functions, 553 primitive gaussians, 358 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 858.4171505790 Hartrees.
NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 6.34D-06 NBF= 345
NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345
Initial guess from the checkpoint file: "."
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999780 0.000564 -0.000027 0.020958 Ang= 2.40 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.33852523 A.U. after 12 cycles
NFock= 12 Conv=0.23D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000191784	-0.000414502	0.000635905
2	6	-0.000444394	0.000034049	0.000360457
3	7	-0.000096714	0.000125006	-0.000202841
4	6	0.000291050	0.000252624	-0.001244027
5	7	-0.000174855	0.000132819	-0.000219319
6	6	-0.000344707	-0.000357898	0.000244910
7	6	-0.000693055	-0.000073696	0.000551027
8	1	0.000132849	0.000264870	-0.000127708
9	1	0.000065581	0.000078489	-0.000044452
10	1	0.000166806	0.000031450	-0.000205920
11	1	0.000109725	-0.000057766	0.000044051
12	1	-0.000195999	0.000249779	-0.000012816
13	1	0.000537826	-0.000163145	-0.000959303

14	35	-0.000329852	-0.000928900	0.000413350
15	1	0.000011793	0.000766472	0.000584358
16	6	0.000154762	-0.000195695	0.000002748
17	6	0.000176317	0.000174815	0.000186518
18	1	0.000012245	-0.000128799	-0.000101801
19	1	0.000010521	-0.000108234	-0.000082226
20	1	-0.000043771	0.000053232	0.000016601
21	8	0.000370874	0.000730079	0.000437909
22	1	0.000091215	-0.000465048	-0.000277422

Cartesian Forces: Max 0.001244027 RMS 0.000366876

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.005192626 RMS 0.000767991
Search for a local minimum.
Step number 33 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 25 29 30 31 32
33
DE= -6.38D-06 DEPred=-2.15D-05 R= 2.97D-01
Trust test= 2.97D-01 RLast= 2.04D-01 DXMaxT set to 6.23D-01
ITU= 0 1 1 1 1 1 1 0 -1 1 1 1 1 1 0 -1 1 1 1 1
ITU= 1 1 1 1 1 1 1 1 0 0 -1 0 0
Eigenvalues --- 0.00010 0.00092 0.00505 0.00579 0.00749
Eigenvalues --- 0.01133 0.01318 0.01675 0.02009 0.02075
Eigenvalues --- 0.02332 0.02536 0.03067 0.03108 0.03692
Eigenvalues --- 0.04423 0.05007 0.05429 0.06149 0.06702
Eigenvalues --- 0.08891 0.09216 0.13984 0.14521 0.14930
Eigenvalues --- 0.15703 0.15956 0.15987 0.16035 0.16123
Eigenvalues --- 0.16768 0.17419 0.20593 0.22380 0.23052
Eigenvalues --- 0.24371 0.24958 0.25842 0.29663 0.33144
Eigenvalues --- 0.33830 0.33877 0.33930 0.34087 0.34257
Eigenvalues --- 0.34495 0.34803 0.36115 0.36316 0.36427
Eigenvalues --- 0.38296 0.43150 0.44880 0.46142 0.50034
Eigenvalues --- 0.53394 0.54872 0.58217 0.61030 3.06555
En-DIIS/RFO-DIIS IScMMF= 0 using points: 33 32 31 30 29
RFO step: Lambda=-3.91634189D-05.
DidBck=F Rises=F RFO-DIIS coefs: 1.49114 -4.83329 6.64121 -2.00994 -0.28911

Iteration 1 RMS(Cart)= 0.05405114 RMS(Int)= 0.00502388
Iteration 2 RMS(Cart)= 0.00801905 RMS(Int)= 0.00010867
Iteration 3 RMS(Cart)= 0.00016117 RMS(Int)= 0.00006127
Iteration 4 RMS(Cart)= 0.00000004 RMS(Int)= 0.00006127

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56186	0.00029	-0.00089	-0.00016	-0.00099	2.56087
R2	2.62514	-0.00043	0.00063	-0.00011	0.00052	2.62566
R3	2.03356	0.00000	-0.00028	-0.00005	-0.00033	2.03323
R4	2.63063	-0.00029	-0.00030	-0.00012	-0.00039	2.63024
R5	2.03117	-0.00002	-0.00001	0.00003	0.00002	2.03120
R6	2.54288	-0.00016	0.00199	-0.00005	0.00190	2.54478
R7	2.69082	-0.00036	-0.00278	0.00077	-0.00201	2.68881
R8	2.52551	0.00001	0.00219	0.00035	0.00248	2.52799
R9	2.03867	0.00092	-0.00738	0.00071	-0.00666	2.03200
R10	2.78110	-0.00020	-0.00213	-0.00054	-0.00266	2.77843
R11	2.90871	-0.00064	-0.00098	0.00010	-0.00088	2.90783
R12	2.05979	-0.00019	-0.00025	0.00003	-0.00021	2.05957
R13	2.06197	0.00009	0.00053	0.00008	0.00061	2.06258
R14	2.06806	-0.00009	-0.00009	-0.00020	-0.00029	2.06776
R15	2.06864	-0.00106	-0.00115	-0.00052	-0.00167	2.06697
R16	2.68195	0.00051	0.00372	-0.00022	0.00350	2.68546
R17	5.24324	-0.00015	-0.01171	0.00850	-0.00322	5.24003
R18	2.50711	-0.00020	0.00009	-0.00004	0.00006	2.50717
R19	2.05020	-0.00016	-0.00019	0.00034	0.00015	2.05035
R20	2.04368	-0.00009	-0.00015	0.00011	-0.00004	2.04364
R21	2.04740	-0.00005	-0.00003	0.00016	0.00014	2.04754
R22	1.82090	-0.00054	-0.00197	0.00000	-0.00197	1.81893
A1	1.87436	-0.00004	0.00067	0.00005	0.00074	1.87510
A2	2.27856	0.00007	-0.00021	0.00005	-0.00016	2.27840
A3	2.13025	-0.00003	-0.00050	-0.00010	-0.00059	2.12966
A4	1.86660	-0.00003	0.00102	0.00000	0.00105	1.86765
A5	2.28373	-0.00001	0.00049	0.00036	0.00084	2.28457
A6	2.13255	0.00004	-0.00171	-0.00039	-0.00211	2.13044
A7	1.89359	0.00002	-0.00108	0.00019	-0.00099	1.89260
A8	2.23730	0.00013	-0.00302	-0.00080	-0.00380	2.23350
A9	2.14730	-0.00015	0.00219	0.00028	0.00247	2.14977
A10	1.89374	0.00001	0.00003	-0.00023	-0.00002	1.89373
A11	2.19084	-0.00016	-0.00038	-0.00034	-0.00032	2.19052
A12	2.19510	0.00014	0.00272	0.00052	0.00365	2.19874
A13	1.89619	0.00004	-0.00138	0.00005	-0.00141	1.89477
A14	2.20943	0.00032	-0.00514	0.00011	-0.00497	2.20446
A15	2.15994	-0.00041	0.00505	0.00039	0.00550	2.16545
A16	1.93856	-0.00235	0.00100	0.00091	0.00190	1.94046

A17	1.87076	0.00074	0.00190	0.00096	0.00285	1.87361
A18	1.89648	0.00089	0.00214	-0.00032	0.00182	1.89830
A19	1.91212	-0.00016	0.00085	-0.00030	0.00054	1.91267
A20	1.94927	0.00121	-0.00482	-0.00089	-0.00571	1.94356
A21	1.89445	-0.00030	-0.00084	-0.00030	-0.00114	1.89331
A22	1.92172	0.00088	-0.00125	0.00081	-0.00043	1.92129
A23	1.89119	-0.00321	0.00487	0.00084	0.00571	1.89690
A24	1.90344	0.00109	-0.00125	0.00066	-0.00060	1.90285
A25	1.91442	0.00064	-0.00719	0.00011	-0.00708	1.90734
A26	1.87932	-0.00045	0.00045	-0.00111	-0.00066	1.87865
A27	1.95386	0.00111	0.00426	-0.00129	0.00297	1.95682
A28	2.58187	-0.00519	0.00222	-0.00329	-0.00106	2.58081
A29	2.15784	0.00010	-0.00133	-0.00071	-0.00204	2.15581
A30	1.95507	-0.00009	-0.00103	0.00014	-0.00088	1.95419
A31	2.16972	-0.00002	0.00208	0.00069	0.00279	2.17250
A32	2.08263	0.00011	0.00161	0.00038	0.00198	2.08462
A33	2.14924	0.00000	-0.00152	-0.00049	-0.00200	2.14724
A34	2.05131	-0.00011	-0.00010	0.00011	0.00002	2.05132
A35	1.88766	0.00020	0.00378	-0.00013	0.00365	1.89131
D1	0.00597	0.00015	-0.00117	0.00044	-0.00072	0.00525
D2	3.12083	-0.00006	-0.00839	-0.00079	-0.00918	3.11166
D3	-3.13942	0.00025	0.01044	0.00016	0.01060	-3.12882
D4	-0.02456	0.00004	0.00321	-0.00107	0.00215	-0.02241
D5	-0.01839	-0.00018	-0.01127	0.00096	-0.01031	-0.02870
D6	-2.96400	0.00014	-0.00424	-0.00207	-0.00628	-2.97028
D7	3.12661	-0.00027	-0.02168	0.00122	-0.02046	3.10615
D8	0.18100	0.00006	-0.01465	-0.00181	-0.01643	0.16456
D9	0.00836	-0.00007	0.01313	-0.00168	0.01145	0.01981
D10	3.04394	-0.00013	-0.00542	-0.00504	-0.01044	3.03349
D11	-3.10934	0.00011	0.01954	-0.00060	0.01894	-3.09040
D12	-0.07377	0.00006	0.00099	-0.00396	-0.00295	-0.07672
D13	-0.01997	-0.00004	-0.02034	0.00231	-0.01802	-0.03800
D14	3.03586	-0.00011	0.08581	0.00176	0.08759	3.12346
D15	-3.06220	-0.00001	-0.00251	0.00554	0.00304	-3.05916
D16	-0.00636	-0.00008	0.10363	0.00498	0.10865	0.10230
D17	0.49932	0.00002	0.05493	0.01098	0.06591	0.56522
D18	-2.60777	0.00004	0.06240	0.00736	0.06976	-2.53802
D19	-2.76227	-0.00003	0.03365	0.00716	0.04081	-2.72146
D20	0.41383	-0.00001	0.04112	0.00354	0.04466	0.45849
D21	0.02373	0.00014	0.01959	-0.00203	0.01756	0.04128
D22	2.97614	-0.00008	0.01134	0.00086	0.01222	2.98837
D23	-3.03185	0.00023	-0.08703	-0.00143	-0.08844	-3.12029
D24	-0.07943	0.00001	-0.09528	0.00146	-0.09377	-0.17320
D25	1.28368	0.00096	-0.04602	0.00262	-0.04340	1.24028

D26	-2.91126	-0.00013	-0.04323	0.00337	-0.03986	-2.95113
D27	-0.86717	0.00038	-0.04207	0.00337	-0.03871	-0.90589
D28	-1.63413	0.00127	-0.03702	-0.00080	-0.03781	-1.67194
D29	0.45411	0.00018	-0.03423	-0.00005	-0.03427	0.41984
D30	2.49820	0.00069	-0.03307	-0.00005	-0.03312	2.46508
D31	-1.20306	0.00004	0.04246	0.00048	0.04294	-1.16012
D32	0.89074	-0.00063	0.03593	0.00161	0.03755	0.92828
D33	3.02164	-0.00059	0.04339	0.00096	0.04435	3.06600
D34	3.01674	0.00066	0.03897	-0.00106	0.03791	3.05465
D35	-1.17265	0.00000	0.03245	0.00006	0.03252	-1.14014
D36	0.95825	0.00004	0.03991	-0.00059	0.03932	0.99758
D37	0.91718	0.00037	0.04255	0.00009	0.04264	0.95982
D38	3.01097	-0.00030	0.03603	0.00122	0.03724	3.04821
D39	-1.14131	-0.00026	0.04349	0.00056	0.04405	-1.09726
D40	0.40423	-0.00020	-0.22499	0.00136	-0.22362	0.18060
D41	2.50258	-0.00070	-0.22782	0.00293	-0.22490	2.27768
D42	-1.69555	-0.00013	-0.22934	0.00079	-0.22855	-1.92410
D43	-1.73734	0.00134	-0.03519	0.01492	-0.02027	-1.75761
D44	2.46085	-0.00007	-0.03325	0.01422	-0.01903	2.44182
D45	0.35527	-0.00124	-0.02723	0.01560	-0.01163	0.34364
D46	-3.09699	0.00003	0.00724	-0.00367	0.00357	-3.09342
D47	0.04382	0.00000	0.00451	-0.00099	0.00352	0.04734
D48	0.00588	0.00001	-0.00123	0.00038	-0.00085	0.00503
D49	-3.13651	-0.00002	-0.00396	0.00306	-0.00090	-3.13741

Item	Value	Threshold	Converged?
Maximum Force	0.005193	0.000450	NO
RMS Force	0.000768	0.000300	NO
Maximum Displacement	0.301387	0.001800	NO
RMS Displacement	0.058592	0.001200	NO

Predicted change in Energy=-7.517833D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.463644	-2.027338	-1.307077
2	6	0	-1.751787	-1.639315	-1.470064
3	7	0	-2.094728	-0.885880	-0.351130
4	6	0	-1.018485	-0.805278	0.454251
5	7	0	-0.026174	-1.518045	-0.090612
6	6	0	1.358099	-1.515566	0.404881
7	6	0	2.227268	-0.516358	-0.378636

8	1	0	0.177308	-2.610114	-1.945199
9	1	0	-2.438751	-1.802619	-2.280462
10	1	0	1.326746	-1.227182	1.455447
11	1	0	1.757454	-2.529025	0.336109
12	1	0	2.337019	-0.846687	-1.416009
13	1	0	1.738737	0.462112	-0.360903
14	35	0	-0.263945	2.068169	0.687352
15	1	0	-0.975228	-0.272762	1.387419
16	6	0	-3.297483	-0.162296	-0.118045
17	6	0	-4.481663	-0.540736	-0.581433
18	1	0	-3.121013	0.747233	0.446611
19	1	0	-5.346639	0.083204	-0.402430
20	1	0	-4.631933	-1.456886	-1.140079
21	8	0	3.524456	-0.477308	0.200377
22	1	0	3.584736	0.305800	0.756785

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.355153	0.000000			
3	N	2.208437	1.391864	0.000000		
4	C	2.214397	2.221787	1.346638	0.000000	
5	N	1.389441	2.212540	2.178627	1.337757	0.000000
6	C	2.551756	3.633473	3.590275	2.480948	1.470283
7	C	3.222743	4.276111	4.337851	3.363345	2.482808
8	H	1.075940	2.211246	3.267443	3.231828	2.161830
9	H	2.213373	1.074863	2.163581	3.238903	3.270619
10	H	3.387814	4.266830	3.884159	2.584667	2.074920
11	H	2.808029	4.045816	4.244000	3.269725	2.094159
12	H	3.041302	4.165275	4.558057	3.841743	2.791429
13	H	3.455878	4.222558	4.063575	3.142138	2.666270
14	Br	4.559694	4.540216	3.627206	2.979994	3.677322
15	H	3.255851	3.261245	2.156791	1.075289	2.153140
16	C	3.594833	2.529568	1.422857	2.436141	3.541225
17	C	4.345229	3.073884	2.422730	3.624393	4.587746
18	H	4.223183	3.353212	2.087273	2.613612	3.872741
19	H	5.395962	4.126726	3.393623	4.500690	5.564941
20	H	4.210456	2.904722	2.717701	4.002935	4.724208
21	O	4.536514	5.655031	5.660947	4.561834	3.711440
22	H	5.108077	6.100886	5.907952	4.745068	4.133179

		6	7	8	9	10
6	C	0.000000				
7	C	1.538756	0.000000			
8	H	2.848715	3.322690	0.000000		

9	H	4.659349	5.200302	2.758299	0.000000	
10	H	1.089880	2.163348	3.846830	5.335457	0.000000
11	H	1.091473	2.186873	2.776293	4.998224	1.770091
12	H	2.172860	1.094214	2.837969	4.946621	3.067684
13	H	2.154651	1.093792	3.792971	5.124951	2.514474
14	Br	3.943853	3.744630	5.386219	5.340477	3.738931
15	H	2.820348	3.665280	4.230590	4.235057	2.492916
16	C	4.876396	5.542215	4.626497	2.846774	4.999335
17	C	6.002160	6.712039	5.277138	2.941520	6.193359
18	H	5.018411	5.557140	5.279342	3.795280	4.969771
19	H	6.939836	7.597638	6.336251	3.941972	7.050027
20	H	6.186343	6.965130	5.010684	2.496008	6.503489
21	O	2.410997	1.421084	4.511736	6.593242	2.639592
22	H	2.898124	1.951370	5.235822	7.067722	2.817212

		11	12	13	14	15
11	H	0.000000				
12	H	2.497213	0.000000			
13	H	3.071332	1.784417	0.000000		
14	Br	5.034245	4.436838	2.772904	0.000000	
15	H	3.696421	4.377166	3.310934	2.544794	0.000000
16	C	5.600005	5.822432	5.080589	3.850454	2.769746
17	C	6.612243	6.876376	6.304579	5.119115	4.030294
18	H	5.877544	5.983313	4.934627	3.156844	2.555367
19	H	7.605085	7.805807	7.095622	5.564304	4.737035
20	H	6.644764	7.001055	6.698889	5.902952	4.600205
21	O	2.711137	2.039400	2.094358	4.590053	4.658119
22	H	3.398847	2.757908	2.163648	4.233570	4.639581

		16	17	18	19	20
16	C	0.000000				
17	C	1.326735	0.000000			
18	H	1.084998	2.137079	0.000000		
19	H	2.083310	1.081446	2.472896	0.000000	
20	H	2.121621	1.083512	3.107830	1.851164	0.000000
21	O	6.836628	8.044451	6.761833	8.909202	8.323646
22	H	6.953373	8.220356	6.727417	9.009039	8.615034

		21	22
21	O	0.000000	
22	H	0.962539	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.436137	-2.319873	-0.508740
2	6	0	-1.688374	-1.828278	-0.672071
3	7	0	-1.791238	-0.699549	0.135813
4	6	0	-0.609187	-0.507419	0.751666
5	7	0	0.218566	-1.497808	0.400172
6	6	0	1.652128	-1.527646	0.725354
7	6	0	2.498248	-0.989100	-0.441616
8	1	0	0.045585	-3.170226	-0.958727
9	1	0	-2.496183	-2.155197	-1.301276
10	1	0	1.799291	-0.899465	1.603745
11	1	0	1.932967	-2.550948	0.980884
12	1	0	2.425903	-1.663137	-1.300536
13	1	0	2.118820	-0.002732	-0.723561
14	35	0	0.457942	2.134482	-0.121236
15	1	0	-0.380452	0.297278	1.427232
16	6	0	-2.869291	0.225773	0.213945
17	6	0	-4.139355	-0.112002	0.032095
18	1	0	-2.523387	1.237117	0.400375
19	1	0	-4.902546	0.653607	0.062242
20	1	0	-4.459279	-1.131251	-0.148955
21	8	0	3.861591	-0.944100	-0.043183
22	1	0	4.079104	-0.036331	0.191606

Rotational constants (GHZ): 0.8111330 0.5713819 0.3534269
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 358 symmetry adapted cartesian basis functions of A symmetry.
There are 345 symmetry adapted basis functions of A symmetry.
345 basis functions, 553 primitive gaussians, 358 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 864.2033487301 Hartrees.
NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 345 RedAO= T EigKep= 6.75D-06 NBF= 345
NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345
Initial guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999035 -0.001531 0.000111 -0.043889 Ang= -5.03 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.33850265 A.U. after 12 cycles
NFock= 12 Conv=0.78D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000027307	-0.000094929	0.000050335
2	6	-0.000043955	-0.000027320	-0.000026165
3	7	0.000249918	0.000188197	-0.000069057
4	6	-0.000133228	-0.000258644	0.000319722
5	7	-0.000068994	0.000190017	-0.000038762
6	6	-0.000004477	-0.000078126	-0.000030138
7	6	-0.000000056	0.000040366	0.000376151
8	1	0.000042474	0.000039061	-0.000044382
9	1	0.000013792	0.000033646	-0.000011256
10	1	-0.000072918	0.000001174	-0.000019189
11	1	0.000016084	-0.000003092	0.000015123
12	1	-0.000091655	0.000000223	-0.000028210
13	1	-0.000010856	-0.000095702	-0.000596239
14	35	-0.000065857	0.000206302	0.000114615
15	1	0.000037203	-0.000061229	-0.000248988
16	6	-0.000034609	-0.000022614	0.000111361

17	6	0.000002869	-0.000011549	0.000035305
18	1	-0.000022752	-0.000041302	0.000020157
19	1	0.000035811	0.000000657	-0.000052332
20	1	-0.000004592	0.000021282	-0.000005874
21	8	0.000096717	0.000031101	0.000172445
22	1	0.000031776	-0.000057518	-0.000044623

Cartesian Forces: Max 0.000596239 RMS 0.000127967

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000550013 RMS 0.000110357
Search for a local minimum.
Step number 34 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 25 24 26 27 28
29 30 31 32 33
34
DE= 2.26D-05 DEPred=-7.52D-05 R=-3.00D-01
Trust test=-3.00D-01 RLast= 4.78D-01 DXMaxT set to 3.11D-01
ITU= -1 0 1 1 1 1 1 1 0 -1 1 1 1 1 1 0 -1 1 1 1
ITU= 1 1 1 1 1 1 1 1 1 0 0 -1 0 0
Eigenvalues --- 0.00011 0.00070 0.00171 0.00421 0.00878
Eigenvalues --- 0.00947 0.01284 0.01615 0.01783 0.02083
Eigenvalues --- 0.02239 0.02345 0.03064 0.03110 0.03571
Eigenvalues --- 0.04343 0.05025 0.05319 0.05953 0.06756
Eigenvalues --- 0.08883 0.09207 0.13993 0.14587 0.14808
Eigenvalues --- 0.15465 0.15909 0.15981 0.16014 0.16089
Eigenvalues --- 0.16888 0.17132 0.20582 0.22129 0.22986
Eigenvalues --- 0.23921 0.24829 0.25848 0.29630 0.33170
Eigenvalues --- 0.33801 0.33881 0.33921 0.34054 0.34225
Eigenvalues --- 0.34372 0.34774 0.36068 0.36295 0.36433
Eigenvalues --- 0.38988 0.43148 0.44637 0.46081 0.49413
Eigenvalues --- 0.53357 0.54773 0.56830 0.60647 3.37489
En-DIIS/RFO-DIIS IScMMF= 0 using points: 34 33 32 31 30
RFO step: Lambda=-3.51865033D-06.
DidBck=T Rises=F RFO-DIIS coefs: 0.08681 1.21685 -2.97612 4.33403 -1.66157
Iteration 1 RMS(Cart)= 0.02864019 RMS(Int)= 0.00056199
Iteration 2 RMS(Cart)= 0.00111473 RMS(Int)= 0.00006140

Iteration 3 RMS(Cart)= 0.00000132 RMS(Int)= 0.00006139

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00006139

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56087	0.00003	0.00031	0.00039	0.00076	2.56163
R2	2.62566	-0.00002	-0.00001	-0.00047	-0.00047	2.62520
R3	2.03323	0.00003	0.00013	-0.00004	0.00009	2.03333
R4	2.63024	0.00005	0.00023	-0.00023	0.00002	2.63026
R5	2.03120	0.00000	-0.00002	0.00001	-0.00001	2.03118
R6	2.54478	-0.00018	-0.00038	-0.00090	-0.00133	2.54344
R7	2.68881	0.00001	0.00014	0.00104	0.00118	2.68999
R8	2.52799	-0.00018	-0.00082	-0.00030	-0.00118	2.52682
R9	2.03200	-0.00025	0.00150	0.00180	0.00329	2.03529
R10	2.77843	-0.00011	0.00092	0.00077	0.00170	2.78013
R11	2.90783	0.00007	0.00012	-0.00009	0.00004	2.90786
R12	2.05957	-0.00002	0.00007	-0.00019	-0.00012	2.05946
R13	2.06258	0.00001	-0.00022	-0.00008	-0.00030	2.06228
R14	2.06776	0.00002	0.00025	0.00007	0.00032	2.06808
R15	2.06697	0.00013	0.00083	-0.00051	0.00032	2.06728
R16	2.68546	0.00017	-0.00080	-0.00042	-0.00122	2.68424
R17	5.24003	0.00021	-0.00044	-0.00612	-0.00655	5.23348
R18	2.50717	-0.00003	0.00004	-0.00022	-0.00018	2.50699
R19	2.05035	-0.00003	-0.00020	0.00012	-0.00008	2.05027
R20	2.04364	-0.00004	-0.00003	-0.00006	-0.00008	2.04356
R21	2.04754	-0.00001	-0.00011	-0.00002	-0.00013	2.04741
R22	1.81893	-0.00007	0.00058	-0.00008	0.00050	1.81943
A1	1.87510	-0.00008	-0.00027	-0.00004	-0.00029	1.87481
A2	2.27840	0.00004	0.00009	-0.00017	-0.00009	2.27832
A3	2.12966	0.00004	0.00017	0.00023	0.00040	2.13006
A4	1.86765	-0.00004	-0.00027	-0.00036	-0.00061	1.86704
A5	2.28457	0.00003	-0.00037	0.00002	-0.00035	2.28422
A6	2.13044	0.00002	0.00072	0.00029	0.00102	2.13145
A7	1.89260	0.00003	0.00019	0.00043	0.00052	1.89312
A8	2.23350	0.00005	0.00139	0.00035	0.00179	2.23528
A9	2.14977	-0.00008	-0.00079	-0.00035	-0.00111	2.14867
A10	1.89373	0.00001	0.00000	0.00010	0.00026	1.89399
A11	2.19052	0.00002	0.00014	-0.00044	0.00010	2.19062
A12	2.19874	-0.00003	-0.00181	0.00077	-0.00064	2.19811
A13	1.89477	0.00008	0.00043	0.00018	0.00052	1.89529
A14	2.20446	-0.00001	0.00133	0.00087	0.00224	2.20670
A15	2.16545	-0.00007	-0.00165	-0.00116	-0.00274	2.16270
A16	1.94046	0.00009	-0.00051	-0.00174	-0.00225	1.93821
A17	1.87361	-0.00012	-0.00120	0.00022	-0.00099	1.87263
A18	1.89830	0.00003	-0.00052	0.00005	-0.00047	1.89784

A19	1.91267	0.00015	0.00008	-0.00076	-0.00068	1.91198
A20	1.94356	-0.00017	0.00173	0.00151	0.00324	1.94680
A21	1.89331	0.00001	0.00033	0.00073	0.00107	1.89438
A22	1.92129	-0.00021	-0.00043	0.00130	0.00087	1.92215
A23	1.89690	0.00055	-0.00178	-0.00176	-0.00353	1.89337
A24	1.90285	-0.00018	-0.00083	0.00033	-0.00051	1.90234
A25	1.90734	-0.00021	0.00195	0.00057	0.00252	1.90986
A26	1.87865	0.00014	0.00103	0.00142	0.00245	1.88110
A27	1.95682	-0.00010	0.00007	-0.00177	-0.00171	1.95511
A28	2.58081	0.00035	0.00129	0.00006	0.00135	2.58216
A29	2.15581	-0.00003	0.00091	-0.00072	0.00019	2.15600
A30	1.95419	0.00003	0.00016	-0.00034	-0.00018	1.95401
A31	2.17250	0.00000	-0.00112	0.00116	0.00004	2.17254
A32	2.08462	0.00000	-0.00085	0.00047	-0.00038	2.08424
A33	2.14724	0.00001	0.00080	-0.00037	0.00043	2.14768
A34	2.05132	-0.00001	0.00005	-0.00010	-0.00005	2.05127
A35	1.89131	0.00006	-0.00090	-0.00030	-0.00119	1.89011
D1	0.00525	-0.00005	-0.00011	0.00064	0.00052	0.00576
D2	3.11166	-0.00005	0.00341	-0.00109	0.00232	3.11398
D3	-3.12882	0.00004	-0.00360	-0.00076	-0.00435	-3.13317
D4	-0.02241	0.00004	-0.00008	-0.00249	-0.00255	-0.02496
D5	-0.02870	0.00006	0.00207	0.00361	0.00568	-0.02302
D6	-2.97028	0.00005	0.00159	0.00434	0.00597	-2.96432
D7	3.10615	-0.00001	0.00519	0.00486	0.01005	3.11619
D8	0.16456	-0.00003	0.00471	0.00560	0.01033	0.17489
D9	0.01981	0.00001	-0.00187	-0.00463	-0.00650	0.01331
D10	3.03349	0.00004	0.00526	-0.00092	0.00436	3.03785
D11	-3.09040	0.00001	-0.00499	-0.00308	-0.00808	-3.09848
D12	-0.07672	0.00004	0.00214	0.00062	0.00277	-0.07394
D13	-0.03800	0.00003	0.00318	0.00693	0.01012	-0.02788
D14	3.12346	-0.00003	-0.02516	-0.01586	-0.04095	3.08251
D15	-3.05916	-0.00001	-0.00370	0.00338	-0.00033	-3.05949
D16	0.10230	-0.00007	-0.03204	-0.01941	-0.05139	0.05090
D17	0.56522	-0.00006	-0.02302	-0.00191	-0.02493	0.54029
D18	-2.53802	-0.00005	-0.02176	-0.00473	-0.02649	-2.56451
D19	-2.72146	-0.00002	-0.01484	0.00235	-0.01249	-2.73394
D20	0.45849	-0.00001	-0.01359	-0.00046	-0.01405	0.44444
D21	0.04128	-0.00006	-0.00325	-0.00653	-0.00979	0.03150
D22	2.98837	-0.00003	-0.00241	-0.00697	-0.00938	2.97899
D23	-3.12029	0.00000	0.02512	0.01637	0.04156	-3.07873
D24	-0.17320	0.00003	0.02596	0.01594	0.04197	-0.13123
D25	1.24028	-0.00021	0.01262	0.00685	0.01946	1.25974
D26	-2.95113	-0.00005	0.01166	0.00505	0.01671	-2.93442
D27	-0.90589	-0.00008	0.01113	0.00607	0.01719	-0.88870

D28	-1.67194	-0.00025	0.01180	0.00751	0.01932	-1.65262
D29	0.41984	-0.00009	0.01084	0.00571	0.01656	0.43641
D30	2.46508	-0.00012	0.01031	0.00672	0.01704	2.48212
D31	-1.16012	-0.00002	-0.01094	-0.00153	-0.01246	-1.17258
D32	0.92828	-0.00006	-0.00990	-0.00113	-0.01104	0.91725
D33	3.06600	0.00004	-0.01144	-0.00420	-0.01564	3.05036
D34	3.05465	-0.00002	-0.00918	-0.00025	-0.00943	3.04522
D35	-1.14014	-0.00007	-0.00815	0.00014	-0.00801	-1.14814
D36	0.99758	0.00004	-0.00968	-0.00293	-0.01261	0.98497
D37	0.95982	-0.00003	-0.01075	-0.00163	-0.01238	0.94743
D38	3.04821	-0.00008	-0.00972	-0.00124	-0.01096	3.03726
D39	-1.09726	0.00003	-0.01125	-0.00431	-0.01556	-1.11281
D40	0.18060	0.00014	0.05356	0.04263	0.09620	0.27680
D41	2.27768	0.00009	0.05312	0.04349	0.09662	2.37429
D42	-1.92410	0.00006	0.05574	0.04453	0.10027	-1.82383
D43	-1.75761	-0.00027	-0.00916	0.00438	-0.00478	-1.76239
D44	2.44182	0.00000	-0.00877	0.00183	-0.00694	2.43488
D45	0.34364	0.00023	-0.01190	0.00127	-0.01063	0.33301
D46	-3.09342	0.00005	0.00140	-0.00251	-0.00111	-3.09453
D47	0.04734	-0.00001	-0.00025	-0.00068	-0.00092	0.04641
D48	0.00503	0.00004	0.00002	0.00062	0.00064	0.00567
D49	-3.13741	-0.00002	-0.00162	0.00245	0.00083	-3.13658

Item	Value	Threshold	Converged?
Maximum Force	0.000550	0.000450	NO
RMS Force	0.000110	0.000300	YES
Maximum Displacement	0.171979	0.001800	NO
RMS Displacement	0.028298	0.001200	NO

Predicted change in Energy=-1.759400D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.469886	-2.054089	-1.301275
2	6	0	-1.756924	-1.661323	-1.464990
3	7	0	-2.091055	-0.891125	-0.354822
4	6	0	-1.014460	-0.812340	0.449087
5	7	0	-0.026001	-1.531226	-0.093202
6	6	0	1.360792	-1.521557	0.397801
7	6	0	2.216855	-0.509630	-0.383858
8	1	0	0.164521	-2.651825	-1.932141
9	1	0	-2.447852	-1.833322	-2.270192

10	1	0	1.330115	-1.237695	1.449555
11	1	0	1.766309	-2.531948	0.322773
12	1	0	2.335391	-0.838269	-1.420976
13	1	0	1.711023	0.460178	-0.365033
14	35	0	-0.226634	2.075082	0.778360
15	1	0	-0.953808	-0.239621	1.359203
16	6	0	-3.290404	-0.160584	-0.122076
17	6	0	-4.474938	-0.527111	-0.593788
18	1	0	-3.110417	0.742635	0.451444
19	1	0	-5.336227	0.101366	-0.413143
20	1	0	-4.629342	-1.437439	-1.160632
21	8	0	3.509408	-0.447566	0.201885
22	1	0	3.553887	0.340529	0.753173

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.355556	0.000000			
3	N	2.208267	1.391876	0.000000		
4	C	2.214107	2.221647	1.345932	0.000000	
5	N	1.389193	2.212424	2.177756	1.337134	0.000000
6	C	2.553787	3.634511	3.588750	2.479403	1.471181
7	C	3.231963	4.276232	4.324866	3.350646	2.481641
8	H	1.075989	2.211623	3.267356	3.231710	2.161882
9	H	2.213569	1.074856	2.164181	3.239058	3.270460
10	H	3.387266	4.266596	3.883335	2.584356	2.074925
11	H	2.804719	4.045646	4.246255	3.271954	2.094482
12	H	3.059759	4.174493	4.553339	3.836575	2.796309
13	H	3.457520	4.211570	4.035086	3.116143	2.656470
14	Br	4.629698	4.618996	3.682194	3.011029	3.715553
15	H	3.256473	3.262254	2.157701	1.077032	2.153729
16	C	3.595996	2.531244	1.423482	2.435351	3.540596
17	C	4.344265	3.071324	2.423327	3.625445	4.588232
18	H	4.226830	3.359119	2.087664	2.609787	3.870492
19	H	5.395927	4.126120	3.394051	4.500663	5.564729
20	H	4.207269	2.897162	2.718582	4.006160	4.726410
21	O	4.546998	5.655611	5.645516	4.545279	3.709517
22	H	5.113287	6.093633	5.883026	4.721374	4.127399

		6	7	8	9	10
6	C	0.000000				
7	C	1.538776	0.000000			
8	H	2.852578	3.346379	0.000000		
9	H	4.660596	5.202875	2.758391	0.000000	
10	H	1.089819	2.162819	3.846328	5.335197	0.000000

11	H	1.091313	2.189084	2.768525	4.997069	1.770591
12	H	2.173632	1.094381	2.874534	4.958902	3.067584
13	H	2.152173	1.093959	3.812093	5.117227	2.514079
14	Br	3.949754	3.741941	5.462917	5.431675	3.721352
15	H	2.815142	3.628259	4.231115	4.236102	2.494117
16	C	4.874027	5.524514	4.628080	2.849973	4.997938
17	C	6.002326	6.695108	5.275432	2.936936	6.195065
18	H	5.012100	5.535857	5.284795	3.805502	4.963493
19	H	6.938412	7.577810	6.336059	3.941364	7.050024
20	H	6.190112	6.952310	5.005106	2.479263	6.509079
21	O	2.410061	1.420437	4.538843	6.597002	2.632547
22	H	2.898848	1.950196	5.258602	7.063090	2.814409

		11	12	13	14	15
11	H	0.000000				
12	H	2.496610	0.000000			
13	H	3.070659	1.786285	0.000000		
14	Br	5.040249	4.459671	2.769436	0.000000	
15	H	3.705129	4.348172	3.250236	2.494797	0.000000
16	C	5.602820	5.813429	5.045656	3.898163	2.767692
17	C	6.619110	6.867433	6.268427	5.167425	4.036730
18	H	5.875534	5.971770	4.898234	3.193507	2.537680
19	H	7.610645	7.794380	7.056542	5.605637	4.739523
20	H	6.656034	6.995304	6.665895	5.956620	4.614530
21	O	2.719864	2.040747	2.092746	4.544677	4.615509
22	H	3.410543	2.757032	2.158900	4.159525	4.585102

		16	17	18	19	20
16	C	0.000000				
17	C	1.326641	0.000000			
18	H	1.084954	2.136980	0.000000		
19	H	2.082962	1.081403	2.472441	0.000000	
20	H	2.121724	1.083443	3.107836	1.851039	0.000000
21	O	6.813571	8.024289	6.730598	8.883966	8.311171
22	H	6.918200	8.187132	6.683238	8.969482	8.590056

		21	22
21	O	0.000000	
22	H	0.962803	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.540904	-2.343398	-0.467334
2	6	0	-1.774512	-1.808553	-0.639627
3	7	0	-1.826232	-0.650054	0.130129
4	6	0	-0.636220	-0.488465	0.737824
5	7	0	0.151621	-1.517688	0.409290
6	6	0	1.587176	-1.585623	0.723834
7	6	0	2.436254	-1.085610	-0.458065
8	1	0	-0.097503	-3.228787	-0.888328
9	1	0	-2.599520	-2.125657	-1.251284
10	1	0	1.759197	-0.949017	1.591502
11	1	0	1.839096	-2.613070	0.991886
12	1	0	2.346616	-1.774010	-1.304080
13	1	0	2.071993	-0.097166	-0.753087
14	35	0	0.567310	2.137609	-0.111614
15	1	0	-0.358870	0.347122	1.358202
16	6	0	-2.867406	0.318845	0.189200
17	6	0	-4.149035	0.029394	0.005839
18	1	0	-2.482336	1.317968	0.364133
19	1	0	-4.880922	0.825329	0.021996
20	1	0	-4.508957	-0.978513	-0.162772
21	8	0	3.801303	-1.055092	-0.066465
22	1	0	4.035070	-0.145136	0.144063

Rotational constants (GHZ): 0.7998659 0.5710415 0.3503022
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 358 symmetry adapted cartesian basis functions of A symmetry.
There are 345 symmetry adapted basis functions of A symmetry.
345 basis functions, 553 primitive gaussians, 358 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 862.0406804295 Hartrees.
NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 345 RedAO= T EigKep= 6.60D-06 NBF= 345
NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345
Initial guess from the checkpoint file: "."
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999822 0.001251 -0.000126 0.018806 Ang= 2.16 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Keep R1 ints in memory in canonical form, NReq=1804729152.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3032.33851541 A.U. after 12 cycles

NFock= 12 Conv=0.24D-08 -V/T= 2.0017

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000053465	-0.000230198	0.000142704
2	6	-0.000030201	-0.000031988	0.000018873
3	7	0.000058100	0.000092415	-0.000132881
4	6	0.000006399	-0.000186156	0.000017298
5	7	-0.000053530	0.000163526	0.000015378
6	6	-0.000280764	-0.000191205	-0.000053348
7	6	-0.000254088	-0.000008639	0.000610828
8	1	0.000119329	0.000144854	-0.000105665
9	1	0.000015816	0.000018638	-0.000010502
10	1	-0.000020629	-0.000028005	-0.000031984
11	1	0.000058913	-0.000026816	0.000002203
12	1	-0.000030991	0.000013802	0.000039674
13	1	0.000234537	0.000012771	-0.000788539
14	35	-0.000159253	0.000271074	0.000203194
15	1	0.000087768	0.000105049	-0.000038883
16	6	0.000163979	-0.000163317	0.000031949
17	6	0.000024329	0.000084596	0.000082208
18	1	-0.000119757	-0.000060356	0.000058732

19	1	0.000007480	-0.000011594	-0.000039273
20	1	-0.000033437	0.000005780	-0.000023204
21	8	0.000254788	0.000190747	0.000054283
22	1	0.000004677	-0.000164978	-0.000053044

Cartesian Forces: Max 0.000788539 RMS 0.000167456

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000683517 RMS 0.000127915
Search for a local minimum.
Step number 35 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 25 26 27 28 29
30 31 32 33 34
35
DE= -1.28D-05 DEPred=-1.76D-05 R= 7.25D-01
TightC=F SS= 1.41D+00 RLast= 2.06D-01 DXNew= 5.2346D-01 6.1784D-01
Trust test= 7.25D-01 RLast= 2.06D-01 DXMaxT set to 5.23D-01
ITU= 1 -1 0 1 1 1 1 1 1 0 -1 1 1 1 1 1 0 -1 1 1
ITU= 1 1 1 1 1 1 1 1 1 1 0 0 -1 0 0
Eigenvalues --- -0.03692 0.00002 0.00148 0.00282 0.00519
Eigenvalues --- 0.00974 0.01145 0.01540 0.01766 0.02045
Eigenvalues --- 0.02082 0.02326 0.03061 0.03073 0.03464
Eigenvalues --- 0.04026 0.04855 0.05262 0.05795 0.06103
Eigenvalues --- 0.08634 0.09192 0.12314 0.14019 0.14426
Eigenvalues --- 0.15395 0.15903 0.15968 0.16006 0.16047
Eigenvalues --- 0.16597 0.17261 0.19950 0.21582 0.23016
Eigenvalues --- 0.24048 0.24630 0.25007 0.29192 0.33085
Eigenvalues --- 0.33619 0.33879 0.33902 0.34025 0.34229
Eigenvalues --- 0.34331 0.34789 0.35978 0.36288 0.36364
Eigenvalues --- 0.36754 0.43026 0.44821 0.45689 0.49700
Eigenvalues --- 0.53202 0.54631 0.57282 0.60757 1.44103
Eigenvalue 2 is 1.72D-05 Eigenvector:

	D42	D40	D41	D16	D23
1	-0.49388	-0.47230	-0.47156	0.24999	-0.19562
	D14	D24	D18	D17	D28
1	0.19229	-0.18575	0.13281	0.12678	-0.08489

Use linear search instead of GDIIS.
RFO step: Lambda=-3.69302955D-02 EMin=-3.69247732D-02

I= 1 Eig= -3.69D-02 Dot1= 2.71D-04

I= 1 Stepn= 6.00D-01 RXN= 6.00D-01 EDone=F

Mixed 1 eigenvectors in step. Raw Step.Grad= 2.71D-04.

RFO eigenvector is Hessian eigenvector with negative curvature.

Taking step of 6.00D-01 in eigenvector direction(s). Step.Grad= -1.95D-05.

Skip linear search -- no minimum in search direction.

Iteration 1 RMS(Cart)= 0.12836480 RMS(Int)= 0.00860283

Iteration 2 RMS(Cart)= 0.01139400 RMS(Int)= 0.00046199

Iteration 3 RMS(Cart)= 0.00013110 RMS(Int)= 0.00045788

Iteration 4 RMS(Cart)= 0.00000002 RMS(Int)= 0.00045788

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56163	0.00001	0.00000	-0.00750	-0.00734	2.55429
R2	2.62520	-0.00003	0.00000	0.00722	0.00721	2.63241
R3	2.03333	0.00005	0.00000	0.00515	0.00515	2.03847
R4	2.63026	0.00001	0.00000	0.00587	0.00597	2.63623
R5	2.03118	0.00000	0.00000	0.00048	0.00048	2.03166
R6	2.54344	-0.00006	0.00000	0.02831	0.02820	2.57165
R7	2.68999	-0.00008	0.00000	-0.02140	-0.02140	2.66859
R8	2.52682	-0.00023	0.00000	-0.00410	-0.00425	2.52257
R9	2.03529	0.00003	0.00000	0.05848	0.05848	2.09378
R10	2.78013	-0.00018	0.00000	-0.03051	-0.03051	2.74962
R11	2.90786	0.00019	0.00000	0.02244	0.02244	2.93030
R12	2.05946	-0.00004	0.00000	0.00294	0.00294	2.06240
R13	2.06228	0.00005	0.00000	0.00639	0.00639	2.06867
R14	2.06808	-0.00004	0.00000	-0.01228	-0.01228	2.05580
R15	2.06728	0.00020	0.00000	0.02387	0.02387	2.09115
R16	2.68424	0.00024	0.00000	-0.00205	-0.00205	2.68219
R17	5.23348	0.00035	0.00000	0.29123	0.29123	5.52470
R18	2.50699	-0.00003	0.00000	0.00533	0.00533	2.51232
R19	2.05027	-0.00004	0.00000	0.00205	0.00205	2.05231
R20	2.04356	-0.00002	0.00000	0.00667	0.00667	2.05023
R21	2.04741	0.00001	0.00000	0.00619	0.00619	2.05360
R22	1.81943	-0.00017	0.00000	0.00494	0.00494	1.82437
A1	1.87481	-0.00005	0.00000	0.00451	0.00411	1.87891
A2	2.27832	0.00006	0.00000	0.01054	0.01066	2.28897
A3	2.13006	0.00000	0.00000	-0.01508	-0.01496	2.11510
A4	1.86704	-0.00005	0.00000	0.00050	0.00019	1.86723
A5	2.28422	0.00002	0.00000	-0.00203	-0.00196	2.28226
A6	2.13145	0.00003	0.00000	0.00211	0.00218	2.13363
A7	1.89312	0.00002	0.00000	-0.00305	-0.00366	1.88946
A8	2.23528	0.00012	0.00000	0.01695	0.01701	2.25229
A9	2.14867	-0.00014	0.00000	-0.01708	-0.01692	2.13174
A10	1.89399	-0.00001	0.00000	-0.00718	-0.00795	1.88604

A11	2.19062	0.00005	0.00000	0.02515	0.02547	2.21609
A12	2.19811	-0.00005	0.00000	-0.01745	-0.01714	2.18096
A13	1.89529	0.00009	0.00000	0.00273	0.00187	1.89716
A14	2.20670	-0.00007	0.00000	-0.00647	-0.00640	2.20030
A15	2.16270	-0.00001	0.00000	0.01081	0.01092	2.17363
A16	1.93821	0.00020	0.00000	0.06387	0.06370	2.00191
A17	1.87263	-0.00007	0.00000	0.01731	0.01710	1.88973
A18	1.89784	-0.00004	0.00000	-0.02291	-0.02242	1.87541
A19	1.91198	0.00007	0.00000	-0.02016	-0.02148	1.89050
A20	1.94680	-0.00018	0.00000	-0.02335	-0.02338	1.92343
A21	1.89438	0.00002	0.00000	-0.01478	-0.01527	1.87910
A22	1.92215	-0.00026	0.00000	-0.01531	-0.01574	1.90641
A23	1.89337	0.00068	0.00000	0.06735	0.06646	1.95982
A24	1.90234	-0.00007	0.00000	0.02855	0.02788	1.93022
A25	1.90986	-0.00021	0.00000	0.01502	0.01392	1.92378
A26	1.88110	0.00006	0.00000	-0.07921	-0.07933	1.80177
A27	1.95511	-0.00022	0.00000	-0.01756	-0.01976	1.93535
A28	2.58216	0.00017	0.00000	-0.15521	-0.15521	2.42695
A29	2.15600	0.00011	0.00000	0.05328	0.05315	2.20915
A30	1.95401	0.00005	0.00000	0.01873	0.01860	1.97261
A31	2.17254	-0.00016	0.00000	-0.07102	-0.07116	2.10139
A32	2.08424	0.00000	0.00000	-0.01610	-0.01613	2.06811
A33	2.14768	0.00004	0.00000	0.02110	0.02108	2.16875
A34	2.05127	-0.00004	0.00000	-0.00499	-0.00502	2.04625
A35	1.89011	0.00006	0.00000	-0.01539	-0.01539	1.87473
D1	0.00576	-0.00003	0.00000	0.01546	0.01518	0.02094
D2	3.11398	-0.00003	0.00000	0.03587	0.03562	-3.13359
D3	-3.13317	0.00008	0.00000	0.03429	0.03426	-3.09891
D4	-0.02496	0.00007	0.00000	0.05471	0.05470	0.02974
D5	-0.02302	0.00000	0.00000	-0.05582	-0.05604	-0.07906
D6	-2.96432	-0.00002	0.00000	-0.09515	-0.09515	-3.05947
D7	3.11619	-0.00009	0.00000	-0.07266	-0.07279	3.04340
D8	0.17489	-0.00011	0.00000	-0.11199	-0.11190	0.06299
D9	0.01331	0.00004	0.00000	0.02959	0.02964	0.04296
D10	3.03785	0.00004	0.00000	-0.00221	-0.00240	3.03545
D11	-3.09848	0.00004	0.00000	0.01145	0.01143	-3.08705
D12	-0.07394	0.00005	0.00000	-0.02034	-0.02061	-0.09455
D13	-0.02788	-0.00003	0.00000	-0.06476	-0.06466	-0.09254
D14	3.08251	-0.00005	0.00000	-0.04784	-0.04748	3.03503
D15	-3.05949	-0.00006	0.00000	-0.03760	-0.03798	-3.09747
D16	0.05090	-0.00008	0.00000	-0.02068	-0.02080	0.03010
D17	0.54029	-0.00008	0.00000	-0.04034	-0.03989	0.50040
D18	-2.56451	-0.00009	0.00000	-0.06697	-0.06740	-2.63191
D19	-2.73394	-0.00006	0.00000	-0.07506	-0.07463	-2.80857

D20	0.44444	-0.00007	0.00000	-0.10169	-0.10213	0.34231
D21	0.03150	0.00002	0.00000	0.07446	0.07419	0.10569
D22	2.97899	0.00004	0.00000	0.11017	0.11015	3.08914
D23	-3.07873	0.00004	0.00000	0.05649	0.05649	-3.02223
D24	-0.13123	0.00005	0.00000	0.09220	0.09245	-0.03878
D25	1.25974	-0.00015	0.00000	0.11352	0.11296	1.37270
D26	-2.93442	0.00000	0.00000	0.13662	0.13713	-2.79729
D27	-0.88870	-0.00004	0.00000	0.11656	0.11647	-0.77223
D28	-1.65262	-0.00019	0.00000	0.06980	0.06934	-1.58328
D29	0.43641	-0.00004	0.00000	0.09291	0.09351	0.52991
D30	2.48212	-0.00007	0.00000	0.07284	0.07285	2.55497
D31	-1.17258	0.00001	0.00000	-0.00710	-0.00710	-1.17968
D32	0.91725	0.00002	0.00000	0.04342	0.04274	0.95999
D33	3.05036	0.00013	0.00000	0.08103	0.08165	3.13201
D34	3.04522	-0.00007	0.00000	-0.05480	-0.05448	2.99073
D35	-1.14814	-0.00006	0.00000	-0.00428	-0.00464	-1.15278
D36	0.98497	0.00005	0.00000	0.03333	0.03427	1.01923
D37	0.94743	-0.00003	0.00000	-0.00797	-0.00823	0.93920
D38	3.03726	-0.00002	0.00000	0.04254	0.04161	3.07887
D39	-1.11281	0.00009	0.00000	0.08016	0.08052	-1.03230
D40	0.27680	0.00020	0.00000	0.00256	0.00180	0.27860
D41	2.37429	0.00017	0.00000	0.03343	0.03412	2.40842
D42	-1.82383	-0.00003	0.00000	-0.06682	-0.06675	-1.89058
D43	-1.76239	-0.00030	0.00000	0.03625	0.03658	-1.72580
D44	2.43488	0.00001	0.00000	0.08423	0.08517	2.52005
D45	0.33301	0.00037	0.00000	0.12839	0.12711	0.46012
D46	-3.09453	0.00002	0.00000	-0.03534	-0.03493	-3.12946
D47	0.04641	-0.00003	0.00000	-0.02183	-0.02143	0.02499
D48	0.00567	0.00004	0.00000	-0.00304	-0.00345	0.00222
D49	-3.13658	-0.00001	0.00000	0.01046	0.01006	-3.12652

Item	Value	Threshold	Converged?
Maximum Force	0.000684	0.000450	NO
RMS Force	0.000128	0.000300	YES
Maximum Displacement	0.605059	0.001800	NO
RMS Displacement	0.128399	0.001200	NO

Predicted change in Energy=-6.908740D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.491244	-2.081851	-1.306368

2	6	0	-1.793827	-1.756895	-1.463521
3	7	0	-2.133939	-0.913572	-0.405573
4	6	0	-1.018365	-0.697951	0.343383
5	7	0	-0.039165	-1.464075	-0.142558
6	6	0	1.328761	-1.467641	0.353316
7	6	0	2.278243	-0.468687	-0.357383
8	1	0	0.169952	-2.678358	-1.915157
9	1	0	-2.499627	-2.034641	-2.225466
10	1	0	1.307864	-1.223573	1.416844
11	1	0	1.711252	-2.488544	0.254243
12	1	0	2.431008	-0.789283	-1.385669
13	1	0	1.891288	0.567763	-0.333287
14	35	0	-0.111503	2.144410	1.098543
15	1	0	-0.915021	-0.003153	1.200235
16	6	0	-3.337803	-0.210786	-0.179765
17	6	0	-4.552014	-0.568246	-0.586439
18	1	0	-3.194165	0.709009	0.379540
19	1	0	-5.389161	0.079513	-0.348374
20	1	0	-4.769132	-1.479649	-1.137040
21	8	0	3.581532	-0.535379	0.200789
22	1	0	3.665413	0.194710	0.826859

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.351672	0.000000			
3	N	2.207885	1.395035	0.000000		
4	C	2.216915	2.233294	1.360857	0.000000	
5	N	1.393010	2.215744	2.181813	1.334885	0.000000
6	C	2.538548	3.624241	3.587924	2.470126	1.455035
7	C	3.342593	4.411889	4.434815	3.378055	2.531269
8	H	1.078714	2.215739	3.271273	3.230342	2.158777
9	H	2.209202	1.075108	2.168533	3.252670	3.273824
10	H	3.374806	4.266312	3.906829	2.615328	2.074624
11	H	2.729815	3.971347	4.207301	3.265727	2.066626
12	H	3.196338	4.334924	4.670629	3.859552	2.846476
13	H	3.693751	4.501281	4.289759	3.244379	2.809162
14	Br	4.877405	4.961306	3.962810	3.077610	3.816639
15	H	3.283844	3.308097	2.212067	1.107980	2.168988
16	C	3.587899	2.534234	1.412156	2.427098	3.528899
17	C	4.393081	3.128859	2.449296	3.656237	4.622267
18	H	4.235206	3.382085	2.091232	2.591322	3.866382
19	H	5.438643	4.188362	3.403816	4.492976	5.572027
20	H	4.323383	3.005976	2.792800	4.107426	4.833407

21	O	4.609838	5.758169	5.759975	4.604978	3.753640
22	H	5.197228	6.233610	6.031555	4.792533	4.173156

		6	7	8	9	10
6	C	0.000000				
7	C	1.550651	0.000000			
8	H	2.820398	3.428439	0.000000		
9	H	4.650609	5.363766	2.763570	0.000000	
10	H	1.091374	2.158557	3.809655	5.331158	0.000000
11	H	1.094695	2.185266	2.667945	4.907798	1.764799
12	H	2.167761	1.087884	2.993549	5.154352	3.050269
13	H	2.220524	1.106590	4.000326	5.443619	2.571424
14	Br	3.959373	3.828691	5.693917	5.849499	3.668682
15	H	2.810081	3.583270	4.247300	4.286414	2.545105
16	C	4.862168	5.624769	4.626537	2.865986	5.015687
17	C	6.022920	6.834821	5.339947	3.008158	6.227421
18	H	5.019498	5.645996	5.296902	3.846564	5.007908
19	H	6.929396	7.686981	6.400344	4.042589	7.047281
20	H	6.277388	7.162080	5.141684	2.577467	6.596800
21	O	2.442817	1.419355	4.550655	6.716770	2.668701
22	H	2.906474	1.940816	5.290691	7.231487	2.813831

		11	12	13	14	15
11	H	0.000000				
12	H	2.468775	0.000000			
13	H	3.117469	1.800105	0.000000		
14	Br	5.049707	4.608929	2.923547	0.000000	
15	H	3.737563	4.301257	3.248539	2.295215	0.000000
16	C	5.556032	5.921828	5.288960	4.194047	2.795959
17	C	6.604755	7.032086	6.547576	5.469534	4.091363
18	H	5.856890	6.083044	5.137111	3.475651	2.524919
19	H	7.574558	7.936362	7.296818	5.849021	4.735288
20	H	6.704394	7.237433	7.014207	6.310716	4.743107
21	O	2.704748	1.976113	2.087842	4.650348	4.636933
22	H	3.368454	2.717955	2.152353	4.259136	4.599884

		16	17	18	19	20
16	C	0.000000				
17	C	1.329462	0.000000			
18	H	1.086037	2.099583	0.000000		
19	H	2.078647	1.084934	2.396691	0.000000	
20	H	2.138946	1.086719	3.093664	1.854027	0.000000
21	O	6.937390	8.171621	6.891337	9.008497	8.509701
22	H	7.086801	8.372910	6.893360	9.131251	8.820539

		21	22
21	O	0.000000	
22	H	0.965417	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.870885	-2.359982	-0.352324
2	6	0	-2.072039	-1.761830	-0.514990
3	7	0	-1.989137	-0.509103	0.093226
4	6	0	-0.723201	-0.347478	0.565680
5	7	0	-0.061560	-1.491272	0.376243
6	6	0	1.343557	-1.694065	0.695066
7	6	0	2.323096	-1.380903	-0.465515
8	1	0	-0.499902	-3.312610	-0.696558
9	1	0	-2.964124	-2.101454	-1.009659
10	1	0	1.598359	-1.053604	1.541223
11	1	0	1.460219	-2.733452	1.018210
12	1	0	2.184191	-2.112256	-1.258812
13	1	0	2.190104	-0.356418	-0.862106
14	35	0	0.929730	2.165126	-0.087253
15	1	0	-0.292568	0.567626	1.018184
16	6	0	-2.932806	0.541443	0.098488
17	6	0	-4.253342	0.420602	0.003341
18	1	0	-2.475380	1.522847	0.182661
19	1	0	-4.857364	1.321821	0.009829
20	1	0	-4.777097	-0.528749	-0.069944
21	8	0	3.665500	-1.595247	-0.057376
22	1	0	4.037619	-0.735294	0.175085

Rotational constants (GHZ): 0.7555616 0.5399151 0.3263380
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 358 symmetry adapted cartesian basis functions of A symmetry.
There are 345 symmetry adapted basis functions of A symmetry.
345 basis functions, 553 primitive gaussians, 358 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 846.3761428607 Hartrees.
NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.

Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 345 RedAO= T EigKep= 6.37D-06 NBF= 345
NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345
Initial guess from the checkpoint file: "."
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.998230 0.005865 0.001744 0.059152 Ang= 6.82 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.33438489 A.U. after 13 cycles
NFock= 13 Conv=0.92D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.005452811	-0.003868380	0.002140193
2	6	-0.004166114	0.000539146	0.001236871
3	7	0.014894365	0.006273009	0.000162174
4	6	-0.009865647	-0.007364578	0.012244900
5	7	-0.004891959	0.009727670	-0.011459767
6	6	0.014393804	0.001543416	0.008322880
7	6	0.000813064	0.002800576	-0.008658596
8	1	-0.002404552	-0.000673708	0.001084033
9	1	-0.000049229	0.000637684	-0.000291000
10	1	-0.002349424	-0.000403522	-0.000459912

11	1	0.000816589	0.002456011	-0.000040291
12	1	-0.006571956	0.001183852	-0.006478584
13	1	-0.002599378	-0.010456745	0.000799372
14	35	0.000755525	0.001114297	0.000295646
15	1	-0.002390654	-0.005195725	-0.010826378
16	6	-0.010244369	0.007106226	0.003661335
17	6	0.001298519	-0.003763213	-0.001757426
18	1	0.003758984	-0.001683648	0.000152408
19	1	0.001850673	-0.001344722	-0.001249542
20	1	0.001312806	0.001523101	0.000898302
21	8	-0.001493705	0.002876205	0.010342481
22	1	0.001679848	-0.003026951	-0.000119099

Cartesian Forces: Max 0.014894365 RMS 0.005456283

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.011854341 RMS 0.003224136
Search for a local minimum.
Step number 36 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 25 29 30 31 32
34 35 36 33
ITU= 0 1 -1 0 1 1 1 1 1 1 0 -1 1 1 1 1 1 0 -1 1
ITU= 1 1 1 1 1 1 1 1 1 1 1 0 0 -1 0 0
Use linear search instead of GDIIS.
Energy rises -- skip Quadratic/GDIIS search.
Quartic linear search produced a step of -0.94865.
Iteration 1 RMS(Cart)= 0.10300814 RMS(Int)= 0.01146804
Iteration 2 RMS(Cart)= 0.02059549 RMS(Int)= 0.00031860
Iteration 3 RMS(Cart)= 0.00047674 RMS(Int)= 0.00002458
Iteration 4 RMS(Cart)= 0.00000029 RMS(Int)= 0.00002458

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55429	0.00183	0.00718	0.00000	0.00718	2.56147
R2	2.63241	-0.00181	-0.00689	0.00000	-0.00689	2.62552
R3	2.03847	-0.00171	-0.00466	0.00000	-0.00466	2.03382
R4	2.63623	-0.00118	-0.00531	0.00000	-0.00532	2.63092
R5	2.03166	0.00007	-0.00046	0.00000	-0.00046	2.03120
R6	2.57165	-0.01108	-0.02729	0.00000	-0.02729	2.54436
R7	2.66859	0.00290	0.02109	0.00000	0.02109	2.68968

R8	2.52257	0.00025	0.00279	0.00000	0.00280	2.52536
R9	2.09378	-0.01185	-0.05228	0.00000	-0.05228	2.04150
R10	2.74962	0.00649	0.02986	0.00000	0.02986	2.77948
R11	2.93030	-0.00633	-0.02049	0.00000	-0.02049	2.90982
R12	2.06240	-0.00049	-0.00248	0.00000	-0.00248	2.05992
R13	2.06867	-0.00200	-0.00636	0.00000	-0.00636	2.06232
R14	2.05580	0.00485	0.01163	0.00000	0.01163	2.06743
R15	2.09115	-0.00808	-0.02136	0.00000	-0.02136	2.06979
R16	2.68219	0.00420	-0.00022	0.00000	-0.00022	2.68197
R17	5.52470	0.00023	-0.26700	0.00000	-0.26700	5.25770
R18	2.51232	-0.00246	-0.00494	0.00000	-0.00494	2.50738
R19	2.05231	-0.00085	-0.00201	0.00000	-0.00201	2.05031
R20	2.05023	-0.00251	-0.00621	0.00000	-0.00621	2.04402
R21	2.05360	-0.00199	-0.00588	0.00000	-0.00588	2.04772
R22	1.82437	-0.00221	-0.00329	0.00000	-0.00329	1.82108
A1	1.87891	-0.00268	-0.00432	0.00000	-0.00429	1.87462
A2	2.28897	0.00006	-0.00988	0.00000	-0.00988	2.27909
A3	2.11510	0.00259	0.01438	0.00000	0.01437	2.12947
A4	1.86723	-0.00044	-0.00059	0.00000	-0.00058	1.86665
A5	2.28226	0.00046	0.00140	0.00000	0.00139	2.28365
A6	2.13363	-0.00002	-0.00103	0.00000	-0.00103	2.13260
A7	1.88946	0.00190	0.00392	0.00000	0.00394	1.89340
A8	2.25229	-0.00309	-0.01422	0.00000	-0.01421	2.23808
A9	2.13174	0.00136	0.01476	0.00000	0.01476	2.14650
A10	1.88604	0.00126	0.00731	0.00000	0.00737	1.89341
A11	2.21609	-0.00276	-0.02395	0.00000	-0.02393	2.19216
A12	2.18096	0.00145	0.01341	0.00000	0.01344	2.19440
A13	1.89716	0.00043	-0.00092	0.00000	-0.00089	1.89627
A14	2.20030	-0.00052	0.00866	0.00000	0.00866	2.20896
A15	2.17363	0.00028	-0.01298	0.00000	-0.01299	2.16064
A16	2.00191	-0.00737	-0.06009	0.00000	-0.06009	1.94182
A17	1.88973	0.00063	-0.01800	0.00000	-0.01799	1.87174
A18	1.87541	0.00348	0.01998	0.00000	0.01996	1.89537
A19	1.89050	0.00430	0.02051	0.00000	0.02058	1.91108
A20	1.92343	-0.00002	0.02452	0.00000	0.02453	1.94795
A21	1.87910	-0.00075	0.01456	0.00000	0.01459	1.89369
A22	1.90641	0.00060	0.01452	0.00000	0.01454	1.92095
A23	1.95982	0.00014	-0.06511	0.00000	-0.06507	1.89475
A24	1.93022	-0.00776	-0.02540	0.00000	-0.02537	1.90485
A25	1.92378	-0.00203	-0.00888	0.00000	-0.00883	1.91496
A26	1.80177	0.00658	0.07357	0.00000	0.07358	1.87535
A27	1.93535	0.00290	0.01756	0.00000	0.01767	1.95302
A28	2.42695	0.00517	0.14697	0.00000	0.14697	2.57391
A29	2.20915	-0.00825	-0.04867	0.00000	-0.04867	2.16048

A30	1.97261	0.00002	-0.01664	0.00000	-0.01664	1.95597
A31	2.10139	0.00823	0.06482	0.00000	0.06482	2.16621
A32	2.06811	0.00103	0.01378	0.00000	0.01378	2.08189
A33	2.16875	-0.00146	-0.01851	0.00000	-0.01851	2.15025
A34	2.04625	0.00044	0.00479	0.00000	0.00480	2.05105
A35	1.87473	0.00440	0.01227	0.00000	0.01227	1.88699
D1	0.02094	-0.00106	-0.01420	0.00000	-0.01418	0.00676
D2	-3.13359	-0.00140	-0.02729	0.00000	-0.02727	3.12232
D3	-3.09891	0.00026	-0.03843	0.00000	-0.03843	-3.13734
D4	0.02974	-0.00008	-0.05151	0.00000	-0.05152	-0.02177
D5	-0.07906	0.00340	0.05756	0.00000	0.05756	-0.02150
D6	-3.05947	0.00216	0.09056	0.00000	0.09056	-2.96891
D7	3.04340	0.00221	0.07894	0.00000	0.07894	3.12234
D8	0.06299	0.00097	0.11194	0.00000	0.11193	0.17492
D9	0.04296	-0.00133	-0.03282	0.00000	-0.03283	0.01013
D10	3.03545	0.00019	0.00805	0.00000	0.00805	3.04350
D11	-3.08705	-0.00103	-0.02114	0.00000	-0.02115	-3.10820
D12	-0.09455	0.00049	0.01972	0.00000	0.01973	-0.07482
D13	-0.09254	0.00338	0.06884	0.00000	0.06884	-0.02370
D14	3.03503	-0.00081	0.00079	0.00000	0.00074	3.03577
D15	-3.09747	0.00245	0.03346	0.00000	0.03349	-3.06398
D16	0.03010	-0.00174	-0.03459	0.00000	-0.03461	-0.00451
D17	0.50040	-0.00153	-0.00103	0.00000	-0.00104	0.49936
D18	-2.63191	-0.00122	0.02289	0.00000	0.02291	-2.60899
D19	-2.80857	0.00014	0.04393	0.00000	0.04391	-2.76466
D20	0.34231	0.00046	0.06785	0.00000	0.06786	0.41017
D21	0.10569	-0.00400	-0.07775	0.00000	-0.07774	0.02795
D22	3.08914	-0.00287	-0.10719	0.00000	-0.10719	2.98195
D23	-3.02223	0.00012	-0.00912	0.00000	-0.00915	-3.03139
D24	-0.03878	0.00125	-0.03856	0.00000	-0.03860	-0.07739
D25	1.37270	-0.00081	-0.08445	0.00000	-0.08442	1.28828
D26	-2.79729	0.00029	-0.10812	0.00000	-0.10815	-2.90544
D27	-0.77223	0.00155	-0.09007	0.00000	-0.09006	-0.86229
D28	-1.58328	-0.00224	-0.04824	0.00000	-0.04821	-1.63150
D29	0.52991	-0.00114	-0.07191	0.00000	-0.07194	0.45797
D30	2.55497	0.00012	-0.05385	0.00000	-0.05386	2.50112
D31	-1.17968	0.00239	-0.02218	0.00000	-0.02218	-1.20186
D32	0.95999	0.00032	-0.06570	0.00000	-0.06567	0.89432
D33	3.13201	-0.00164	-0.10470	0.00000	-0.10473	3.02728
D34	2.99073	0.00330	0.02467	0.00000	0.02466	3.01539
D35	-1.15278	0.00123	-0.01885	0.00000	-0.01883	-1.17162
D36	1.01923	-0.00072	-0.05785	0.00000	-0.05790	0.96134
D37	0.93920	0.00169	-0.02089	0.00000	-0.02088	0.91832
D38	3.07887	-0.00038	-0.06441	0.00000	-0.06436	3.01450

D39	-1.03230	-0.00234	-0.10341	0.00000	-0.10343	-1.13573
D40	0.27860	-0.00124	0.11918	0.00000	0.11921	0.39781
D41	2.40842	-0.00182	0.08933	0.00000	0.08930	2.49771
D42	-1.89058	0.00662	0.18502	0.00000	0.18502	-1.70556
D43	-1.72580	0.00202	-0.01095	0.00000	-0.01096	-1.73677
D44	2.52005	0.00129	-0.05616	0.00000	-0.05620	2.46385
D45	0.46012	-0.00136	-0.09947	0.00000	-0.09941	0.36072
D46	-3.12946	0.00079	0.03080	0.00000	0.03078	-3.09867
D47	0.02499	0.00006	0.01786	0.00000	0.01784	0.04283
D48	0.00222	0.00040	0.00346	0.00000	0.00348	0.00570
D49	-3.12652	-0.00032	-0.00948	0.00000	-0.00946	-3.13598

Item	Value	Threshold	Converged?
Maximum Force	0.011854	0.000450	NO
RMS Force	0.003224	0.000300	NO
Maximum Displacement	0.443347	0.001800	NO
RMS Displacement	0.116249	0.001200	NO

Predicted change in Energy=-7.770107D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.478810	-2.079263	-1.299096
2	6	0	-1.766748	-1.688134	-1.458874
3	7	0	-2.091112	-0.899857	-0.358108
4	6	0	-1.008871	-0.812460	0.438101
5	7	0	-0.025570	-1.538394	-0.102281
6	6	0	1.362763	-1.525341	0.383235
7	6	0	2.214697	-0.501278	-0.389110
8	1	0	0.149883	-2.690391	-1.923258
9	1	0	-2.465589	-1.877717	-2.253236
10	1	0	1.333591	-1.252475	1.438191
11	1	0	1.770922	-2.533841	0.297556
12	1	0	2.357126	-0.834087	-1.421519
13	1	0	1.694554	0.462580	-0.379961
14	35	0	-0.171073	2.109728	0.863934
15	1	0	-0.924900	-0.193479	1.319513
16	6	0	-3.288799	-0.168372	-0.120819
17	6	0	-4.474061	-0.516160	-0.605297
18	1	0	-3.111740	0.721974	0.473406
19	1	0	-5.330599	0.115530	-0.412233
20	1	0	-4.635087	-1.412042	-1.193237

21	8	0	3.497792	-0.416098	0.211425
22	1	0	3.511983	0.362701	0.778822

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.355469	0.000000			
3	N	2.208161	1.392220	0.000000		
4	C	2.214409	2.222543	1.346416	0.000000	
5	N	1.389364	2.212344	2.177071	1.336365	0.000000
6	C	2.555084	3.635066	3.587488	2.477065	1.470838
7	C	3.251628	4.290096	4.324328	3.342529	2.485292
8	H	1.076249	2.212159	3.267685	3.231927	2.161907
9	H	2.213209	1.074864	2.165168	3.240385	3.270389
10	H	3.385426	4.265546	3.883249	2.584747	2.074155
11	H	2.795931	4.039229	4.244420	3.272636	2.092407
12	H	3.099674	4.211547	4.574056	3.845593	2.813126
13	H	3.468325	4.215475	4.023429	3.098944	2.653267
14	Br	4.724516	4.729205	3.773267	3.069597	3.776710
15	H	3.257651	3.265293	2.161813	1.080313	2.153854
16	C	3.596649	2.533122	1.423317	2.434197	3.539204
17	C	4.345881	3.071101	2.426267	3.630981	4.592065
18	H	4.233322	3.369174	2.088883	2.603420	3.868478
19	H	5.398472	4.129127	3.395322	4.501285	5.565506
20	H	4.210823	2.893814	2.726092	4.021220	4.738543
21	O	4.567400	5.667747	5.638638	4.529734	3.711070
22	H	5.119312	6.089188	5.855027	4.683504	4.111543

		6	7	8	9	10
6	C	0.000000				
7	C	1.539810	0.000000			
8	H	2.854528	3.377763	0.000000		
9	H	4.661698	5.222511	2.758626	0.000000	
10	H	1.090064	2.163255	3.842929	5.333978	0.000000
11	H	1.091332	2.190835	2.753959	4.988493	1.770368
12	H	2.173414	1.094037	2.927376	5.003948	3.066042
13	H	2.155083	1.095287	3.835231	5.127664	2.525349
14	Br	3.974601	3.752249	5.559911	5.557093	3.728029
15	H	2.807824	3.587645	4.231465	4.239684	2.497266
16	C	4.871598	5.520079	4.629677	2.854249	4.997227
17	C	6.005344	6.692267	5.276852	2.933173	6.200550
18	H	5.007967	5.532739	5.293999	3.822366	4.958853
19	H	6.937313	7.570500	6.339722	3.945961	7.050314
20	H	6.202604	6.956698	5.006301	2.459101	6.524951
21	O	2.412113	1.419236	4.575781	6.616101	2.624547

22	H	2.887965	1.947685	5.284536	7.067122	2.790870
		11	12	13	14	15
11	H	0.000000				
12	H	2.487573	0.000000			
13	H	3.073011	1.790304	0.000000		
14	Br	5.065063	4.503458	2.782254	0.000000	
15	H	3.713373	4.323809	3.190637	2.465882	0.000000
16	C	5.601005	5.831935	5.029817	3.984934	2.768250
17	C	6.624650	6.887119	6.249842	5.250680	4.050378
18	H	5.871255	5.993376	4.888351	3.275041	2.517185
19	H	7.612789	7.811628	7.033793	5.676807	4.743903
20	H	6.672169	7.019771	6.651314	6.046672	4.643737
21	O	2.733923	2.035274	2.091287	4.501793	4.564824
22	H	3.413629	2.758169	2.157731	4.077285	4.504177
		16	17	18	19	20
16	C	0.000000				
17	C	1.326846	0.000000			
18	H	1.084975	2.133658	0.000000		
19	H	2.081938	1.081648	2.464846	0.000000	
20	H	2.123508	1.083608	3.106817	1.851264	0.000000
21	O	6.799233	8.014205	6.711911	8.866344	8.313164
22	H	6.880555	8.152612	6.640486	8.925859	8.568166
		21	22			
21	O	0.000000				
22	H	0.963675	0.000000			

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.696007	-2.353485	-0.434755
2	6	0	-1.901530	-1.758624	-0.608392
3	7	0	-1.880567	-0.576591	0.126888
4	6	0	-0.676454	-0.463235	0.718580
5	7	0	0.050726	-1.540941	0.409339
6	6	0	1.482932	-1.676863	0.715403
7	6	0	2.352926	-1.224000	-0.471627
8	1	0	-0.306521	-3.275206	-0.831040

9	1	0	-2.752336	-2.052529	-1.195828
10	1	0	1.689933	-1.045833	1.579805
11	1	0	1.683626	-2.714359	0.988039
12	1	0	2.248898	-1.927413	-1.303074
13	1	0	2.022346	-0.228343	-0.786331
14	35	0	0.729316	2.138717	-0.103661
15	1	0	-0.329131	0.392627	1.278885
16	6	0	-2.867944	0.447336	0.176778
17	6	0	-4.162884	0.233794	-0.018295
18	1	0	-2.433112	1.424392	0.359677
19	1	0	-4.845585	1.072635	-0.003240
20	1	0	-4.582066	-0.749734	-0.194835
21	8	0	3.716438	-1.229157	-0.077879
22	1	0	3.969034	-0.324902	0.139350

Rotational constants (GHZ): 0.7837687 0.5657765 0.3444034

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 857.5903109326 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 6.33D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Lowest energy guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999996 0.000337 0.000109 0.002736 Ang= 0.32 deg.

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999494 -0.005243 -0.001514 -0.031332 Ang= -3.65 deg.

Keep R1 ints in memory in canonical form, NReq=1804729152.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3032.33853710 A.U. after 9 cycles

NFock= 9 Conv=0.71D-08 -V/T= 2.0017

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000455908	-0.000602403	0.000726111
2	6	-0.000627931	0.000058219	0.000400986
3	7	0.000704662	0.000460688	-0.000101094
4	6	-0.000232131	-0.000072474	-0.000466054
5	7	-0.000372251	0.000681898	-0.000791936
6	6	0.000381071	-0.000208704	0.000636562
7	6	-0.000642662	0.000089130	0.000086838
8	1	-0.000001807	0.000223268	-0.000064701
9	1	0.000058928	0.000106245	-0.000053315
10	1	0.000056542	0.000013123	-0.000226059
11	1	0.000140595	0.000076212	0.000035176
12	1	-0.000516160	0.000255481	-0.000321029
13	1	0.000416387	-0.000728452	-0.000834817
14	35	-0.000313924	-0.000959345	0.000374946
15	1	-0.000122771	0.000449256	-0.000167551
16	6	-0.000365018	0.000183714	0.000187579
17	6	0.000258834	-0.000016502	0.000085985
18	1	0.000190744	-0.000214803	-0.000087647
19	1	0.000111844	-0.000167786	-0.000138870
20	1	0.000023884	0.000124266	0.000070636
21	8	0.000217532	0.000844157	0.000907040
22	1	0.000177724	-0.000595189	-0.000258786

Cartesian Forces: Max 0.000959345 RMS 0.000404173

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.005187510 RMS 0.000836424

Search for a local minimum.

Step number 37 out of a maximum of 116

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 25 29 30 31 32
34 35 36 33 37

ITU= 0 0 1 -1 0 1 1 1 1 1 1 0 -1 1 1 1 1 1 0 -1

ITU= 1 1 1 1 1 1 1 1 1 1 1 1 0 0 -1 0 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00001	0.00163	0.00356	0.00456	0.00626
Eigenvalues ---	0.00999	0.01240	0.01712	0.01758	0.02058
Eigenvalues ---	0.02246	0.02358	0.03062	0.03106	0.03714
Eigenvalues ---	0.04587	0.05018	0.05341	0.06265	0.06383
Eigenvalues ---	0.08588	0.09197	0.12228	0.14123	0.14971
Eigenvalues ---	0.15623	0.15816	0.15946	0.16020	0.16111
Eigenvalues ---	0.16838	0.17158	0.21024	0.22503	0.23102
Eigenvalues ---	0.23842	0.24862	0.25275	0.29592	0.33007
Eigenvalues ---	0.33849	0.33881	0.33995	0.34152	0.34266
Eigenvalues ---	0.34641	0.34830	0.36223	0.36330	0.36411
Eigenvalues ---	0.36635	0.43213	0.44490	0.45986	0.49886
Eigenvalues ---	0.53708	0.54599	0.57201	0.60839	2.51057

RFO step: Lambda=-1.68893333D-04 EMin= 1.47859162D-05

Quartic linear search produced a step of -0.01432.

Iteration 1 RMS(Cart)= 0.09694652 RMS(Int)= 0.02932647

Iteration 2 RMS(Cart)= 0.04962929 RMS(Int)= 0.00272907

Iteration 3 RMS(Cart)= 0.00372745 RMS(Int)= 0.00115950

Iteration 4 RMS(Cart)= 0.00001528 RMS(Int)= 0.00115946

Iteration 5 RMS(Cart)= 0.00000000 RMS(Int)= 0.00115946

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56147	0.00037	0.00001	0.00095	-0.00025	2.56121
R2	2.62552	-0.00055	-0.00001	-0.00015	-0.00051	2.62501
R3	2.03382	-0.00009	0.00000	0.00137	0.00137	2.03518
R4	2.63092	-0.00031	0.00000	0.00154	0.00117	2.63209
R5	2.03120	-0.00002	0.00000	0.00016	0.00016	2.03135
R6	2.54436	-0.00078	-0.00002	0.00070	0.00165	2.54601
R7	2.68968	-0.00021	0.00002	0.00176	0.00178	2.69146
R8	2.52536	0.00003	0.00000	-0.00465	-0.00367	2.52169
R9	2.04150	0.00011	-0.00004	0.02443	0.02439	2.06589
R10	2.77948	0.00005	0.00002	-0.00025	-0.00022	2.77926
R11	2.90982	-0.00108	-0.00002	0.00403	0.00401	2.91383
R12	2.05992	-0.00021	0.00000	0.00055	0.00055	2.06047
R13	2.06232	-0.00002	0.00000	-0.00009	-0.00009	2.06223
R14	2.06743	0.00016	0.00001	-0.00103	-0.00102	2.06641
R15	2.06979	-0.00154	-0.00002	0.00580	0.00579	2.07558
R16	2.68197	0.00065	0.00000	-0.00572	-0.00572	2.67625
R17	5.25770	-0.00019	-0.00021	0.06739	0.06718	5.32488
R18	2.50738	-0.00034	0.00000	0.00048	0.00048	2.50786
R19	2.05031	-0.00019	0.00000	0.00062	0.00062	2.05093
R20	2.04402	-0.00021	0.00000	0.00116	0.00116	2.04518
R21	2.04772	-0.00014	0.00000	0.00092	0.00092	2.04864
R22	1.82108	-0.00063	0.00000	0.00374	0.00373	1.82481
A1	1.87462	-0.00020	0.00000	-0.00093	-0.00125	1.87338

A2	2.27909	0.00008	-0.00001	0.00223	0.00229	2.28138
A3	2.12947	0.00012	0.00001	-0.00135	-0.00127	2.12820
A4	1.86665	-0.00005	0.00000	-0.00222	-0.00252	1.86413
A5	2.28365	0.00001	0.00000	-0.00090	-0.00080	2.28285
A6	2.13260	0.00003	0.00000	0.00346	0.00356	2.13615
A7	1.89340	0.00011	0.00000	0.00227	0.00390	1.89730
A8	2.23808	-0.00003	-0.00001	0.00791	0.00688	2.24496
A9	2.14650	-0.00008	0.00001	-0.00728	-0.00829	2.13821
A10	1.89341	0.00006	0.00000	-0.00222	-0.00528	1.88813
A11	2.19216	-0.00032	-0.00002	-0.00006	-0.00797	2.18419
A12	2.19440	0.00023	0.00001	-0.01299	-0.02029	2.17411
A13	1.89627	0.00009	0.00000	0.00381	0.00550	1.90177
A14	2.20896	0.00039	0.00001	0.00741	0.00659	2.21555
A15	2.16064	-0.00052	-0.00001	-0.00781	-0.00884	2.15180
A16	1.94182	-0.00294	-0.00005	0.00729	0.00724	1.94906
A17	1.87174	0.00079	-0.00001	-0.00013	-0.00014	1.87160
A18	1.89537	0.00119	0.00002	-0.00705	-0.00705	1.88832
A19	1.91108	0.00009	0.00001	-0.00569	-0.00567	1.90542
A20	1.94795	0.00128	0.00002	0.00496	0.00499	1.95294
A21	1.89369	-0.00036	0.00001	0.00029	0.00030	1.89399
A22	1.92095	0.00103	0.00001	0.00000	-0.00002	1.92093
A23	1.89475	-0.00350	-0.00005	0.00065	0.00057	1.89533
A24	1.90485	0.00073	-0.00002	0.00166	0.00163	1.90648
A25	1.91496	0.00058	-0.00001	0.01400	0.01397	1.92893
A26	1.87535	-0.00016	0.00006	-0.00638	-0.00630	1.86904
A27	1.95302	0.00140	0.00001	-0.00993	-0.00991	1.94311
A28	2.57391	-0.00519	0.00011	-0.03475	-0.03464	2.53928
A29	2.16048	-0.00034	-0.00004	0.00920	0.00914	2.16963
A30	1.95597	-0.00006	-0.00001	0.00352	0.00348	1.95946
A31	2.16621	0.00041	0.00005	-0.01237	-0.01234	2.15387
A32	2.08189	0.00015	0.00001	-0.00494	-0.00493	2.07696
A33	2.15025	-0.00008	-0.00001	0.00514	0.00513	2.15538
A34	2.05105	-0.00008	0.00000	-0.00020	-0.00020	2.05085
A35	1.88699	0.00041	0.00001	-0.00759	-0.00758	1.87941
D1	0.00676	0.00010	-0.00001	0.00397	0.00411	0.01087
D2	3.12232	-0.00013	-0.00002	0.01937	0.01954	-3.14132
D3	-3.13734	0.00027	-0.00003	-0.01626	-0.01645	3.12939
D4	-0.02177	0.00004	-0.00004	-0.00085	-0.00103	-0.02280
D5	-0.02150	0.00000	0.00004	0.01201	0.01169	-0.00980
D6	-2.96891	0.00030	0.00007	-0.00589	-0.00629	-2.97520
D7	3.12234	-0.00016	0.00006	0.03011	0.03006	-3.13079
D8	0.17492	0.00014	0.00009	0.01221	0.01208	0.18700
D9	0.01013	-0.00016	-0.00003	-0.01854	-0.01846	-0.00833
D10	3.04350	-0.00013	0.00001	0.01102	0.01112	3.05462

D11	-3.10820	0.00005	-0.00002	-0.03224	-0.03222	-3.14042
D12	-0.07482	0.00007	0.00002	-0.00268	-0.00264	-0.07747
D13	-0.02370	0.00016	0.00005	0.02628	0.02599	0.00228
D14	3.03577	-0.00015	0.00000	-0.16973	-0.17012	2.86565
D15	-3.06398	0.00013	0.00003	-0.00249	-0.00249	-3.06647
D16	-0.00451	-0.00018	-0.00003	-0.19851	-0.19860	-0.20310
D17	0.49936	-0.00006	0.00000	-0.09315	-0.09306	0.40629
D18	-2.60899	-0.00002	0.00002	-0.10412	-0.10408	-2.71307
D19	-2.76466	-0.00002	0.00003	-0.05899	-0.05898	-2.82365
D20	0.41017	0.00001	0.00005	-0.06997	-0.07000	0.34017
D21	0.02795	-0.00010	-0.00006	-0.02377	-0.02338	0.00457
D22	2.98195	-0.00026	-0.00008	-0.00446	-0.00418	2.97777
D23	-3.03139	0.00025	-0.00001	0.17180	0.17059	-2.86080
D24	-0.07739	0.00008	-0.00003	0.19111	0.18979	0.11241
D25	1.28828	0.00095	-0.00007	0.10803	0.10805	1.39634
D26	-2.90544	-0.00016	-0.00008	0.10523	0.10525	-2.80019
D27	-0.86229	0.00046	-0.00007	0.10183	0.10188	-0.76041
D28	-1.63150	0.00121	-0.00004	0.08603	0.08587	-1.54562
D29	0.45797	0.00010	-0.00006	0.08323	0.08307	0.54104
D30	2.50112	0.00072	-0.00004	0.07983	0.07970	2.58081
D31	-1.20186	0.00009	-0.00002	-0.04783	-0.04786	-1.24972
D32	0.89432	-0.00075	-0.00005	-0.03033	-0.03040	0.86393
D33	3.02728	-0.00076	-0.00008	-0.04107	-0.04117	2.98611
D34	3.01539	0.00086	0.00002	-0.04853	-0.04851	2.96688
D35	-1.17162	0.00002	-0.00001	-0.03103	-0.03104	-1.20266
D36	0.96134	0.00002	-0.00004	-0.04177	-0.04181	0.91953
D37	0.91832	0.00044	-0.00002	-0.04829	-0.04829	0.87003
D38	3.01450	-0.00040	-0.00005	-0.03079	-0.03083	2.98368
D39	-1.13573	-0.00040	-0.00008	-0.04152	-0.04160	-1.17732
D40	0.39781	-0.00035	0.00009	0.35388	0.35396	0.75176
D41	2.49771	-0.00090	0.00007	0.36265	0.36277	2.86048
D42	-1.70556	0.00018	0.00014	0.35761	0.35772	-1.34784
D43	-1.73677	0.00156	-0.00001	-0.00201	-0.00202	-1.73878
D44	2.46385	0.00001	-0.00004	0.00075	0.00072	2.46457
D45	0.36072	-0.00144	-0.00008	-0.00640	-0.00649	0.35423
D46	-3.09867	0.00008	0.00002	-0.00981	-0.00975	-3.10843
D47	0.04283	0.00001	0.00001	-0.00751	-0.00746	0.03537
D48	0.00570	0.00003	0.00000	0.00285	0.00282	0.00852
D49	-3.13598	-0.00004	-0.00001	0.00515	0.00511	-3.13087

Item	Value	Threshold	Converged?
Maximum Force	0.005188	0.000450	NO
RMS Force	0.000836	0.000300	NO
Maximum Displacement	0.680075	0.001800	NO
RMS Displacement	0.118190	0.001200	NO

Predicted change in Energy=-1.118298D-04
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.509549	-2.175905	-1.282517
2	6	0	-1.798221	-1.786318	-1.438988
3	7	0	-2.091428	-0.929933	-0.380385
4	6	0	-0.999305	-0.818728	0.400697
5	7	0	-0.031116	-1.569644	-0.127902
6	6	0	1.362359	-1.537801	0.341385
7	6	0	2.186036	-0.460772	-0.392860
8	1	0	0.100445	-2.839006	-1.872498
9	1	0	-2.518180	-2.029680	-2.199214
10	1	0	1.339278	-1.306552	1.406686
11	1	0	1.788245	-2.534207	0.212169
12	1	0	2.369296	-0.768303	-1.426094
13	1	0	1.628699	0.485281	-0.365838
14	35	0	0.085700	2.226596	1.223814
15	1	0	-0.840907	-0.042692	1.154229
16	6	0	-3.279857	-0.180884	-0.145711
17	6	0	-4.469574	-0.489237	-0.646395
18	1	0	-3.100680	0.690747	0.475609
19	1	0	-5.310798	0.158785	-0.437354
20	1	0	-4.652119	-1.364681	-1.259203
21	8	0	3.449713	-0.332318	0.233453
22	1	0	3.412313	0.438373	0.814071

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.355337	0.000000			
3	N	2.206498	1.392842	0.000000		
4	C	2.216980	2.226868	1.347289	0.000000	
5	N	1.389096	2.211008	2.172064	1.334422	0.000000
6	C	2.558960	3.636036	3.580377	2.469421	1.470720
7	C	3.316527	4.327328	4.303135	3.302160	2.493103
8	H	1.076974	2.213824	3.267303	3.233943	2.161527
9	H	2.212762	1.074946	2.167880	3.245447	3.269167
10	H	3.377240	4.262856	3.886542	2.592095	2.074165
11	H	2.764476	4.018507	4.239892	3.278543	2.087129

12	H	3.207757	4.290073	4.584506	3.832386	2.844193
13	H	3.534730	4.249188	3.980250	3.032230	2.652229
14	Br	5.100788	5.171379	4.156563	3.335979	4.031405
15	H	3.255477	3.268250	2.169341	1.093221	2.152023
16	C	3.598200	2.538746	1.424257	2.430293	3.533170
17	C	4.351012	3.073557	2.433219	3.639744	4.597393
18	H	4.245310	3.390860	2.092347	2.588417	3.859509
19	H	5.405282	4.138223	3.398955	4.499648	5.564015
20	H	4.221317	2.890473	2.741982	4.049245	4.761882
21	O	4.623066	5.696665	5.606977	4.478652	3.711836
22	H	5.158597	6.097146	5.795701	4.605817	4.095930

		6	7	8	9	10
6	C	0.000000				
7	C	1.541932	0.000000			
8	H	2.861265	3.492136	0.000000		
9	H	4.664244	5.277692	2.760244	0.000000	
10	H	1.090355	2.161182	3.825724	5.329673	0.000000
11	H	1.091283	2.196231	2.699520	4.961312	1.770756
12	H	2.174864	1.093496	3.103993	5.106487	3.061910
13	H	2.159621	1.098349	3.956825	5.184872	2.536981
14	Br	4.071760	3.774519	5.936976	6.050885	3.753403
15	H	2.783962	3.425005	4.226889	4.243459	2.532644
16	C	4.860932	5.478632	4.633988	2.866195	5.001348
17	C	6.007216	6.660499	5.282974	2.931237	6.214975
18	H	4.990306	5.479927	5.312246	3.859366	4.956746
19	H	6.929348	7.522523	6.350428	3.961344	7.054871
20	H	6.226219	6.951832	5.013644	2.424776	6.557987
21	O	2.412859	1.416209	4.683600	6.664432	2.603755
22	H	2.886348	1.941365	5.378413	7.095204	2.773703

		11	12	13	14	15
11	H	0.000000				
12	H	2.477891	0.000000			
13	H	3.078450	1.801139	0.000000		
14	Br	5.156290	4.605024	2.817804	0.000000	
15	H	3.742668	4.182103	2.947594	2.452165	0.000000
16	C	5.599274	5.822145	4.958442	4.358731	2.767204
17	C	6.639228	6.888829	6.182017	5.623519	4.075399
18	H	5.862705	5.972097	4.808042	3.615476	2.470836
19	H	7.620400	7.798779	6.947541	6.013112	4.749069
20	H	6.709025	7.048673	6.608263	6.442793	4.700814
21	O	2.758485	2.027679	2.084158	4.341134	4.397855
22	H	3.440365	2.749962	2.139080	3.798945	4.293833

		16	17	18	19	20
16	C	0.000000				

17	C	1.327100	0.000000			
18	H	1.085303	2.127234	0.000000		
19	H	2.079700	1.082260	2.449715	0.000000	
20	H	2.127051	1.084094	3.105048	1.852092	0.000000
21	O	6.741944	7.969559	6.634226	8.799871	8.302619
22	H	6.788946	8.069545	6.526662	8.816853	8.519656

		21	22
21	O	0.000000	
22	H	0.965650	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.401480	-2.232216	-0.301393
2	6	0	-2.439167	-1.380983	-0.489924
3	7	0	-2.082333	-0.173052	0.104702
4	6	0	-0.856611	-0.304480	0.648318
5	7	0	-0.428944	-1.546912	0.415627
6	6	0	0.946445	-1.991345	0.687297
7	6	0	1.872322	-1.749507	-0.521760
8	1	0	-1.274900	-3.261086	-0.593415
9	1	0	-3.379357	-1.520042	-0.992135
10	1	0	1.310286	-1.414438	1.537986
11	1	0	0.914383	-3.044601	0.971060
12	1	0	1.630574	-2.450472	-1.325464
13	1	0	1.740743	-0.713488	-0.861941
14	35	0	1.471672	1.975753	-0.064698
15	1	0	-0.215727	0.523360	0.963090
16	6	0	-2.787627	1.064288	0.096978
17	6	0	-4.094992	1.178911	-0.100131
18	1	0	-2.129581	1.913736	0.249612
19	1	0	-4.538179	2.166082	-0.119284
20	1	0	-4.755062	0.330909	-0.243166
21	8	0	3.212943	-2.000138	-0.140226
22	1	0	3.630341	-1.148490	0.041308

Rotational constants (GHZ): 0.7594125 0.5223184 0.3211177

Standard basis: 6-311++G(d,p) (5D, 7F)
There are 358 symmetry adapted cartesian basis functions of A symmetry.
There are 345 symmetry adapted basis functions of A symmetry.
345 basis functions, 553 primitive gaussians, 358 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 840.9140017899 Hartrees.
NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 345 RedAO= T EigKep= 5.83D-06 NBF= 345
NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345
Initial guess from the checkpoint file: "."
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.991701 0.001519 0.000428 0.128554 Ang= 14.77 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.33741105 A.U. after 13 cycles
NFock= 13 Conv=0.77D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Atomic Forces (Hartrees/Bohr)
Number Number X Y Z
---
1 6 0.002108594 -0.001598436 0.003040544

2	6	-0.002524218	0.001188230	0.001786002
3	7	-0.000112203	-0.000154343	0.000147986
4	6	0.001105909	0.006276096	-0.006255658
5	7	-0.000388452	-0.000028183	-0.001748939
6	6	0.002243452	-0.000381083	0.002021557
7	6	-0.001248605	0.000616401	-0.000322591
8	1	-0.000257758	0.000566506	-0.000013862
9	1	0.000095629	0.000149038	-0.000062366
10	1	0.000033724	-0.000068100	-0.000465616
11	1	0.000439841	0.000358673	0.000108518
12	1	-0.001674666	0.000676372	-0.001146519
13	1	0.001127062	-0.002179919	-0.001319238
14	35	-0.001606762	-0.006800934	-0.000747040
15	1	-0.000111228	0.000981463	0.003066757
16	6	-0.001163450	0.000758624	0.000156379
17	6	0.000634981	-0.000185947	0.000062635
18	1	0.000436399	-0.000888319	-0.000299087
19	1	0.000337183	-0.000550288	-0.000370154
20	1	0.000202678	0.000525607	0.000338108
21	8	0.000052405	0.002039276	0.002302077
22	1	0.000269484	-0.001300733	-0.000279494

Cartesian Forces: Max 0.006800934 RMS 0.001785406

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.019649443 RMS 0.004086122
Search for a local minimum.
Step number 38 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 25 29 30 31 32
34 35 36 33 38
37
DE= 1.13D-03 DEPred=-1.12D-04 R=-1.01D+01
Trust test=-1.01D+01 RLast= 7.92D-01 DXMaxT set to 2.62D-01
ITU= -1 0 0 1 -1 0 1 1 1 1 1 1 0 -1 1 1 1 1 1 0
ITU= -1 1 1 1 1 1 1 1 1 1 1 1 1 0 0 -1 0 0
Use linear search instead of GDIIS.
Energy rises -- skip Quadratic/GDIIS search.
Quartic linear search produced a step of -0.84244.
Iteration 1 RMS(Cart)= 0.08137608 RMS(Int)= 0.01677806

Iteration 2 RMS(Cart)= 0.02617658 RMS(Int)= 0.00075194
Iteration 3 RMS(Cart)= 0.00121393 RMS(Int)= 0.00015362
Iteration 4 RMS(Cart)= 0.00000167 RMS(Int)= 0.00015362
Iteration 5 RMS(Cart)= 0.00000000 RMS(Int)= 0.00015362

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56121	0.00250	0.00021	0.00000	0.00037	2.56159
R2	2.62501	-0.00268	0.00043	0.00000	0.00048	2.62549
R3	2.03518	-0.00049	-0.00115	0.00000	-0.00115	2.03403
R4	2.63209	-0.00118	-0.00099	0.00000	-0.00094	2.63115
R5	2.03135	-0.00005	-0.00013	0.00000	-0.00013	2.03122
R6	2.54601	-0.00100	-0.00139	0.00000	-0.00152	2.54449
R7	2.69146	-0.00057	-0.00150	0.00000	-0.00150	2.68996
R8	2.52169	0.00233	0.00309	0.00000	0.00296	2.52465
R9	2.06589	0.00279	-0.02055	0.00000	-0.02055	2.04534
R10	2.77926	-0.00045	0.00019	0.00000	0.00019	2.77945
R11	2.91383	-0.00578	-0.00338	0.00000	-0.00338	2.91045
R12	2.06047	-0.00047	-0.00046	0.00000	-0.00046	2.06001
R13	2.06223	-0.00017	0.00008	0.00000	0.00008	2.06230
R14	2.06641	0.00061	0.00086	0.00000	0.00086	2.06727
R15	2.07558	-0.00755	-0.00488	0.00000	-0.00488	2.07070
R16	2.67625	0.00125	0.00482	0.00000	0.00482	2.68107
R17	5.32488	-0.00374	-0.05659	0.00000	-0.05659	5.26828
R18	2.50786	-0.00102	-0.00040	0.00000	-0.00040	2.50745
R19	2.05093	-0.00081	-0.00052	0.00000	-0.00052	2.05040
R20	2.04518	-0.00066	-0.00098	0.00000	-0.00098	2.04420
R21	2.04864	-0.00065	-0.00077	0.00000	-0.00077	2.04787
R22	1.82481	-0.00122	-0.00315	0.00000	-0.00315	1.82167
A1	1.87338	-0.00072	0.00105	0.00000	0.00109	1.87447
A2	2.28138	0.00024	-0.00193	0.00000	-0.00194	2.27944
A3	2.12820	0.00049	0.00107	0.00000	0.00106	2.12926
A4	1.86413	0.00068	0.00212	0.00000	0.00216	1.86629
A5	2.28285	-0.00034	0.00067	0.00000	0.00066	2.28351
A6	2.13615	-0.00034	-0.00300	0.00000	-0.00301	2.13314
A7	1.89730	-0.00035	-0.00328	0.00000	-0.00350	1.89380
A8	2.24496	-0.00035	-0.00580	0.00000	-0.00566	2.23930
A9	2.13821	0.00071	0.00698	0.00000	0.00712	2.14533
A10	1.88813	0.00013	0.00445	0.00000	0.00486	1.89299
A11	2.18419	0.00005	0.00672	0.00000	0.00774	2.19193
A12	2.17411	0.00014	0.01710	0.00000	0.01809	2.19220
A13	1.90177	0.00026	-0.00463	0.00000	-0.00486	1.89691
A14	2.21555	0.00489	-0.00555	0.00000	-0.00544	2.21011
A15	2.15180	-0.00534	0.00745	0.00000	0.00758	2.15938
A16	1.94906	-0.01348	-0.00610	0.00000	-0.00610	1.94296

A17	1.87160	0.00195	0.00012	0.00000	0.00012	1.87172
A18	1.88832	0.00681	0.00594	0.00000	0.00594	1.89426
A19	1.90542	0.00064	0.00477	0.00000	0.00477	1.91019
A20	1.95294	0.00589	-0.00420	0.00000	-0.00420	1.94874
A21	1.89399	-0.00170	-0.00025	0.00000	-0.00025	1.89374
A22	1.92093	0.00721	0.00002	0.00000	0.00002	1.92095
A23	1.89533	-0.01965	-0.00048	0.00000	-0.00048	1.89485
A24	1.90648	0.00265	-0.00137	0.00000	-0.00137	1.90511
A25	1.92893	0.00280	-0.01177	0.00000	-0.01177	1.91716
A26	1.86904	-0.00144	0.00531	0.00000	0.00531	1.87435
A27	1.94311	0.00901	0.00835	0.00000	0.00835	1.95146
A28	2.53928	-0.01861	0.02918	0.00000	0.02918	2.56846
A29	2.16963	-0.00116	-0.00770	0.00000	-0.00770	2.16193
A30	1.95946	-0.00006	-0.00293	0.00000	-0.00293	1.95653
A31	2.15387	0.00122	0.01040	0.00000	0.01040	2.16427
A32	2.07696	0.00050	0.00416	0.00000	0.00416	2.08111
A33	2.15538	-0.00034	-0.00432	0.00000	-0.00432	2.15106
A34	2.05085	-0.00016	0.00017	0.00000	0.00017	2.05102
A35	1.87941	0.00071	0.00639	0.00000	0.00639	1.88580
D1	0.01087	0.00049	-0.00346	0.00000	-0.00348	0.00739
D2	-3.14132	0.00015	-0.01646	0.00000	-0.01647	3.12539
D3	3.12939	0.00052	0.01386	0.00000	0.01387	-3.13992
D4	-0.02280	0.00018	0.00087	0.00000	0.00089	-0.02192
D5	-0.00980	-0.00080	-0.00985	0.00000	-0.00982	-0.01962
D6	-2.97520	0.00101	0.00530	0.00000	0.00534	-2.96986
D7	-3.13079	-0.00083	-0.02532	0.00000	-0.02531	3.12709
D8	0.18700	0.00098	-0.01017	0.00000	-0.01015	0.17685
D9	-0.00833	-0.00001	0.01555	0.00000	0.01556	0.00722
D10	3.05462	0.00007	-0.00937	0.00000	-0.00936	3.04526
D11	-3.14042	0.00030	0.02715	0.00000	0.02715	-3.11327
D12	-0.07747	0.00038	0.00223	0.00000	0.00223	-0.07524
D13	0.00228	-0.00049	-0.02189	0.00000	-0.02187	-0.01959
D14	2.86565	0.00073	0.14331	0.00000	0.14340	3.00905
D15	-3.06647	-0.00051	0.00210	0.00000	0.00208	-3.06439
D16	-0.20310	0.00072	0.16730	0.00000	0.16736	-0.03575
D17	0.40629	-0.00014	0.07840	0.00000	0.07839	0.48468
D18	-2.71307	-0.00015	0.08768	0.00000	0.08768	-2.62539
D19	-2.82365	-0.00010	0.04969	0.00000	0.04969	-2.77396
D20	0.34017	-0.00012	0.05897	0.00000	0.05898	0.39915
D21	0.00457	0.00081	0.01970	0.00000	0.01967	0.02423
D22	2.97777	0.00030	0.00352	0.00000	0.00350	2.98127
D23	-2.86080	-0.00039	-0.14371	0.00000	-0.14359	-3.00439
D24	0.11241	-0.00089	-0.15989	0.00000	-0.15976	-0.04735
D25	1.39634	0.00481	-0.09103	0.00000	-0.09104	1.30529

D26	-2.80019	-0.00101	-0.08866	0.00000	-0.08868	-2.88887
D27	-0.76041	0.00152	-0.08582	0.00000	-0.08584	-0.84626
D28	-1.54562	0.00614	-0.07234	0.00000	-0.07233	-1.61795
D29	0.54104	0.00032	-0.06998	0.00000	-0.06996	0.47108
D30	2.58081	0.00285	-0.06714	0.00000	-0.06713	2.51369
D31	-1.24972	-0.00170	0.04032	0.00000	0.04032	-1.20940
D32	0.86393	-0.00622	0.02561	0.00000	0.02561	0.88953
D33	2.98611	-0.00571	0.03468	0.00000	0.03468	3.02079
D34	2.96688	0.00370	0.04086	0.00000	0.04086	3.00774
D35	-1.20266	-0.00082	0.02615	0.00000	0.02615	-1.17651
D36	0.91953	-0.00031	0.03522	0.00000	0.03522	0.95475
D37	0.87003	0.00165	0.04068	0.00000	0.04068	0.91071
D38	2.98368	-0.00286	0.02597	0.00000	0.02597	3.00965
D39	-1.17732	-0.00235	0.03504	0.00000	0.03504	-1.14228
D40	0.75176	-0.00551	-0.29819	0.00000	-0.29818	0.45358
D41	2.86048	-0.00742	-0.30561	0.00000	-0.30562	2.55487
D42	-1.34784	-0.00161	-0.30136	0.00000	-0.30135	-1.64920
D43	-1.73878	0.00902	0.00170	0.00000	0.00170	-1.73708
D44	2.46457	-0.00019	-0.00061	0.00000	-0.00061	2.46396
D45	0.35423	-0.00803	0.00546	0.00000	0.00547	0.35969
D46	-3.10843	0.00007	0.00822	0.00000	0.00821	-3.10021
D47	0.03537	-0.00003	0.00629	0.00000	0.00628	0.04165
D48	0.00852	0.00006	-0.00238	0.00000	-0.00237	0.00615
D49	-3.13087	-0.00004	-0.00431	0.00000	-0.00430	-3.13517

Item	Value	Threshold	Converged?
Maximum Force	0.019649	0.000450	NO
RMS Force	0.004086	0.000300	NO
Maximum Displacement	0.557790	0.001800	NO
RMS Displacement	0.099570	0.001200	NO

Predicted change in Energy=-6.024421D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.483260	-2.094344	-1.297520
2	6	0	-1.771248	-1.703087	-1.457137
3	7	0	-2.090902	-0.904056	-0.362610
4	6	0	-1.007255	-0.813504	0.431448
5	7	0	-0.026216	-1.543389	-0.106787
6	6	0	1.362753	-1.527729	0.376771
7	6	0	2.210804	-0.495141	-0.389138

8	1	0	0.142502	-2.713855	-1.916539
9	1	0	-2.473219	-1.900971	-2.246718
10	1	0	1.334010	-1.261603	1.433507
11	1	0	1.773651	-2.534498	0.284214
12	1	0	2.360112	-0.823963	-1.421762
13	1	0	1.684856	0.466080	-0.377185
14	35	0	-0.137905	2.122731	0.928645
15	1	0	-0.911552	-0.168587	1.295391
16	6	0	-3.287022	-0.169577	-0.125776
17	6	0	-4.473045	-0.510726	-0.613213
18	1	0	-3.109472	0.717636	0.473067
19	1	0	-5.327063	0.123763	-0.417645
20	1	0	-4.637620	-1.403250	-1.205404
21	8	0	3.490771	-0.403216	0.215933
22	1	0	3.496670	0.374409	0.785612

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.355534	0.000000			
3	N	2.208021	1.392344	0.000000		
4	C	2.214600	2.223015	1.346484	0.000000	
5	N	1.389347	2.212258	2.176493	1.335989	0.000000
6	C	2.555791	3.635372	3.586556	2.475893	1.470819
7	C	3.261991	4.296102	4.321179	3.336258	2.486524
8	H	1.076363	2.212497	3.267747	3.232077	2.161865
9	H	2.213212	1.074877	2.165611	3.241020	3.270320
10	H	3.384440	4.265367	3.883799	2.585814	2.074156
11	H	2.790926	4.036069	4.243995	3.273673	2.091579
12	H	3.116740	4.224008	4.575996	3.843651	2.818030
13	H	3.479011	4.220928	4.016694	3.088476	2.653083
14	Br	4.781088	4.795482	3.826614	3.102330	3.811171
15	H	3.258092	3.266524	2.163503	1.082347	2.154066
16	C	3.597054	2.534117	1.423465	2.433614	3.538442
17	C	4.346781	3.071423	2.427367	3.632449	4.593162
18	H	4.235469	3.372896	2.089431	2.601045	3.867160
19	H	5.399686	4.130587	3.395906	4.501130	5.565519
20	H	4.212458	2.892985	2.728601	4.025746	4.742535
21	O	4.576393	5.672537	5.633882	4.521839	3.711245
22	H	5.125819	6.090720	5.845840	4.671393	4.109142

		6	7	8	9	10
6	C	0.000000				
7	C	1.540144	0.000000			
8	H	2.855727	3.396103	0.000000		

9	H	4.662262	5.231351	2.758949	0.000000	
10	H	1.090110	2.162929	3.840772	5.333651	0.000000
11	H	1.091324	2.191685	2.745201	4.984263	1.770429
12	H	2.173645	1.093951	2.955383	5.020118	3.065448
13	H	2.155800	1.095770	3.854926	5.136894	2.527170
14	Br	3.985272	3.755827	5.618386	5.632655	3.724934
15	H	2.804210	3.562777	4.231538	4.241049	2.501261
16	C	4.870066	5.513750	4.630532	2.856291	4.997781
17	C	6.005905	6.687622	5.277851	2.932648	6.202802
18	H	5.005170	5.524451	5.297233	3.828727	4.958262
19	H	6.936293	7.563286	6.341522	3.948351	7.050950
20	H	6.206709	6.956425	5.007291	2.452894	6.530258
21	O	2.412231	1.418759	4.593190	6.623979	2.621247
22	H	2.887712	1.946691	5.299947	7.071913	2.788082

		11	12	13	14	15
11	H	0.000000				
12	H	2.486005	0.000000			
13	H	3.073891	1.792017	0.000000		
14	Br	5.075344	4.521891	2.787855	0.000000	
15	H	3.718915	4.303048	3.153037	2.446052	0.000000
16	C	5.601014	5.830773	5.018649	4.035271	2.768135
17	C	6.627385	6.887953	6.239359	5.301496	4.055127
18	H	5.870002	5.990262	4.875632	3.318441	2.508477
19	H	7.614401	7.810191	7.020386	5.721515	4.745176
20	H	6.678553	7.025000	6.644850	6.101978	4.654239
21	O	2.737796	2.034076	2.090166	4.478354	4.538803
22	H	3.417884	2.756875	2.154802	4.035743	4.470698

		16	17	18	19	20
16	C	0.000000				
17	C	1.326886	0.000000			
18	H	1.085027	2.132653	0.000000		
19	H	2.081587	1.081744	2.462471	0.000000	
20	H	2.124067	1.083685	3.106550	1.851395	0.000000
21	O	6.790422	8.007584	6.699674	8.856259	8.312100
22	H	6.866224	8.139811	6.622432	8.908924	8.561009

		21	22
21	O	0.000000	
22	H	0.963986	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.794361	-2.353705	-0.409980
2	6	0	-1.980428	-1.721786	-0.587166
3	7	0	-1.912741	-0.525913	0.122712
4	6	0	-0.701885	-0.442948	0.705775
5	7	0	-0.013944	-1.549760	0.411548
6	6	0	1.414916	-1.727145	0.711887
7	6	0	2.294255	-1.306781	-0.480632
8	1	0	-0.440131	-3.297370	-0.787571
9	1	0	-2.846255	-1.999870	-1.160204
10	1	0	1.644847	-1.097998	1.571914
11	1	0	1.584277	-2.768848	0.989665
12	1	0	2.171742	-2.015044	-1.305304
13	1	0	1.989654	-0.304649	-0.802595
14	35	0	0.831982	2.131371	-0.097086
15	1	0	-0.311574	0.421741	1.226778
16	6	0	-2.863956	0.532373	0.161096
17	6	0	-4.165794	0.363910	-0.032468
18	1	0	-2.396105	1.495644	0.335757
19	1	0	-4.817221	1.227481	-0.024870
20	1	0	-4.621010	-0.605120	-0.200198
21	8	0	3.657524	-1.343095	-0.089409
22	1	0	3.932510	-0.442975	0.119005

Rotational constants (GHZ): 0.7765353 0.5618271 0.3410197
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 358 symmetry adapted cartesian basis functions of A symmetry.
There are 345 symmetry adapted basis functions of A symmetry.
345 basis functions, 553 primitive gaussians, 358 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 855.1908764210 Hartrees.
NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 345 RedAO= T EigKep= 6.24D-06 NBF= 345
NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345
Lowest energy guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999842 0.000531 0.000035 0.017755 Ang= 2.04 deg.
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.993828 -0.001019 -0.000400 -0.110927 Ang= -12.74 deg.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.33856340 A.U. after 11 cycles
NFock= 11 Conv=0.22D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000623677	-0.000774992	0.001011288
2	6	-0.000852682	0.000161237	0.000554835
3	7	0.000775465	0.000460876	-0.000107088
4	6	-0.000206008	0.000219442	-0.000857815
5	7	-0.000471572	0.000751450	-0.001085620
6	6	0.000659767	-0.000229148	0.000886908
7	6	-0.000781341	0.000175701	-0.000020316
8	1	-0.000048322	0.000276798	-0.000051976
9	1	0.000079146	0.000109667	-0.000064765
10	1	0.000078750	0.000028110	-0.000290304
11	1	0.000182425	0.000128731	0.000032952
12	1	-0.000671013	0.000326017	-0.000460028
13	1	0.000394212	-0.000996090	-0.000855326
14	35	-0.000352134	-0.001549428	0.000386229
15	1	-0.000169642	0.000674527	-0.000031116
16	6	-0.000507969	0.000299648	0.000210679
17	6	0.000334507	-0.000040512	0.000069692
18	1	0.000283986	-0.000289635	-0.000142451
19	1	0.000149106	-0.000228825	-0.000170542
20	1	0.000043871	0.000186567	0.000129442
21	8	0.000226870	0.001073762	0.001153671
22	1	0.000228901	-0.000763903	-0.000298349

Cartesian Forces: Max 0.001549428 RMS 0.000533314

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.007367777 RMS 0.001230027
Search for a local minimum.
Step number 39 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 30 31 32 34 35
33 37 39
ITU= 0 -1 0 0 1 -1 0 1 1 1 1 1 1 0 -1 1 1 1 1 1
ITU= 0 -1 1 1 1 1 1 1 1 1 1 1 1 1 0 0 -1 0 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00032	0.00155	0.00251	0.00355	0.00494
Eigenvalues ---	0.00992	0.01313	0.01573	0.01778	0.02033
Eigenvalues ---	0.02074	0.02347	0.03032	0.03068	0.03467
Eigenvalues ---	0.04006	0.04919	0.05301	0.05755	0.06581
Eigenvalues ---	0.08153	0.09157	0.11229	0.14081	0.14597
Eigenvalues ---	0.15353	0.15886	0.15929	0.16015	0.16275
Eigenvalues ---	0.16828	0.17191	0.19853	0.21893	0.22911
Eigenvalues ---	0.23727	0.24783	0.25365	0.29132	0.32350
Eigenvalues ---	0.33566	0.33861	0.33882	0.34054	0.34233
Eigenvalues ---	0.34363	0.34773	0.35970	0.36274	0.36405
Eigenvalues ---	0.37265	0.43185	0.43830	0.46107	0.49405
Eigenvalues ---	0.53136	0.54708	0.56595	0.60616	3.67666

RFO step: Lambda=-1.49641489D-04 EMin= 3.21070181D-04
Quartic linear search produced a step of 0.26096.
Iteration 1 RMS(Cart)= 0.06641596 RMS(Int)= 0.00320583
Iteration 2 RMS(Cart)= 0.00421491 RMS(Int)= 0.00037871
Iteration 3 RMS(Cart)= 0.00002787 RMS(Int)= 0.00037831
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00037831

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56159	0.00053	0.00003	0.00125	0.00088	2.56247
R2	2.62549	-0.00077	-0.00001	-0.00198	-0.00212	2.62337
R3	2.03403	-0.00016	0.00006	0.00019	0.00025	2.03428
R4	2.63115	-0.00045	0.00006	-0.00084	-0.00088	2.63027
R5	2.03122	-0.00002	0.00001	0.00004	0.00005	2.03127
R6	2.54449	-0.00092	0.00003	-0.00224	-0.00188	2.54261
R7	2.68996	-0.00028	0.00007	0.00067	0.00074	2.69070
R8	2.52465	0.00022	-0.00019	-0.00189	-0.00176	2.52289
R9	2.04534	0.00036	0.00100	0.01052	0.01152	2.05686
R10	2.77945	0.00013	-0.00001	0.00238	0.00237	2.78181
R11	2.91045	-0.00166	0.00016	-0.00024	-0.00008	2.91037

R12	2.06001	-0.00027	0.00002	-0.00113	-0.00111	2.05890
R13	2.06230	-0.00005	0.00000	-0.00024	-0.00024	2.06206
R14	2.06727	0.00024	-0.00004	0.00027	0.00023	2.06750
R15	2.07070	-0.00226	0.00024	-0.00111	-0.00087	2.06983
R16	2.68107	0.00080	-0.00024	0.00014	-0.00009	2.68097
R17	5.26828	-0.00051	0.00276	0.00595	0.00871	5.27699
R18	2.50745	-0.00045	0.00002	-0.00083	-0.00081	2.50664
R19	2.05040	-0.00027	0.00003	-0.00054	-0.00052	2.04988
R20	2.04420	-0.00028	0.00005	-0.00056	-0.00051	2.04369
R21	2.04787	-0.00023	0.00004	-0.00026	-0.00023	2.04764
R22	1.82167	-0.00079	0.00015	-0.00092	-0.00076	1.82091
A1	1.87447	-0.00023	-0.00004	-0.00085	-0.00102	1.87345
A2	2.27944	0.00008	0.00009	0.00039	0.00054	2.27999
A3	2.12926	0.00015	-0.00005	0.00047	0.00048	2.12973
A4	1.86629	-0.00003	-0.00009	-0.00185	-0.00205	1.86424
A5	2.28351	-0.00002	-0.00004	-0.00030	-0.00029	2.28322
A6	2.13314	0.00004	0.00014	0.00208	0.00227	2.13541
A7	1.89380	0.00012	0.00010	0.00271	0.00329	1.89709
A8	2.23930	-0.00007	0.00032	0.00370	0.00365	2.24295
A9	2.14533	-0.00005	-0.00031	-0.00419	-0.00489	2.14044
A10	1.89299	0.00006	-0.00011	-0.00204	-0.00322	1.88978
A11	2.19193	-0.00042	-0.00006	-0.00590	-0.00843	2.18350
A12	2.19220	0.00032	-0.00057	-0.00318	-0.00629	2.18592
A13	1.89691	0.00008	0.00017	0.00258	0.00327	1.90018
A14	2.21011	0.00068	0.00030	0.00260	0.00263	2.21275
A15	2.15938	-0.00082	-0.00033	-0.00550	-0.00609	2.15329
A16	1.94296	-0.00422	0.00030	-0.00628	-0.00599	1.93697
A17	1.87172	0.00111	-0.00001	0.00094	0.00091	1.87263
A18	1.89426	0.00172	-0.00029	0.00138	0.00110	1.89536
A19	1.91019	0.00006	-0.00023	-0.00359	-0.00383	1.90636
A20	1.94874	0.00190	0.00020	0.00423	0.00444	1.95318
A21	1.89374	-0.00051	0.00001	0.00346	0.00348	1.89721
A22	1.92095	0.00166	0.00000	0.00273	0.00273	1.92368
A23	1.89485	-0.00539	0.00002	-0.00346	-0.00345	1.89140
A24	1.90511	0.00106	0.00007	-0.00012	-0.00007	1.90504
A25	1.91716	0.00094	0.00058	0.00030	0.00089	1.91805
A26	1.87435	-0.00030	-0.00026	0.00608	0.00582	1.88016
A27	1.95146	0.00217	-0.00041	-0.00535	-0.00577	1.94569
A28	2.56846	-0.00737	-0.00142	-0.01557	-0.01700	2.55146
A29	2.16193	-0.00046	0.00038	-0.00005	0.00032	2.16225
A30	1.95653	-0.00011	0.00014	-0.00089	-0.00074	1.95578
A31	2.16427	0.00057	-0.00051	0.00091	0.00040	2.16467
A32	2.08111	0.00021	-0.00020	0.00057	0.00037	2.08148
A33	2.15106	-0.00012	0.00021	0.00022	0.00043	2.15148

A34	2.05102	-0.00009	-0.00001	-0.00079	-0.00080	2.05022
A35	1.88580	0.00053	-0.00031	-0.00036	-0.00067	1.88513
D1	0.00739	0.00015	0.00016	0.00084	0.00100	0.00839
D2	3.12539	-0.00015	0.00080	-0.00319	-0.00233	3.12306
D3	-3.13992	0.00034	-0.00067	0.00163	0.00093	-3.13899
D4	-0.02192	0.00004	-0.00004	-0.00240	-0.00241	-0.02433
D5	-0.01962	-0.00005	0.00049	0.01288	0.01332	-0.00630
D6	-2.96986	0.00041	-0.00025	0.01534	0.01508	-2.95478
D7	3.12709	-0.00022	0.00124	0.01218	0.01339	3.14048
D8	0.17685	0.00024	0.00050	0.01463	0.01515	0.19200
D9	0.00722	-0.00020	-0.00076	-0.01418	-0.01490	-0.00767
D10	3.04526	-0.00019	0.00046	0.00975	0.01033	3.05559
D11	-3.11327	0.00007	-0.00132	-0.01055	-0.01187	-3.12514
D12	-0.07524	0.00008	-0.00011	0.01338	0.01336	-0.06188
D13	-0.01959	0.00018	0.00107	0.02242	0.02339	0.00380
D14	3.00905	-0.00017	-0.00697	-0.08098	-0.08777	2.92129
D15	-3.06439	0.00017	-0.00011	-0.00048	-0.00063	-3.06502
D16	-0.03575	-0.00018	-0.00815	-0.10388	-0.11178	-0.14753
D17	0.48468	-0.00005	-0.00383	-0.03580	-0.03963	0.44505
D18	-2.62539	0.00000	-0.00428	-0.03461	-0.03890	-2.66429
D19	-2.77396	-0.00003	-0.00242	-0.00830	-0.01072	-2.78467
D20	0.39915	0.00002	-0.00288	-0.00712	-0.00999	0.38917
D21	0.02423	-0.00008	-0.00097	-0.02189	-0.02274	0.00149
D22	2.98127	-0.00032	-0.00018	-0.02320	-0.02331	2.95796
D23	-3.00439	0.00033	0.00705	0.08176	0.08878	-2.91561
D24	-0.04735	0.00009	0.00784	0.08044	0.08821	0.04086
D25	1.30529	0.00148	0.00444	0.03229	0.03675	1.34204
D26	-2.88887	-0.00020	0.00432	0.02486	0.02920	-2.85967
D27	-0.84626	0.00068	0.00418	0.03015	0.03435	-0.81191
D28	-1.61795	0.00188	0.00354	0.03409	0.03761	-1.58034
D29	0.47108	0.00020	0.00342	0.02666	0.03006	0.50114
D30	2.51369	0.00108	0.00328	0.03195	0.03521	2.54890
D31	-1.20940	0.00007	-0.00197	0.01911	0.01715	-1.19224
D32	0.88953	-0.00112	-0.00125	0.01898	0.01774	0.90727
D33	3.02079	-0.00116	-0.00169	0.01021	0.00852	3.02932
D34	3.00774	0.00125	-0.00199	0.02407	0.02207	3.02981
D35	-1.17651	0.00005	-0.00128	0.02394	0.02265	-1.15386
D36	0.95475	0.00001	-0.00172	0.01517	0.01344	0.96819
D37	0.91071	0.00064	-0.00199	0.01942	0.01743	0.92815
D38	3.00965	-0.00056	-0.00127	0.01929	0.01802	3.02766
D39	-1.14228	-0.00060	-0.00171	0.01051	0.00880	-1.13348
D40	0.45358	-0.00070	0.01455	0.14226	0.15682	0.61040
D41	2.55487	-0.00143	0.01491	0.14364	0.15856	2.71343
D42	-1.64920	0.00019	0.01471	0.14804	0.16274	-1.48645

D43	-1.73708	0.00243	-0.00008	0.01203	0.01194	-1.72514
D44	2.46396	0.00003	0.00003	0.00533	0.00536	2.46932
D45	0.35969	-0.00223	-0.00027	0.00423	0.00397	0.36366
D46	-3.10021	0.00009	-0.00040	0.00527	0.00487	-3.09534
D47	0.04165	0.00003	-0.00031	0.00120	0.00089	0.04255
D48	0.00615	0.00002	0.00012	0.00392	0.00404	0.01019
D49	-3.13517	-0.00004	0.00021	-0.00015	0.00006	-3.13511

Item	Value	Threshold	Converged?
Maximum Force	0.007368	0.000450	NO
RMS Force	0.001230	0.000300	NO
Maximum Displacement	0.446865	0.001800	NO
RMS Displacement	0.065887	0.001200	NO

Predicted change in Energy=-1.220375D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.495247	-2.149345	-1.277992
2	6	0	-1.780804	-1.752036	-1.445992
3	7	0	-2.087079	-0.916447	-0.375800
4	6	0	-1.007568	-0.824169	0.422000
5	7	0	-0.031457	-1.565668	-0.106928
6	6	0	1.361438	-1.528806	0.367920
7	6	0	2.178072	-0.472760	-0.400063
8	1	0	0.123796	-2.793079	-1.879020
9	1	0	-2.486104	-1.966836	-2.228185
10	1	0	1.336514	-1.264347	1.424565
11	1	0	1.789971	-2.527260	0.267146
12	1	0	2.309952	-0.780723	-1.441582
13	1	0	1.637520	0.478956	-0.358363
14	35	0	0.003546	2.154367	1.165115
15	1	0	-0.880831	-0.097176	1.222079
16	6	0	-3.277761	-0.170190	-0.146123
17	6	0	-4.463580	-0.498584	-0.641579
18	1	0	-3.094608	0.714544	0.454199
19	1	0	-5.311438	0.146305	-0.454934
20	1	0	-4.633929	-1.388915	-1.235215
21	8	0	3.466088	-0.364702	0.184811
22	1	0	3.463857	0.399992	0.771095

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.356000	0.000000			
3	N	2.206335	1.391878	0.000000		
4	C	2.215522	2.224461	1.345490	0.000000	
5	N	1.388226	2.210891	2.172409	1.335057	0.000000
6	C	2.557611	3.635078	3.580555	2.472171	1.472072
7	C	3.275412	4.289896	4.288234	3.308712	2.482416
8	H	1.076496	2.213320	3.266402	3.232845	2.161239
9	H	2.213524	1.074901	2.166533	3.242720	3.268939
10	H	3.382659	4.265631	3.883727	2.587202	2.075477
11	H	2.784330	4.035622	4.247306	3.278830	2.093368
12	H	3.125545	4.204492	4.526388	3.805360	2.807069
13	H	3.507474	4.224357	3.977447	3.050179	2.651262
14	Br	4.973882	5.026109	4.021820	3.232066	3.931664
15	H	3.257366	3.266056	2.163205	1.088443	2.155033
16	C	3.597299	2.536292	1.423859	2.429861	3.533749
17	C	4.344847	3.068470	2.427551	3.630595	4.590014
18	H	4.237809	3.379471	2.089054	2.593147	3.859679
19	H	5.398438	4.129319	3.395909	4.498236	5.561489
20	H	4.208179	2.883853	2.729151	4.026883	4.742048
21	O	4.584420	5.666929	5.608597	4.503439	3.709481
22	H	5.135405	6.087131	5.819044	4.649095	4.105114

		6	7	8	9	10
6	C	0.000000				
7	C	1.540104	0.000000			
8	H	2.859875	3.433838	0.000000		
9	H	4.662104	5.227698	2.759741	0.000000	
10	H	1.089521	2.159651	3.836845	5.333711	0.000000
11	H	1.091195	2.194711	2.729987	4.982526	1.772058
12	H	2.175685	1.094073	3.003366	5.002776	3.065334
13	H	2.152862	1.095307	3.912795	5.146105	2.511681
14	Br	4.005641	3.752352	5.810202	5.890430	3.678549
15	H	2.794088	3.482714	4.230129	4.239912	2.513943
16	C	4.861301	5.470113	4.631745	2.861754	4.995575
17	C	6.000940	6.646091	5.276361	2.929760	6.204549
18	H	4.989630	5.471801	5.301458	3.841258	4.948986
19	H	6.928951	7.515252	6.341117	3.948708	7.051079
20	H	6.207579	6.923884	5.002210	2.435802	6.537288
21	O	2.412098	1.418710	4.618152	6.619514	2.623249
22	H	2.881488	1.945907	5.326802	7.071039	2.778963

		11	12	13	14	15
11	H	0.000000				
12	H	2.498104	0.000000			

13	H	3.074384	1.792294	0.000000		
14	Br	5.090707	4.552926	2.792465	0.000000	
15	H	3.735023	4.212295	3.028501	2.419672	0.000000
16	C	5.604326	5.768319	4.962501	4.229644	2.760902
17	C	6.636882	6.826444	6.185403	5.500682	4.058378
18	H	5.865441	5.919382	4.807160	3.489563	2.479785
19	H	7.622294	7.740701	6.957586	5.908124	4.743620
20	H	6.694730	6.973519	6.602187	6.310516	4.668257
21	O	2.737298	2.038351	2.085775	4.392710	4.476963
22	H	3.409496	2.760711	2.148818	3.899595	4.396235

		16	17	18	19	20
16	C	0.000000				
17	C	1.326456	0.000000			
18	H	1.084752	2.132250	0.000000		
19	H	2.081196	1.081472	2.462470	0.000000	
20	H	2.123818	1.083565	3.106151	1.850610	0.000000
21	O	6.754764	7.973736	6.654327	8.815631	8.287083
22	H	6.827577	8.102305	6.573647	8.864159	8.532268

		21	22
21	O	0.000000	
22	H	0.963582	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.172022	-2.298456	-0.309244
2	6	0	-2.268932	-1.527719	-0.512932
3	7	0	-2.021704	-0.304597	0.103650
4	6	0	-0.803629	-0.347329	0.673572
5	7	0	-0.272004	-1.548647	0.435689
6	6	0	1.135275	-1.880561	0.712088
7	6	0	2.020426	-1.595592	-0.515601
8	1	0	-0.955355	-3.305821	-0.620873
9	1	0	-3.178183	-1.727586	-1.050267
10	1	0	1.459250	-1.252712	1.541487
11	1	0	1.192092	-2.925492	1.021274
12	1	0	1.784747	-2.295935	-1.322428

13	1	0	1.831578	-0.568649	-0.846393
14	35	0	1.236536	2.046762	-0.069598
15	1	0	-0.260856	0.515166	1.055943
16	6	0	-2.823464	0.872021	0.092474
17	6	0	-4.136816	0.870322	-0.093505
18	1	0	-2.229871	1.770705	0.221713
19	1	0	-4.666620	1.812393	-0.130809
20	1	0	-4.718740	-0.035543	-0.215518
21	8	0	3.381261	-1.785658	-0.162414
22	1	0	3.764022	-0.921365	0.024624

Rotational constants (GHZ): 0.7648999 0.5411617 0.3299500

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 847.5777866500 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 6.13D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Initial guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.997529 0.001962 -0.000042 0.070228 Ang= 8.06 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Keep R1 ints in memory in canonical form, NReq=1804729152.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.33840018 A.U. after 12 cycles
NFock= 12 Conv=0.79D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000979424	-0.000727394	0.001402705
2	6	-0.001269457	0.000660344	0.000659317
3	7	-0.000663058	-0.000952742	0.000420875
4	6	0.001031469	0.003721055	-0.004410573
5	7	0.000087746	-0.000159472	0.000034346
6	6	0.001037920	-0.000114935	0.000488547
7	6	-0.000040582	0.000344638	0.000734592
8	1	-0.000055543	0.000260531	-0.000033786
9	1	-0.000006082	-0.000074207	0.000061300
10	1	-0.000130387	-0.000217802	0.000096152
11	1	0.000138076	0.000199033	-0.000103018
12	1	-0.000199389	0.000060250	-0.000250342
13	1	0.000365196	-0.000527912	-0.000970643
14	35	-0.001205614	-0.004158321	-0.000104508
15	1	0.000576768	0.001378521	0.002121948
16	6	-0.000311706	0.000516745	-0.000456430
17	6	0.000124547	0.000122322	-0.000193966
18	1	-0.000129018	-0.000333299	0.000112097
19	1	-0.000028767	-0.000227985	0.000092790
20	1	0.000097648	0.000161532	0.000157952
21	8	-0.000267600	-0.000010040	-0.000094403
22	1	-0.000131591	0.000079137	0.000235047

Cartesian Forces: Max 0.004410573 RMS 0.001045106

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.014182899 RMS 0.002672574
Search for a local minimum.
Step number 40 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 30 31 32 34 35
33 37 40 39
DE= 1.63D-04 DEPred=-1.22D-04 R=-1.34D+00
Trust test=-1.34D+00 RLast= 3.59D-01 DXMaxT set to 1.31D-01
ITU= -1 0 -1 0 0 1 -1 0 1 1 1 1 1 1 0 -1 1 1 1 1
ITU= 1 0 -1 1 1 1 1 1 1 1 1 1 1 1 1 0 0 -1 0 0
Use linear search instead of GDIIS.
Energy rises -- skip Quadratic/GDIIS search.
Quartic linear search produced a step of -0.62733.
Iteration 1 RMS(Cart)= 0.04058173 RMS(Int)= 0.00117879
Iteration 2 RMS(Cart)= 0.00175330 RMS(Int)= 0.00008685
Iteration 3 RMS(Cart)= 0.00000303 RMS(Int)= 0.00008683
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00008683

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56247	0.00155	-0.00055	0.00000	-0.00046	2.56201
R2	2.62337	-0.00116	0.00133	0.00000	0.00136	2.62473
R3	2.03428	-0.00017	-0.00016	0.00000	-0.00016	2.03412
R4	2.63027	-0.00039	0.00055	0.00000	0.00058	2.63084
R5	2.03127	-0.00002	-0.00003	0.00000	-0.00003	2.03124
R6	2.54261	0.00020	0.00118	0.00000	0.00110	2.54371
R7	2.69070	0.00030	-0.00047	0.00000	-0.00047	2.69024
R8	2.52289	0.00118	0.00110	0.00000	0.00103	2.52392
R9	2.05686	0.00255	-0.00723	0.00000	-0.00723	2.04963
R10	2.78181	-0.00051	-0.00149	0.00000	-0.00149	2.78033
R11	2.91037	-0.00346	0.00005	0.00000	0.00005	2.91042
R12	2.05890	0.00004	0.00070	0.00000	0.00070	2.05959
R13	2.06206	-0.00011	0.00015	0.00000	0.00015	2.06221
R14	2.06750	0.00020	-0.00014	0.00000	-0.00014	2.06735
R15	2.06983	-0.00371	0.00055	0.00000	0.00055	2.07038
R16	2.68097	-0.00030	0.00006	0.00000	0.00006	2.68103
R17	5.27699	-0.00185	-0.00547	0.00000	-0.00547	5.27153
R18	2.50664	-0.00022	0.00051	0.00000	0.00051	2.50715
R19	2.04988	-0.00023	0.00033	0.00000	0.00033	2.05021
R20	2.04369	-0.00009	0.00032	0.00000	0.00032	2.04401
R21	2.04764	-0.00024	0.00014	0.00000	0.00014	2.04778
R22	1.82091	0.00020	0.00048	0.00000	0.00048	1.82139
A1	1.87345	-0.00025	0.00064	0.00000	0.00067	1.87412
A2	2.27999	0.00009	-0.00034	0.00000	-0.00036	2.27963
A3	2.12973	0.00017	-0.00030	0.00000	-0.00031	2.12942
A4	1.86424	0.00041	0.00129	0.00000	0.00131	1.86555
A5	2.28322	-0.00021	0.00018	0.00000	0.00017	2.28339
A6	2.13541	-0.00021	-0.00142	0.00000	-0.00143	2.13398

A7	1.89709	-0.00046	-0.00206	0.00000	-0.00217	1.89492
A8	2.24295	-0.00010	-0.00229	0.00000	-0.00221	2.24075
A9	2.14044	0.00055	0.00306	0.00000	0.00316	2.14360
A10	1.88978	0.00026	0.00202	0.00000	0.00226	1.89204
A11	2.18350	0.00037	0.00529	0.00000	0.00586	2.18936
A12	2.18592	-0.00048	0.00394	0.00000	0.00452	2.19044
A13	1.90018	0.00003	-0.00205	0.00000	-0.00217	1.89801
A14	2.21275	0.00326	-0.00165	0.00000	-0.00159	2.21116
A15	2.15329	-0.00342	0.00382	0.00000	0.00388	2.15717
A16	1.93697	-0.00753	0.00376	0.00000	0.00376	1.94073
A17	1.87263	0.00077	-0.00057	0.00000	-0.00056	1.87206
A18	1.89536	0.00388	-0.00069	0.00000	-0.00069	1.89467
A19	1.90636	0.00019	0.00240	0.00000	0.00241	1.90877
A20	1.95318	0.00365	-0.00279	0.00000	-0.00279	1.95039
A21	1.89721	-0.00098	-0.00218	0.00000	-0.00218	1.89503
A22	1.92368	0.00434	-0.00171	0.00000	-0.00171	1.92197
A23	1.89140	-0.01305	0.00216	0.00000	0.00217	1.89356
A24	1.90504	0.00243	0.00005	0.00000	0.00005	1.90509
A25	1.91805	0.00229	-0.00056	0.00000	-0.00056	1.91749
A26	1.88016	-0.00160	-0.00365	0.00000	-0.00365	1.87652
A27	1.94569	0.00586	0.00362	0.00000	0.00362	1.94931
A28	2.55146	-0.01418	0.01066	0.00000	0.01066	2.56212
A29	2.16225	-0.00022	-0.00020	0.00000	-0.00020	2.16205
A30	1.95578	0.00015	0.00047	0.00000	0.00047	1.95625
A31	2.16467	0.00008	-0.00025	0.00000	-0.00025	2.16442
A32	2.08148	0.00018	-0.00023	0.00000	-0.00023	2.08125
A33	2.15148	-0.00016	-0.00027	0.00000	-0.00027	2.15122
A34	2.05022	-0.00002	0.00050	0.00000	0.00050	2.05072
A35	1.88513	-0.00015	0.00042	0.00000	0.00042	1.88555
D1	0.00839	0.00046	-0.00063	0.00000	-0.00063	0.00776
D2	3.12306	0.00030	0.00146	0.00000	0.00145	3.12451
D3	-3.13899	0.00025	-0.00058	0.00000	-0.00058	-3.13957
D4	-0.02433	0.00008	0.00151	0.00000	0.00151	-0.02282
D5	-0.00630	-0.00081	-0.00835	0.00000	-0.00835	-0.01465
D6	-2.95478	0.00043	-0.00946	0.00000	-0.00946	-2.96424
D7	3.14048	-0.00062	-0.00840	0.00000	-0.00839	3.13208
D8	0.19200	0.00062	-0.00950	0.00000	-0.00951	0.18249
D9	-0.00767	0.00005	0.00934	0.00000	0.00934	0.00167
D10	3.05559	-0.00006	-0.00648	0.00000	-0.00651	3.04908
D11	-3.12514	0.00019	0.00745	0.00000	0.00745	-3.11769
D12	-0.06188	0.00009	-0.00838	0.00000	-0.00840	-0.07028
D13	0.00380	-0.00056	-0.01467	0.00000	-0.01465	-0.01085
D14	2.92129	0.00010	0.05506	0.00000	0.05502	2.97631
D15	-3.06502	-0.00043	0.00039	0.00000	0.00040	-3.06462

D16	-0.14753	0.00023	0.07012	0.00000	0.07007	-0.07745
D17	0.44505	0.00005	0.02486	0.00000	0.02486	0.46991
D18	-2.66429	-0.00016	0.02440	0.00000	0.02440	-2.63989
D19	-2.78467	-0.00012	0.00672	0.00000	0.00672	-2.77795
D20	0.38917	-0.00033	0.00627	0.00000	0.00626	0.39543
D21	0.00149	0.00085	0.01427	0.00000	0.01425	0.01574
D22	2.95796	0.00054	0.01463	0.00000	0.01462	2.97257
D23	-2.91561	0.00005	-0.05569	0.00000	-0.05570	-2.97131
D24	0.04086	-0.00025	-0.05533	0.00000	-0.05533	-0.01447
D25	1.34204	0.00327	-0.02305	0.00000	-0.02306	1.31898
D26	-2.85967	-0.00032	-0.01832	0.00000	-0.01832	-2.87799
D27	-0.81191	0.00098	-0.02155	0.00000	-0.02155	-0.83346
D28	-1.58034	0.00418	-0.02360	0.00000	-0.02359	-1.60393
D29	0.50114	0.00059	-0.01886	0.00000	-0.01886	0.48228
D30	2.54890	0.00189	-0.02209	0.00000	-0.02209	2.52681
D31	-1.19224	-0.00136	-0.01076	0.00000	-0.01076	-1.20301
D32	0.90727	-0.00406	-0.01113	0.00000	-0.01113	0.89614
D33	3.02932	-0.00343	-0.00535	0.00000	-0.00535	3.02397
D34	3.02981	0.00209	-0.01384	0.00000	-0.01384	3.01597
D35	-1.15386	-0.00061	-0.01421	0.00000	-0.01421	-1.16806
D36	0.96819	0.00001	-0.00843	0.00000	-0.00843	0.95976
D37	0.92815	0.00084	-0.01094	0.00000	-0.01094	0.91721
D38	3.02766	-0.00186	-0.01130	0.00000	-0.01130	3.01636
D39	-1.13348	-0.00123	-0.00552	0.00000	-0.00552	-1.13900
D40	0.61040	-0.00296	-0.09838	0.00000	-0.09838	0.51202
D41	2.71343	-0.00433	-0.09947	0.00000	-0.09947	2.61396
D42	-1.48645	-0.00110	-0.10209	0.00000	-0.10209	-1.58854
D43	-1.72514	0.00564	-0.00749	0.00000	-0.00749	-1.73263
D44	2.46932	-0.00001	-0.00336	0.00000	-0.00336	2.46596
D45	0.36366	-0.00533	-0.00249	0.00000	-0.00249	0.36117
D46	-3.09534	-0.00030	-0.00306	0.00000	-0.00306	-3.09840
D47	0.04255	-0.00009	-0.00056	0.00000	-0.00056	0.04198
D48	0.01019	-0.00007	-0.00253	0.00000	-0.00253	0.00766
D49	-3.13511	0.00014	-0.00004	0.00000	-0.00004	-3.13515

Item	Value	Threshold	Converged?
Maximum Force	0.014183	0.000450	NO
RMS Force	0.002673	0.000300	NO
Maximum Displacement	0.275252	0.001800	NO
RMS Displacement	0.041234	0.001200	NO

Predicted change in Energy=-1.270277D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.487687	-2.115271	-1.290278
2	6	0	-1.774790	-1.721640	-1.453054
3	7	0	-2.089387	-0.908509	-0.367688
4	6	0	-1.007173	-0.817324	0.427554
5	7	0	-0.027997	-1.551738	-0.106942
6	6	0	1.362447	-1.528099	0.373467
7	6	0	2.198966	-0.486977	-0.393540
8	1	0	0.135486	-2.744125	-1.902537
9	1	0	-2.478038	-1.926028	-2.239849
10	1	0	1.335065	-1.262259	1.430084
11	1	0	1.779902	-2.531863	0.278216
12	1	0	2.341944	-0.808315	-1.429459
13	1	0	1.667515	0.470822	-0.370854
14	35	0	-0.088824	2.133358	1.019458
15	1	0	-0.899911	-0.140904	1.268595
16	6	0	-3.283383	-0.169424	-0.133601
17	6	0	-4.469443	-0.505802	-0.623818
18	1	0	-3.103569	0.717009	0.465535
19	1	0	-5.321092	0.132730	-0.431666
20	1	0	-4.636346	-1.397653	-1.216289
21	8	0	3.481954	-0.388958	0.204089
22	1	0	3.484711	0.384092	0.779732

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.355756	0.000000			
3	N	2.207462	1.392182	0.000000		
4	C	2.214832	2.223446	1.346073	0.000000	
5	N	1.388946	2.211825	2.175100	1.335603	0.000000
6	C	2.556523	3.635366	3.584460	2.474515	1.471286
7	C	3.267045	4.293914	4.309098	3.326056	2.484998
8	H	1.076412	2.212841	3.267309	3.232269	2.161637
9	H	2.213367	1.074886	2.165960	3.241560	3.269876
10	H	3.383848	4.265526	3.883812	2.586332	2.074653
11	H	2.788491	4.036036	4.245452	3.275627	2.092245
12	H	3.119987	4.216897	4.557861	3.829513	2.813956
13	H	3.489716	4.222264	4.002109	3.074205	2.652387
14	Br	4.852300	4.880246	3.896073	3.146464	3.853882
15	H	3.258203	3.266728	2.163675	1.084619	2.154713
16	C	3.597240	2.534992	1.423612	2.432242	3.536813

17	C	4.346141	3.070351	2.427436	3.631769	4.592123
18	H	4.236452	3.375448	2.089291	2.598172	3.864465
19	H	5.399308	4.130155	3.395908	4.500084	5.564148
20	H	4.210917	2.889555	2.728807	4.026152	4.742497
21	O	4.579447	5.670583	5.624651	4.515052	3.710599
22	H	5.129493	6.089482	5.835919	4.663095	4.107644

		6	7	8	9	10
6	C	0.000000				
7	C	1.540129	0.000000			
8	H	2.857332	3.410240	0.000000		
9	H	4.662305	5.230114	2.759270	0.000000	
10	H	1.089890	2.161710	3.839438	5.333737	0.000000
11	H	1.091276	2.192813	2.739497	4.983748	1.771037
12	H	2.174407	1.093997	2.973150	5.013806	3.065429
13	H	2.154708	1.095597	3.876732	5.140393	2.521403
14	Br	3.991209	3.754557	5.690186	5.728005	3.704900
15	H	2.800683	3.533482	4.231416	4.241029	2.505720
16	C	4.866913	5.497686	4.631078	2.858412	4.996945
17	C	6.004216	6.672411	5.277366	2.931603	6.203472
18	H	4.999428	5.504949	5.298933	3.833541	4.954728
19	H	6.933706	7.545645	6.341451	3.948540	7.050996
20	H	6.207242	6.944619	5.005428	2.446456	6.532945
21	O	2.412186	1.418741	4.602557	6.622455	2.621993
22	H	2.885399	1.946399	5.310143	7.071697	2.784674

		11	12	13	14	15
11	H	0.000000				
12	H	2.490515	0.000000			
13	H	3.074092	1.792119	0.000000		
14	Br	5.079946	4.534233	2.789573	0.000000	
15	H	3.725443	4.270194	3.107038	2.427385	0.000000
16	C	5.602460	5.807903	4.997759	4.103359	2.765485
17	C	6.631207	6.865535	6.219328	5.371717	4.056592
18	H	5.868436	5.964162	4.850092	3.376620	2.497404
19	H	7.617618	7.784811	6.997045	5.786614	4.744745
20	H	6.684924	7.006376	6.629074	6.176290	4.659937
21	O	2.737611	2.035671	2.088533	4.447174	4.516132
22	H	3.414774	2.758309	2.152573	3.985919	4.442918

		16	17	18	19	20
16	C	0.000000				
17	C	1.326726	0.000000			
18	H	1.084924	2.132503	0.000000		
19	H	2.081441	1.081643	2.462471	0.000000	
20	H	2.123974	1.083640	3.106402	1.851103	0.000000
21	O	6.777316	7.995236	6.682861	8.841378	8.303116

22 H 6.851836 8.125911 6.604164 8.892291 8.550455

21 22

21 O 0.000000

22 H 0.963836 0.000000

Stoichiometry C7H11BrN2O

Framework group C1[X(C7H11BrN2O)]

Deg. of freedom 60

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.929266	-2.343531	-0.370791
2	6	0	-2.085553	-1.660981	-0.558408
3	7	0	-1.954078	-0.449744	0.115232
4	6	0	-0.738900	-0.410186	0.692891
5	7	0	-0.105313	-1.554093	0.421080
6	6	0	1.318121	-1.785504	0.712569
7	6	0	2.200877	-1.415854	-0.494121
8	1	0	-0.623265	-3.313670	-0.722726
9	1	0	-2.968011	-1.913751	-1.117652
10	1	0	1.581608	-1.153167	1.560263
11	1	0	1.447774	-2.829178	1.003805
12	1	0	2.037611	-2.124892	-1.311090
13	1	0	1.936725	-0.404055	-0.820955
14	35	0	0.976256	2.109901	-0.086622
15	1	0	-0.293563	0.460449	1.162005
16	6	0	-2.853603	0.653512	0.133983
17	6	0	-4.162104	0.544124	-0.055915
18	1	0	-2.339733	1.596190	0.290046
19	1	0	-4.771172	1.437927	-0.066067
20	1	0	-4.663665	-0.404826	-0.204935
21	8	0	3.565706	-1.505507	-0.117254
22	1	0	3.879373	-0.616112	0.081664

Rotational constants (GHZ): 0.7702698 0.5556903 0.3370161

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 852.4503255199 Hartrees.
NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 345 RedAO= T EigKep= 6.20D-06 NBF= 345
NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345
Lowest energy guess from the checkpoint file: "."
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999687 0.000875 -0.000003 0.024995 Ang= 2.87 deg.
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.998974 -0.001095 0.000038 -0.045274 Ang= -5.19 deg.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.33861705 A.U. after 10 cycles
NFock= 10 Conv=0.53D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000692910	-0.000761850	0.001129667
2	6	-0.000965247	0.000326258	0.000561805
3	7	0.000326701	-0.000023013	0.000060150
4	6	0.000149324	0.001131180	-0.001893364
5	7	-0.000293361	0.000476788	-0.000757304
6	6	0.000794523	-0.000186669	0.000751198
7	6	-0.000527891	0.000244271	0.000245330
8	1	-0.000045878	0.000281377	-0.000038941
9	1	0.000062177	0.000029627	-0.000026003
10	1	-0.000004523	-0.000033407	-0.000166540
11	1	0.000165733	0.000162518	-0.000025777
12	1	-0.000475310	0.000232206	-0.000390472
13	1	0.000264465	-0.000840292	-0.000832653
14	35	-0.000529295	-0.002354161	0.000249669
15	1	0.000061358	0.001014993	0.000602629
16	6	-0.000441169	0.000397868	-0.000028724

17	6	0.000265211	0.000016497	-0.000041075
18	1	0.000178384	-0.000282861	-0.000069747
19	1	0.000086143	-0.000227463	-0.000068888
20	1	0.000050105	0.000186055	0.000166684
21	8	0.000049092	0.000683100	0.000706633
22	1	0.000136548	-0.000473023	-0.000134279

Cartesian Forces: Max 0.002354161 RMS 0.000583345

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.009760850 RMS 0.001670966
Search for a local minimum.
Step number 41 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 32 35 33 38 37
40 39 41
ITU= 0 -1 0 -1 0 0 1 -1 0 1 1 1 1 1 1 0 -1 1 1 1
ITU= 1 1 0 -1 1 1 1 1 1 1 1 1 1 1 1 1 0 0 -1 0
ITU= 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00084	0.00148	0.00266	0.00473	0.00639
Eigenvalues ---	0.01034	0.01293	0.01485	0.01732	0.02032
Eigenvalues ---	0.02097	0.02312	0.03032	0.03085	0.03423
Eigenvalues ---	0.03930	0.04927	0.05423	0.05721	0.06391
Eigenvalues ---	0.08164	0.09129	0.11041	0.14069	0.14233
Eigenvalues ---	0.15327	0.15864	0.15943	0.16025	0.16205
Eigenvalues ---	0.16877	0.17188	0.19751	0.22195	0.22883
Eigenvalues ---	0.23744	0.24750	0.25222	0.29008	0.32361
Eigenvalues ---	0.33521	0.33856	0.33881	0.34041	0.34229
Eigenvalues ---	0.34345	0.34769	0.36109	0.36280	0.36460
Eigenvalues ---	0.37091	0.43063	0.43947	0.46123	0.49302
Eigenvalues ---	0.53066	0.54665	0.57012	0.60619	2.29010

RFO step: Lambda=-2.52273901D-04 EMin= 8.38544768D-04
Quartic linear search produced a step of -0.04465.
Iteration 1 RMS(Cart)= 0.04377124 RMS(Int)= 0.00087354
Iteration 2 RMS(Cart)= 0.00115165 RMS(Int)= 0.00009483
Iteration 3 RMS(Cart)= 0.00000102 RMS(Int)= 0.00009482
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00009482

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X

R1	2.56201	0.00081	-0.00002	0.00005	-0.00007	2.56194
R2	2.62473	-0.00087	0.00003	-0.00032	-0.00032	2.62441
R3	2.03412	-0.00017	0.00000	0.00069	0.00069	2.03481
R4	2.63084	-0.00042	0.00001	-0.00005	-0.00007	2.63078
R5	2.03124	-0.00003	0.00000	0.00004	0.00004	2.03128
R6	2.54371	-0.00055	0.00003	0.00172	0.00184	2.54555
R7	2.69024	-0.00008	-0.00001	-0.00174	-0.00176	2.68848
R8	2.52392	0.00050	0.00003	-0.00129	-0.00117	2.52275
R9	2.04963	0.00110	-0.00019	0.01198	0.01179	2.06142
R10	2.78033	-0.00002	-0.00004	-0.00204	-0.00208	2.77824
R11	2.91042	-0.00223	0.00000	-0.00022	-0.00022	2.91020
R12	2.05959	-0.00017	0.00002	-0.00009	-0.00007	2.05952
R13	2.06221	-0.00008	0.00000	0.00025	0.00025	2.06247
R14	2.06735	0.00023	0.00000	-0.00028	-0.00028	2.06707
R15	2.07038	-0.00268	0.00001	0.00127	0.00129	2.07167
R16	2.68103	0.00043	0.00000	0.00064	0.00065	2.68168
R17	5.27153	-0.00094	-0.00014	0.06496	0.06482	5.33635
R18	2.50715	-0.00037	0.00001	0.00006	0.00008	2.50723
R19	2.05021	-0.00024	0.00001	-0.00033	-0.00032	2.04989
R20	2.04401	-0.00022	0.00001	0.00010	0.00010	2.04411
R21	2.04778	-0.00025	0.00000	0.00027	0.00027	2.04806
R22	1.82139	-0.00045	0.00001	0.00002	0.00003	1.82141
A1	1.87412	-0.00020	0.00002	-0.00058	-0.00058	1.87354
A2	2.27963	0.00007	-0.00001	0.00180	0.00179	2.28142
A3	2.12942	0.00013	-0.00001	-0.00120	-0.00121	2.12822
A4	1.86555	0.00008	0.00003	-0.00071	-0.00070	1.86486
A5	2.28339	-0.00008	0.00001	-0.00043	-0.00042	2.28297
A6	2.13398	-0.00001	-0.00004	0.00123	0.00119	2.13517
A7	1.89492	-0.00004	-0.00005	0.00143	0.00151	1.89642
A8	2.24075	-0.00004	-0.00006	0.00380	0.00363	2.24437
A9	2.14360	0.00008	0.00008	-0.00397	-0.00401	2.13959
A10	1.89204	0.00012	0.00004	-0.00246	-0.00264	1.88940
A11	2.18936	-0.00024	0.00011	-0.00010	-0.00063	2.18873
A12	2.19044	0.00010	0.00008	-0.00589	-0.00639	2.18405
A13	1.89801	0.00004	-0.00005	0.00235	0.00242	1.90044
A14	2.21116	0.00140	-0.00005	0.00045	0.00031	2.21147
A15	2.15717	-0.00153	0.00010	-0.00050	-0.00051	2.15666
A16	1.94073	-0.00524	0.00010	0.00394	0.00404	1.94477
A17	1.87206	0.00106	-0.00002	0.00085	0.00083	1.87289
A18	1.89467	0.00233	-0.00002	-0.00142	-0.00143	1.89324
A19	1.90877	0.00007	0.00006	-0.00087	-0.00081	1.90796
A20	1.95039	0.00247	-0.00007	-0.00294	-0.00301	1.94738
A21	1.89503	-0.00065	-0.00006	0.00052	0.00046	1.89549
A22	1.92197	0.00247	-0.00005	-0.00190	-0.00194	1.92003

A23	1.89356	-0.00782	0.00006	0.00492	0.00498	1.89854
A24	1.90509	0.00157	0.00000	-0.00173	-0.00173	1.90336
A25	1.91749	0.00143	-0.00001	0.00069	0.00068	1.91816
A26	1.87652	-0.00076	-0.00010	0.00013	0.00003	1.87655
A27	1.94931	0.00329	0.00010	-0.00225	-0.00215	1.94716
A28	2.56212	-0.00976	0.00028	-0.03425	-0.03396	2.52816
A29	2.16205	-0.00033	-0.00001	0.00496	0.00495	2.16700
A30	1.95625	-0.00008	0.00001	0.00203	0.00204	1.95829
A31	2.16442	0.00040	-0.00001	-0.00687	-0.00688	2.15754
A32	2.08125	0.00019	-0.00001	-0.00156	-0.00157	2.07968
A33	2.15122	-0.00012	-0.00001	0.00268	0.00268	2.15389
A34	2.05072	-0.00008	0.00001	-0.00113	-0.00111	2.04960
A35	1.88555	0.00034	0.00001	-0.00085	-0.00084	1.88471
D1	0.00776	0.00026	-0.00002	0.00080	0.00080	0.00856
D2	3.12451	-0.00002	0.00004	0.00473	0.00479	3.12930
D3	-3.13957	0.00033	-0.00002	0.00402	0.00400	-3.13557
D4	-0.02282	0.00005	0.00004	0.00796	0.00799	-0.01483
D5	-0.01465	-0.00028	-0.00022	0.00064	0.00038	-0.01427
D6	-2.96424	0.00042	-0.00025	-0.01228	-0.01258	-2.97681
D7	3.13208	-0.00034	-0.00022	-0.00226	-0.00249	3.12959
D8	0.18249	0.00035	-0.00025	-0.01518	-0.01545	0.16705
D9	0.00167	-0.00014	0.00025	-0.00198	-0.00174	-0.00007
D10	3.04908	-0.00020	-0.00017	0.01285	0.01270	3.06178
D11	-3.11769	0.00011	0.00020	-0.00547	-0.00528	-3.12298
D12	-0.07028	0.00005	-0.00022	0.00936	0.00915	-0.06112
D13	-0.01085	-0.00003	-0.00039	0.00242	0.00201	-0.00884
D14	2.97631	-0.00014	0.00146	-0.05521	-0.05384	2.92247
D15	-3.06462	0.00003	0.00001	-0.01190	-0.01185	-3.07647
D16	-0.07745	-0.00008	0.00186	-0.06953	-0.06770	-0.14516
D17	0.46991	0.00002	0.00066	-0.04134	-0.04066	0.42925
D18	-2.63989	-0.00002	0.00065	-0.04521	-0.04456	-2.68445
D19	-2.77795	-0.00005	0.00018	-0.02426	-0.02408	-2.80204
D20	0.39543	-0.00009	0.00017	-0.02813	-0.02798	0.36745
D21	0.01574	0.00019	0.00038	-0.00191	-0.00150	0.01424
D22	2.97257	-0.00009	0.00039	0.01063	0.01106	2.98363
D23	-2.97131	0.00034	-0.00148	0.05513	0.05353	-2.91778
D24	-0.01447	0.00005	-0.00147	0.06767	0.06609	0.05161
D25	1.31898	0.00207	-0.00061	0.03494	0.03433	1.35332
D26	-2.87799	-0.00021	-0.00049	0.03668	0.03621	-2.84178
D27	-0.83346	0.00081	-0.00057	0.03701	0.03645	-0.79701
D28	-1.60393	0.00264	-0.00063	0.01992	0.01928	-1.58465
D29	0.48228	0.00036	-0.00050	0.02167	0.02116	0.50344
D30	2.52681	0.00138	-0.00059	0.02199	0.02140	2.54821
D31	-1.20301	-0.00032	-0.00029	0.02737	0.02709	-1.17592

D32	0.89614	-0.00193	-0.00030	0.03013	0.02983	0.92598
D33	3.02397	-0.00178	-0.00014	0.02936	0.02922	3.05318
D34	3.01597	0.00152	-0.00037	0.02448	0.02411	3.04008
D35	-1.16806	-0.00010	-0.00038	0.02723	0.02686	-1.14121
D36	0.95976	0.00005	-0.00022	0.02647	0.02624	0.98600
D37	0.91721	0.00070	-0.00029	0.02628	0.02599	0.94320
D38	3.01636	-0.00091	-0.00030	0.02904	0.02874	3.04510
D39	-1.13900	-0.00077	-0.00015	0.02827	0.02812	-1.11088
D40	0.51202	-0.00129	-0.00261	0.00765	0.00504	0.51705
D41	2.61396	-0.00223	-0.00264	0.00878	0.00614	2.62010
D42	-1.58854	-0.00015	-0.00271	0.00796	0.00525	-1.58329
D43	-1.73263	0.00342	-0.00020	-0.02177	-0.02197	-1.75460
D44	2.46596	0.00003	-0.00009	-0.01861	-0.01870	2.44726
D45	0.36117	-0.00322	-0.00007	-0.01819	-0.01826	0.34291
D46	-3.09840	-0.00005	-0.00008	-0.00194	-0.00201	-3.10041
D47	0.04198	0.00001	-0.00001	-0.00389	-0.00390	0.03808
D48	0.00766	-0.00002	-0.00007	0.00259	0.00252	0.01017
D49	-3.13515	0.00004	0.00000	0.00063	0.00063	-3.13452

Item	Value	Threshold	Converged?
Maximum Force	0.009761	0.000450	NO
RMS Force	0.001671	0.000300	NO
Maximum Displacement	0.309401	0.001800	NO
RMS Displacement	0.044266	0.001200	NO

Predicted change in Energy=-1.257466D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.495734	-2.139946	-1.277141
2	6	0	-1.784400	-1.753278	-1.443906
3	7	0	-2.093619	-0.910259	-0.380058
4	6	0	-1.007666	-0.795662	0.408681
5	7	0	-0.031685	-1.542768	-0.112350
6	6	0	1.357594	-1.515306	0.367847
7	6	0	2.196121	-0.473108	-0.395265
8	1	0	0.127892	-2.782290	-1.875416
9	1	0	-2.492280	-1.984002	-2.219211
10	1	0	1.330118	-1.251863	1.425024
11	1	0	1.777337	-2.517980	0.269676
12	1	0	2.317738	-0.781213	-1.437755
13	1	0	1.683069	0.494628	-0.349544

14	35	0	-0.039872	2.124497	1.183186
15	1	0	-0.878799	-0.059935	1.203706
16	6	0	-3.289941	-0.176002	-0.148313
17	6	0	-4.475550	-0.508249	-0.642534
18	1	0	-3.118171	0.706500	0.458628
19	1	0	-5.326184	0.130410	-0.446048
20	1	0	-4.644603	-1.394275	-1.243340
21	8	0	3.489885	-0.405423	0.183862
22	1	0	3.519099	0.368645	0.757424

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.355721	0.000000			
3	N	2.206836	1.392147	0.000000		
4	C	2.216115	2.225404	1.347047	0.000000	
5	N	1.388777	2.211191	2.173318	1.334983	0.000000
6	C	2.555580	3.634722	3.582781	2.472653	1.470184
7	C	3.286660	4.310803	4.311983	3.318828	2.487434
8	H	1.076777	2.214029	3.267371	3.233153	2.161083
9	H	2.213145	1.074908	2.166643	3.243770	3.269263
10	H	3.379959	4.264082	3.885484	2.589654	2.074283
11	H	2.775321	4.025805	4.241607	3.277491	2.090346
12	H	3.128511	4.215742	4.538221	3.803662	2.802936
13	H	3.542401	4.274816	4.029642	3.078930	2.673504
14	Br	4.944340	4.998213	3.983887	3.172352	3.889385
15	H	3.260028	3.270684	2.169596	1.090856	2.156015
16	C	3.597071	2.536339	1.422682	2.429609	3.533494
17	C	4.347884	3.071577	2.429835	3.635090	4.593394
18	H	4.241736	3.383651	2.089739	2.590988	3.861557
19	H	5.401710	4.133792	3.396590	4.498641	5.562608
20	H	4.215481	2.889615	2.736246	4.039160	4.751863
21	O	4.585658	5.681938	5.634571	4.520044	3.712512
22	H	5.152802	6.121724	5.867884	4.687092	4.125296

		6	7	8	9	10
6	C	0.000000				
7	C	1.540014	0.000000			
8	H	2.854758	3.435220	0.000000		
9	H	4.661982	5.252683	2.760573	0.000000	
10	H	1.089853	2.160989	3.831508	5.331716	0.000000
11	H	1.091411	2.190668	2.718814	4.970848	1.771408
12	H	2.172779	1.093849	2.998546	5.019327	3.064704
13	H	2.158800	1.096278	3.935105	5.203154	2.514736
14	Br	3.983197	3.773423	5.784440	5.871148	3.651735

15	H	2.796108	3.490351	4.231505	4.245199	2.519719
16	C	4.864128	5.499648	4.632192	2.862472	4.997781
17	C	6.005049	6.676344	5.280430	2.932085	6.207539
18	H	4.997714	5.510200	5.306255	3.847254	4.955440
19	H	6.931356	7.546647	6.346169	3.955485	7.051095
20	H	6.215862	6.954371	5.010271	2.435692	6.545054
21	O	2.410882	1.419083	4.603598	6.637241	2.630882
22	H	2.893638	1.946153	5.325459	7.108585	2.804171

		11	12	13	14	15
11	H	0.000000				
12	H	2.494737	0.000000			
13	H	3.077033	1.792981	0.000000		
14	Br	5.068466	4.568458	2.823873	0.000000	
15	H	3.737574	4.208968	3.046850	2.340078	0.000000
16	C	5.597936	5.785759	5.022059	4.198588	2.766774
17	C	6.630969	6.845119	6.246615	5.471732	4.067703
18	H	5.865065	5.946316	4.873392	3.465780	2.481401
19	H	7.614870	7.761706	7.019373	5.880126	4.747331
20	H	6.692776	6.991983	6.663802	6.282781	4.685059
21	O	2.720860	2.035875	2.087869	4.456269	4.499427
22	H	3.406499	2.753952	2.147616	3.991311	4.441211

		16	17	18	19	20
16	C	0.000000				
17	C	1.326767	0.000000			
18	H	1.084755	2.128533	0.000000		
19	H	2.080581	1.081698	2.454718	0.000000	
20	H	2.125648	1.083784	3.104826	1.850646	0.000000
21	O	6.791835	8.008849	6.706585	8.854772	8.317730
22	H	6.890575	8.163531	6.652577	8.929957	8.588188

		21	22
21	O	0.000000	
22	H	0.963851	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.081920	-2.328830	-0.295501

2	6	0	-2.209667	-1.603594	-0.495998
3	7	0	-2.002346	-0.362344	0.099308
4	6	0	-0.771383	-0.346900	0.646140
5	7	0	-0.201577	-1.534134	0.427102
6	6	0	1.212034	-1.822006	0.710428
7	6	0	2.100594	-1.537871	-0.514876
8	1	0	-0.828375	-3.330947	-0.597040
9	1	0	-3.119087	-1.847955	-1.014331
10	1	0	1.515855	-1.175764	1.533741
11	1	0	1.295243	-2.860929	1.034303
12	1	0	1.875131	-2.250029	-1.313940
13	1	0	1.908235	-0.515557	-0.860850
14	35	0	1.137915	2.083394	-0.069447
15	1	0	-0.252386	0.541084	1.009584
16	6	0	-2.850158	0.780069	0.087900
17	6	0	-4.164016	0.731005	-0.090094
18	1	0	-2.295287	1.703565	0.214255
19	1	0	-4.726310	1.654503	-0.122431
20	1	0	-4.715878	-0.194057	-0.209671
21	8	0	3.460725	-1.718703	-0.152746
22	1	0	3.844583	-0.848977	0.006124

Rotational constants (GHZ): 0.7631041 0.5449850 0.3305272

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 848.7233492080 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 6.03D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Initial guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999616 0.002559 -0.000216 0.027580 Ang= 3.17 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.33881572 A.U. after 13 cycles
NFock= 13 Conv=0.29D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.001137804	-0.000920507	0.001346800
2	6	-0.001539474	0.000266695	0.000527902
3	7	0.001067700	0.000015392	0.000314020
4	6	-0.000521409	0.000870385	-0.003002335
5	7	-0.000445980	0.000636863	-0.001517282
6	6	0.001706373	0.000169040	0.001383644
7	6	-0.000363023	0.000343441	0.000085611
8	1	-0.000383751	0.000159823	0.000077645
9	1	0.000063622	0.000002481	-0.000037629
10	1	-0.000080368	-0.000120400	-0.000120725
11	1	0.000169809	0.000303979	-0.000073090
12	1	-0.000564839	0.000333815	-0.000667739
13	1	0.000189062	-0.001555858	-0.000755531
14	35	-0.000286152	-0.001782234	0.000054158
15	1	0.000015285	0.000815809	0.001791235
16	6	-0.001034212	0.000892309	-0.000128993
17	6	0.000227388	-0.000162310	-0.000394407
18	1	0.000395808	-0.000482516	0.000062793
19	1	0.000096715	-0.000310478	-0.000023702
20	1	0.000196092	0.000247296	0.000275034
21	8	-0.000165708	0.000975046	0.000697285
22	1	0.000119258	-0.000698071	0.000105306

Cartesian Forces: Max 0.003002335 RMS 0.000798957

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.007165412 RMS 0.001325344

Search for a local minimum.

Step number 42 out of a maximum of 116

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 32 33 38 37 40 39 41 42

DE= -1.99D-04 DEPred=-1.26D-04 R= 1.58D+00

TightC=F SS= 1.41D+00 RLast= 1.99D-01 DXNew= 2.2009D-01 5.9746D-01

Trust test= 1.58D+00 RLast= 1.99D-01 DXMaxT set to 2.20D-01

ITU= 1 0 -1 0 -1 0 0 1 -1 0 1 1 1 1 1 1 0 -1 1 1

ITU= 1 1 1 0 -1 1 1 1 1 1 1 1 1 1 1 1 1 0 0 -1

ITU= 0 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00123	0.00185	0.00242	0.00559	0.00659
Eigenvalues ---	0.01061	0.01252	0.01332	0.01717	0.02060
Eigenvalues ---	0.02228	0.02401	0.02935	0.03073	0.03347
Eigenvalues ---	0.03872	0.04899	0.05479	0.05627	0.06066
Eigenvalues ---	0.08111	0.09119	0.10959	0.13320	0.14165
Eigenvalues ---	0.15226	0.15767	0.15947	0.16024	0.16154
Eigenvalues ---	0.17006	0.17330	0.19571	0.22144	0.22840
Eigenvalues ---	0.23787	0.24782	0.25087	0.28885	0.32043
Eigenvalues ---	0.33466	0.33840	0.33883	0.33990	0.34224
Eigenvalues ---	0.34340	0.34737	0.35529	0.36152	0.36326
Eigenvalues ---	0.36508	0.42860	0.43934	0.45957	0.48895
Eigenvalues ---	0.52895	0.54474	0.56916	0.60580	1.20548

RFO step: Lambda=-8.74151949D-04 EMin= 1.23067958D-03

Quartic linear search produced a step of 0.14987.

Iteration 1 RMS(Cart)= 0.05455924 RMS(Int)= 0.00251558

Iteration 2 RMS(Cart)= 0.00260959 RMS(Int)= 0.00009962

Iteration 3 RMS(Cart)= 0.00001299 RMS(Int)= 0.00009931

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00009931

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56194	0.00106	-0.00001	0.00437	0.00430	2.56624
R2	2.62441	-0.00084	-0.00005	-0.00602	-0.00611	2.61830
R3	2.03481	-0.00036	0.00010	-0.00240	-0.00230	2.03251

R4	2.63078	-0.00051	-0.00001	-0.00508	-0.00508	2.62569
R5	2.03128	-0.00001	0.00001	-0.00015	-0.00014	2.03114
R6	2.54555	-0.00080	0.00028	-0.00885	-0.00851	2.53704
R7	2.68848	0.00016	-0.00026	0.00453	0.00427	2.69274
R8	2.52275	0.00084	-0.00018	0.00403	0.00389	2.52664
R9	2.06142	0.00185	0.00177	0.00472	0.00648	2.06790
R10	2.77824	0.00088	-0.00031	0.01010	0.00979	2.78804
R11	2.91020	-0.00197	-0.00003	-0.01128	-0.01132	2.89889
R12	2.05952	-0.00015	-0.00001	-0.00220	-0.00221	2.05732
R13	2.06247	-0.00020	0.00004	-0.00280	-0.00276	2.05971
R14	2.06707	0.00048	-0.00004	0.00382	0.00378	2.07085
R15	2.07167	-0.00293	0.00019	-0.01756	-0.01737	2.05430
R16	2.68168	0.00030	0.00010	0.00516	0.00525	2.68693
R17	5.33635	-0.00082	0.00971	0.01610	0.02582	5.36216
R18	2.50723	-0.00036	0.00001	-0.00300	-0.00299	2.50423
R19	2.04989	-0.00029	-0.00005	-0.00300	-0.00305	2.04684
R20	2.04411	-0.00026	0.00002	-0.00441	-0.00440	2.03972
R21	2.04806	-0.00039	0.00004	-0.00374	-0.00370	2.04435
R22	1.82141	-0.00049	0.00000	-0.00443	-0.00443	1.81699
A1	1.87354	-0.00017	-0.00009	-0.00224	-0.00242	1.87112
A2	2.28142	-0.00014	0.00027	-0.00312	-0.00284	2.27859
A3	2.12822	0.00031	-0.00018	0.00539	0.00522	2.13343
A4	1.86486	0.00003	-0.00010	-0.00167	-0.00180	1.86305
A5	2.28297	-0.00007	-0.00006	0.00151	0.00145	2.28442
A6	2.13517	0.00004	0.00018	0.00007	0.00026	2.13543
A7	1.89642	0.00008	0.00023	0.00524	0.00534	1.90176
A8	2.24437	-0.00047	0.00054	-0.00585	-0.00557	2.23881
A9	2.13959	0.00040	-0.00060	0.00312	0.00227	2.14186
A10	1.88940	0.00018	-0.00040	-0.00332	-0.00395	1.88545
A11	2.18873	-0.00007	-0.00009	-0.00931	-0.00979	2.17895
A12	2.18405	-0.00006	-0.00096	0.00587	0.00446	2.18851
A13	1.90044	-0.00011	0.00036	0.00253	0.00268	1.90312
A14	2.21147	0.00136	0.00005	0.00363	0.00343	2.21490
A15	2.15666	-0.00127	-0.00008	-0.00008	-0.00041	2.15624
A16	1.94477	-0.00404	0.00061	-0.02035	-0.01977	1.92500
A17	1.87289	0.00071	0.00012	-0.00197	-0.00184	1.87105
A18	1.89324	0.00191	-0.00021	0.01097	0.01068	1.90392
A19	1.90796	0.00023	-0.00012	0.00830	0.00814	1.91610
A20	1.94738	0.00172	-0.00045	-0.00383	-0.00427	1.94311
A21	1.89549	-0.00050	0.00007	0.00756	0.00761	1.90310
A22	1.92003	0.00216	-0.00029	0.01122	0.01086	1.93089
A23	1.89854	-0.00598	0.00075	-0.01626	-0.01561	1.88293
A24	1.90336	0.00080	-0.00026	-0.01030	-0.01067	1.89268
A25	1.91816	0.00085	0.00010	-0.01204	-0.01192	1.90624

A26	1.87655	-0.00031	0.00000	0.02764	0.02764	1.90419
A27	1.94716	0.00263	-0.00032	0.00041	-0.00010	1.94706
A28	2.52816	-0.00717	-0.00509	-0.01616	-0.02125	2.50691
A29	2.16700	-0.00082	0.00074	-0.02237	-0.02163	2.14537
A30	1.95829	-0.00010	0.00031	-0.00671	-0.00640	1.95188
A31	2.15754	0.00092	-0.00103	0.02915	0.02812	2.18566
A32	2.07968	0.00030	-0.00023	0.00874	0.00850	2.08819
A33	2.15389	-0.00031	0.00040	-0.00972	-0.00932	2.14458
A34	2.04960	0.00000	-0.00017	0.00097	0.00080	2.05040
A35	1.88471	0.00052	-0.00013	0.00981	0.00969	1.89440
D1	0.00856	0.00011	0.00012	-0.01080	-0.01074	-0.00218
D2	3.12930	0.00000	0.00072	-0.01612	-0.01546	3.11384
D3	-3.13557	0.00013	0.00060	0.00111	0.00165	-3.13392
D4	-0.01483	0.00001	0.00120	-0.00422	-0.00306	-0.01789
D5	-0.01427	-0.00006	0.00006	0.02919	0.02930	0.01503
D6	-2.97681	0.00027	-0.00188	-0.00766	-0.00955	-2.98636
D7	3.12959	-0.00007	-0.00037	0.01857	0.01818	-3.13542
D8	0.16705	0.00026	-0.00231	-0.01828	-0.02067	0.14637
D9	-0.00007	-0.00012	-0.00026	-0.01098	-0.01126	-0.01133
D10	3.06178	0.00001	0.00190	0.02512	0.02698	3.08876
D11	-3.12298	-0.00001	-0.00079	-0.00623	-0.00706	-3.13004
D12	-0.06112	0.00011	0.00137	0.02986	0.03117	-0.02995
D13	-0.00884	0.00008	0.00030	0.02933	0.02959	0.02075
D14	2.92247	0.00034	-0.00807	-0.00308	-0.01093	2.91155
D15	-3.07647	0.00001	-0.00178	-0.00365	-0.00564	-3.08211
D16	-0.14516	0.00027	-0.01015	-0.03606	-0.04616	-0.19132
D17	0.42925	-0.00013	-0.00609	-0.02203	-0.02811	0.40114
D18	-2.68445	-0.00026	-0.00668	-0.02558	-0.03222	-2.71666
D19	-2.80204	-0.00001	-0.00361	0.01858	0.01493	-2.78711
D20	0.36745	-0.00014	-0.00419	0.01502	0.01082	0.37827
D21	0.01424	-0.00001	-0.00022	-0.03613	-0.03638	-0.02214
D22	2.98363	0.00000	0.00166	-0.00023	0.00135	2.98498
D23	-2.91778	-0.00026	0.00802	-0.00155	0.00658	-2.91120
D24	0.05161	-0.00026	0.00990	0.03435	0.04431	0.09592
D25	1.35332	0.00159	0.00515	0.03448	0.03957	1.39288
D26	-2.84178	-0.00003	0.00543	0.03155	0.03699	-2.80479
D27	-0.79701	0.00076	0.00546	0.04512	0.05060	-0.74641
D28	-1.58465	0.00180	0.00289	-0.00775	-0.00490	-1.58955
D29	0.50344	0.00018	0.00317	-0.01068	-0.00748	0.49596
D30	2.54821	0.00097	0.00321	0.00288	0.00613	2.55434
D31	-1.17592	-0.00018	0.00406	0.06544	0.06948	-1.10643
D32	0.92598	-0.00155	0.00447	0.04739	0.05174	0.97772
D33	3.05318	-0.00153	0.00438	0.03151	0.03589	3.08908
D34	3.04008	0.00126	0.00361	0.07502	0.07868	3.11876

D35	-1.14121	-0.00010	0.00402	0.05697	0.06094	-1.08027
D36	0.98600	-0.00009	0.00393	0.04109	0.04509	1.03109
D37	0.94320	0.00063	0.00390	0.06253	0.06648	1.00969
D38	3.04510	-0.00073	0.00431	0.04448	0.04874	3.09384
D39	-1.11088	-0.00072	0.00421	0.02860	0.03289	-1.07799
D40	0.51705	-0.00117	0.00075	-0.07722	-0.07653	0.44053
D41	2.62010	-0.00172	0.00092	-0.08088	-0.07985	2.54025
D42	-1.58329	0.00011	0.00079	-0.05398	-0.05324	-1.63653
D43	-1.75460	0.00296	-0.00329	0.16584	0.16256	-1.59205
D44	2.44726	0.00011	-0.00280	0.14233	0.13955	2.58681
D45	0.34291	-0.00231	-0.00274	0.13907	0.13629	0.47920
D46	-3.10041	-0.00018	-0.00030	0.00769	0.00737	-3.09304
D47	0.03808	-0.00001	-0.00058	0.00391	0.00331	0.04140
D48	0.01017	-0.00006	0.00038	0.01095	0.01135	0.02152
D49	-3.13452	0.00011	0.00009	0.00718	0.00729	-3.12723

Item	Value	Threshold	Converged?
Maximum Force	0.007165	0.000450	NO
RMS Force	0.001325	0.000300	NO
Maximum Displacement	0.237371	0.001800	NO
RMS Displacement	0.054487	0.001200	NO

Predicted change in Energy=-5.220866D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.504440	-2.157453	-1.249795
2	6	0	-1.791581	-1.760916	-1.423526
3	7	0	-2.082731	-0.881353	-0.388061
4	6	0	-1.002028	-0.761531	0.399435
5	7	0	-0.027215	-1.516283	-0.118030
6	6	0	1.366969	-1.490236	0.363918
7	6	0	2.182940	-0.457131	-0.423558
8	1	0	0.106089	-2.825257	-1.831278
9	1	0	-2.505856	-2.005182	-2.188648
10	1	0	1.338737	-1.212931	1.416316
11	1	0	1.795050	-2.488247	0.270553
12	1	0	2.239863	-0.735468	-1.481940
13	1	0	1.682162	0.503445	-0.332581
14	35	0	-0.062779	2.024188	1.308797
15	1	0	-0.868345	0.009266	1.164592
16	6	0	-3.284530	-0.149515	-0.163243

17	6	0	-4.456611	-0.519848	-0.658411
18	1	0	-3.109867	0.739212	0.430769
19	1	0	-5.325656	0.098444	-0.492528
20	1	0	-4.590355	-1.424001	-1.237174
21	8	0	3.497064	-0.414570	0.117700
22	1	0	3.523472	0.258488	0.803844

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357997	0.000000			
3	N	2.204999	1.389456	0.000000		
4	C	2.217240	2.223815	1.342545	0.000000	
5	N	1.385545	2.208428	2.168224	1.337042	0.000000
6	C	2.559574	3.639322	3.582826	2.478795	1.475365
7	C	3.285692	4.300768	4.286860	3.303634	2.469805
8	H	1.075560	2.213647	3.263828	3.234652	2.160186
9	H	2.215920	1.074833	2.164288	3.241349	3.266519
10	H	3.376028	4.261910	3.882288	2.591716	2.076551
11	H	2.776424	4.032720	4.248890	3.289651	2.101514
12	H	3.099537	4.160228	4.461241	3.748347	2.758544
13	H	3.564111	4.287701	4.011878	3.056287	2.654676
14	Br	4.922152	4.978088	3.924500	3.077232	3.817333
15	H	3.264409	3.268680	2.163023	1.094287	2.163312
16	C	3.597404	2.532554	1.424939	2.429194	3.532733
17	C	4.318697	3.037768	2.416419	3.620993	4.572137
18	H	4.243020	3.380374	2.086078	2.587701	3.858909
19	H	5.376490	4.100447	3.389318	4.497656	5.551672
20	H	4.151242	2.825133	2.702524	3.999181	4.699281
21	O	4.573808	5.670784	5.622081	4.521237	3.699984
22	H	5.126234	6.106468	5.843747	4.656623	4.075174

		6	7	8	9	10
6	C	0.000000				
7	C	1.534025	0.000000			
8	H	2.861989	3.450073	0.000000		
9	H	4.666855	5.243741	2.760887	0.000000	
10	H	1.088685	2.160798	3.829606	5.329570	0.000000
11	H	1.089952	2.181211	2.717325	4.977832	1.774098
12	H	2.176880	1.095849	3.007033	4.963211	3.072439
13	H	2.135233	1.087088	3.976223	5.222805	2.474374
14	Br	3.910007	3.768454	5.779767	5.868268	3.529128
15	H	2.808241	3.471323	4.237839	4.240715	2.535418
16	C	4.869484	5.482301	4.630144	2.855189	5.000046
17	C	5.991735	6.643999	5.244879	2.890205	6.194425

18	H	5.001697	5.493170	5.307040	3.841598	4.957040
19	H	6.931712	7.529437	6.312221	3.905552	7.055318
20	H	6.169084	6.890162	4.936908	2.363939	6.499207
21	O	2.398955	1.421863	4.594414	6.624526	2.642377
22	H	2.811063	1.953369	5.303947	7.101550	2.704304

		11	12	13	14	15
11	H	0.000000				
12	H	2.518198	0.000000			
13	H	3.053970	1.779595	0.000000		
14	Br	4.989143	4.550392	2.837535	0.000000	
15	H	3.759062	4.149664	2.998471	2.174774	0.000000
16	C	5.608919	5.709748	5.012291	4.155907	2.761577
17	C	6.619730	6.750367	6.232000	5.444978	4.059428
18	H	5.873701	5.869646	4.858172	3.421526	2.468955
19	H	7.614309	7.675377	7.021333	5.886521	4.756219
20	H	6.646747	6.869197	6.624033	6.234655	4.655759
21	O	2.687072	2.059703	2.083116	4.476464	4.509148
22	H	3.288829	2.803642	2.177587	4.029127	4.413650

		16	17	18	19	20
16	C	0.000000				
17	C	1.325184	0.000000			
18	H	1.083140	2.141323	0.000000		
19	H	2.082332	1.079371	2.484508	0.000000	
20	H	2.117268	1.081826	3.106987	1.847432	0.000000
21	O	6.792584	7.992144	6.714221	8.858665	8.262020
22	H	6.888440	8.150197	6.661191	8.945013	8.534091

		21	22
21	O	0.000000	
22	H	0.961508	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.050333	-2.349904	-0.194515
2	6	0	-2.189419	-1.646413	-0.421980
3	7	0	-1.975551	-0.366642	0.075046
4	6	0	-0.742605	-0.303925	0.602622

5	7	0	-0.158732	-1.494678	0.432678
6	6	0	1.267090	-1.750834	0.712175
7	6	0	2.107433	-1.514140	-0.549186
8	1	0	-0.799139	-3.368998	-0.429414
9	1	0	-3.107770	-1.930691	-0.902692
10	1	0	1.571799	-1.056725	1.493585
11	1	0	1.380760	-2.771010	1.078667
12	1	0	1.827754	-2.221676	-1.337891
13	1	0	1.915490	-0.500845	-0.892919
14	35	0	1.090361	2.080021	-0.050366
15	1	0	-0.227277	0.620901	0.879386
16	6	0	-2.848990	0.757993	0.022572
17	6	0	-4.161501	0.644480	-0.120751
18	1	0	-2.306327	1.692994	0.089511
19	1	0	-4.768828	1.533319	-0.199235
20	1	0	-4.666310	-0.311044	-0.170638
21	8	0	3.477447	-1.703116	-0.218970
22	1	0	3.847572	-0.856348	0.046530

Rotational constants (GHZ): 0.7734310 0.5516678 0.3340663

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 853.6354310184 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 6.08D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Initial guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999966 0.003353 -0.001325 -0.007462 Ang= 0.95 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.33814413 A.U. after 13 cycles
NFock= 13 Conv=0.37D-08 -V/T= 2.0016
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.001226838	0.001160696	-0.001121775
2	6	0.000454347	-0.001192292	-0.000918407
3	7	-0.003346038	-0.001475459	0.000072367
4	6	0.001854627	-0.001259793	-0.005555549
5	7	0.000295293	-0.002951215	0.004369550
6	6	-0.003050066	-0.000442529	-0.002772287
7	6	0.002233115	-0.001235133	0.004522757
8	1	0.000400523	-0.000202461	-0.000390378
9	1	0.000319822	-0.000306547	-0.000109582
10	1	0.000169766	0.000042585	0.000455756
11	1	-0.000645288	-0.000947101	-0.000026050
12	1	0.002935525	-0.000473408	0.001972454
13	1	-0.001356378	0.004656152	-0.001050000
14	35	0.001646058	0.004518289	0.001445809
15	1	0.000956161	0.000330504	0.004228533
16	6	0.002576881	-0.002341476	-0.001352569
17	6	-0.000852796	0.001557148	0.000098130
18	1	-0.001216245	0.000712764	0.000409954
19	1	-0.001161199	0.000563917	0.000609249
20	1	-0.000442238	-0.000597370	-0.000400708
21	8	0.000171335	-0.002138717	-0.005106384
22	1	-0.000716367	0.002021445	0.000619132

Cartesian Forces: Max 0.005555549 RMS 0.002019456

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.014663505 RMS 0.003413771
Search for a local minimum.
Step number 43 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 32 33 38 37 40
39 41 43 42
DE= 6.72D-04 DEPred=-5.22D-04 R=-1.29D+00
Trust test=-1.29D+00 RLast= 3.64D-01 DXMaxT set to 1.10D-01
ITU= -1 1 0 -1 0 -1 0 0 1 -1 0 1 1 1 1 1 1 0 -1 1
ITU= 1 1 1 1 0 -1 1 1 1 1 1 1 1 1 1 1 1 1 0 0
ITU= -1 0 0
Use linear search instead of GDIIS.
Energy rises -- skip Quadratic/GDIIS search.
Quartic linear search produced a step of -0.70447.
Iteration 1 RMS(Cart)= 0.03833833 RMS(Int)= 0.00125668
Iteration 2 RMS(Cart)= 0.00128981 RMS(Int)= 0.00001913
Iteration 3 RMS(Cart)= 0.00000297 RMS(Int)= 0.00001901
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001901

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56624	-0.00063	-0.00303	0.00000	-0.00302	2.56322
R2	2.61830	0.00196	0.00430	0.00000	0.00431	2.62261
R3	2.03251	0.00056	0.00162	0.00000	0.00162	2.03413
R4	2.62569	0.00063	0.00358	0.00000	0.00358	2.62927
R5	2.03114	-0.00006	0.00010	0.00000	0.00010	2.03124
R6	2.53704	0.00403	0.00599	0.00000	0.00598	2.54302
R7	2.69274	0.00076	-0.00300	0.00000	-0.00300	2.68974
R8	2.52664	-0.00162	-0.00274	0.00000	-0.00275	2.52390
R9	2.06790	0.00331	-0.00457	0.00000	-0.00457	2.06333
R10	2.78804	0.00144	-0.00690	0.00000	-0.00690	2.78114
R11	2.89889	0.00633	0.00797	0.00000	0.00797	2.90686
R12	2.05732	0.00045	0.00155	0.00000	0.00155	2.05887
R13	2.05971	0.00061	0.00194	0.00000	0.00194	2.06165
R14	2.07085	-0.00163	-0.00266	0.00000	-0.00266	2.06819
R15	2.05430	0.00801	0.01223	0.00000	0.01223	2.06653
R16	2.68693	-0.00222	-0.00370	0.00000	-0.00370	2.68323
R17	5.36216	0.00225	-0.01819	0.00000	-0.01819	5.34398
R18	2.50423	0.00164	0.00211	0.00000	0.00211	2.50634
R19	2.04684	0.00061	0.00215	0.00000	0.00215	2.04899

R20	2.03972	0.00135	0.00310	0.00000	0.00310	2.04281
R21	2.04435	0.00077	0.00261	0.00000	0.00261	2.04696
R22	1.81699	0.00184	0.00312	0.00000	0.00312	1.82011
A1	1.87112	0.00173	0.00170	0.00000	0.00172	1.87285
A2	2.27859	-0.00083	0.00200	0.00000	0.00200	2.28058
A3	2.13343	-0.00090	-0.00368	0.00000	-0.00368	2.12976
A4	1.86305	-0.00051	0.00127	0.00000	0.00128	1.86433
A5	2.28442	-0.00019	-0.00102	0.00000	-0.00103	2.28340
A6	2.13543	0.00071	-0.00018	0.00000	-0.00018	2.13524
A7	1.90176	-0.00080	-0.00376	0.00000	-0.00373	1.89803
A8	2.23881	0.00109	0.00392	0.00000	0.00397	2.24278
A9	2.14186	-0.00030	-0.00160	0.00000	-0.00155	2.14031
A10	1.88545	0.00082	0.00278	0.00000	0.00282	1.88828
A11	2.17895	0.00116	0.00689	0.00000	0.00695	2.18590
A12	2.18851	-0.00153	-0.00314	0.00000	-0.00307	2.18544
A13	1.90312	-0.00122	-0.00189	0.00000	-0.00184	1.90128
A14	2.21490	-0.00402	-0.00242	0.00000	-0.00237	2.21253
A15	2.15624	0.00531	0.00029	0.00000	0.00034	2.15659
A16	1.92500	0.01076	0.01393	0.00000	0.01393	1.93894
A17	1.87105	-0.00081	0.00130	0.00000	0.00129	1.87235
A18	1.90392	-0.00633	-0.00752	0.00000	-0.00751	1.89641
A19	1.91610	-0.00126	-0.00574	0.00000	-0.00573	1.91037
A20	1.94311	-0.00367	0.00301	0.00000	0.00301	1.94612
A21	1.90310	0.00131	-0.00536	0.00000	-0.00536	1.89774
A22	1.93089	-0.00567	-0.00765	0.00000	-0.00764	1.92325
A23	1.88293	0.01466	0.01100	0.00000	0.01102	1.89395
A24	1.89268	0.00096	0.00752	0.00000	0.00754	1.90023
A25	1.90624	-0.00099	0.00840	0.00000	0.00840	1.91464
A26	1.90419	-0.00078	-0.01947	0.00000	-0.01947	1.88471
A27	1.94706	-0.00819	0.00007	0.00000	0.00011	1.94717
A28	2.50691	0.01399	0.01497	0.00000	0.01497	2.52188
A29	2.14537	0.00362	0.01524	0.00000	0.01524	2.16061
A30	1.95188	-0.00045	0.00451	0.00000	0.00451	1.95639
A31	2.18566	-0.00316	-0.01981	0.00000	-0.01981	2.16585
A32	2.08819	-0.00027	-0.00599	0.00000	-0.00599	2.08220
A33	2.14458	0.00049	0.00656	0.00000	0.00656	2.15114
A34	2.05040	-0.00022	-0.00056	0.00000	-0.00056	2.04984
A35	1.89440	-0.00182	-0.00683	0.00000	-0.00683	1.88758
D1	-0.00218	-0.00006	0.00757	0.00000	0.00758	0.00540
D2	3.11384	0.00035	0.01089	0.00000	0.01090	3.12474
D3	-3.13392	-0.00054	-0.00116	0.00000	-0.00115	-3.13507
D4	-0.01789	-0.00013	0.00216	0.00000	0.00216	-0.01573
D5	0.01503	-0.00040	-0.02064	0.00000	-0.02065	-0.00562
D6	-2.98636	-0.00153	0.00673	0.00000	0.00673	-2.97964

D7	-3.13542	0.00003	-0.01280	0.00000	-0.01280	3.13497
D8	0.14637	-0.00110	0.01456	0.00000	0.01458	0.16095
D9	-0.01133	0.00052	0.00793	0.00000	0.00794	-0.00339
D10	3.08876	0.00031	-0.01901	0.00000	-0.01900	3.06976
D11	-3.13004	0.00017	0.00498	0.00000	0.00498	-3.12505
D12	-0.02995	-0.00004	-0.02196	0.00000	-0.02195	-0.05190
D13	0.02075	-0.00075	-0.02085	0.00000	-0.02084	-0.00009
D14	2.91155	0.00082	0.00770	0.00000	0.00765	2.91920
D15	-3.08211	-0.00060	0.00397	0.00000	0.00402	-3.07809
D16	-0.19132	0.00098	0.03252	0.00000	0.03251	-0.15881
D17	0.40114	0.00007	0.01980	0.00000	0.01980	0.42094
D18	-2.71666	-0.00012	0.02270	0.00000	0.02269	-2.69398
D19	-2.78711	-0.00017	-0.01051	0.00000	-0.01051	-2.79762
D20	0.37827	-0.00037	-0.00762	0.00000	-0.00762	0.37065
D21	-0.02214	0.00074	0.02563	0.00000	0.02563	0.00350
D22	2.98498	0.00093	-0.00095	0.00000	-0.00093	2.98405
D23	-2.91120	-0.00134	-0.00464	0.00000	-0.00466	-2.91586
D24	0.09592	-0.00114	-0.03121	0.00000	-0.03123	0.06469
D25	1.39288	-0.00294	-0.02787	0.00000	-0.02786	1.36502
D26	-2.80479	0.00114	-0.02606	0.00000	-0.02606	-2.83085
D27	-0.74641	-0.00115	-0.03565	0.00000	-0.03565	-0.78207
D28	-1.58955	-0.00359	0.00346	0.00000	0.00346	-1.58609
D29	0.49596	0.00049	0.00527	0.00000	0.00527	0.50122
D30	2.55434	-0.00180	-0.00432	0.00000	-0.00433	2.55001
D31	-1.10643	0.00155	-0.04895	0.00000	-0.04895	-1.15538
D32	0.97772	0.00604	-0.03645	0.00000	-0.03643	0.94129
D33	3.08908	0.00530	-0.02528	0.00000	-0.02529	3.06379
D34	3.11876	-0.00318	-0.05543	0.00000	-0.05543	3.06333
D35	-1.08027	0.00131	-0.04293	0.00000	-0.04292	-1.12319
D36	1.03109	0.00058	-0.03176	0.00000	-0.03177	0.99931
D37	1.00969	-0.00159	-0.04684	0.00000	-0.04685	0.96284
D38	3.09384	0.00290	-0.03434	0.00000	-0.03433	3.05951
D39	-1.07799	0.00216	-0.02317	0.00000	-0.02319	-1.10117
D40	0.44053	0.00532	0.05391	0.00000	0.05392	0.49445
D41	2.54025	0.00659	0.05625	0.00000	0.05623	2.59648
D42	-1.63653	-0.00029	0.03751	0.00000	0.03752	-1.59901
D43	-1.59205	-0.00729	-0.11452	0.00000	-0.11452	-1.70656
D44	2.58681	-0.00052	-0.09831	0.00000	-0.09832	2.48849
D45	0.47920	0.00647	-0.09601	0.00000	-0.09600	0.38320
D46	-3.09304	-0.00054	-0.00519	0.00000	-0.00519	-3.09823
D47	0.04140	-0.00009	-0.00233	0.00000	-0.00233	0.03907
D48	0.02152	-0.00027	-0.00799	0.00000	-0.00800	0.01352
D49	-3.12723	0.00018	-0.00513	0.00000	-0.00514	-3.13237

Item	Value	Threshold	Converged?

Maximum Force	0.014664	0.000450	NO
RMS Force	0.003414	0.000300	NO
Maximum Displacement	0.165398	0.001800	NO
RMS Displacement	0.038374	0.001200	NO

Predicted change in Energy=-1.685115D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.498385	-2.145455	-1.269181
2	6	0	-1.786600	-1.755765	-1.437890
3	7	0	-2.090352	-0.901689	-0.382359
4	6	0	-1.005886	-0.785571	0.405923
5	7	0	-0.030315	-1.535040	-0.114034
6	6	0	1.360452	-1.508095	0.366575
7	6	0	2.192376	-0.468647	-0.403907
8	1	0	0.121290	-2.795492	-1.862585
9	1	0	-2.496449	-1.990552	-2.210138
10	1	0	1.332845	-1.240466	1.422340
11	1	0	1.782575	-2.509444	0.269880
12	1	0	2.294834	-0.768126	-1.451578
13	1	0	1.682705	0.497069	-0.344701
14	35	0	-0.046775	2.095101	1.221272
15	1	0	-0.875501	-0.039298	1.192215
16	6	0	-3.288229	-0.168014	-0.152718
17	6	0	-4.469973	-0.511517	-0.647243
18	1	0	-3.115508	0.716411	0.450289
19	1	0	-5.326086	0.121387	-0.459933
20	1	0	-4.628711	-1.403155	-1.241481
21	8	0	3.492360	-0.408357	0.164013
22	1	0	3.519682	0.337836	0.772392

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.356399	0.000000			
3	N	2.206301	1.391351	0.000000		
4	C	2.216487	2.224957	1.345711	0.000000	
5	N	1.387826	2.210396	2.171839	1.335589	0.000000
6	C	2.556795	3.636120	3.582831	2.474499	1.471715
7	C	3.286423	4.307905	4.304620	3.314385	2.482253

8	H	1.076417	2.213921	3.266332	3.233642	2.160823
9	H	2.213969	1.074886	2.165945	3.243075	3.268480
10	H	3.378860	4.263495	3.884583	2.590309	2.074952
11	H	2.775603	4.027843	4.243802	3.281122	2.093663
12	H	3.119675	4.199252	4.515631	3.787527	2.789892
13	H	3.548908	4.278598	4.024165	3.071990	2.667792
14	Br	4.938484	4.992725	3.965929	3.143718	3.867976
15	H	3.261378	3.270140	2.167687	1.091870	2.158210
16	C	3.597220	2.535253	1.423349	2.429515	3.533307
17	C	4.339363	3.061661	2.425900	3.631000	4.587207
18	H	4.242192	3.382732	2.088659	2.590062	3.860817
19	H	5.394456	4.124083	3.394507	4.498489	5.559549
20	H	4.196590	2.870628	2.726320	4.027432	4.736430
21	O	4.582314	5.678822	5.631037	4.520513	3.708904
22	H	5.145835	6.117609	5.860235	4.677298	4.110462

		6	7	8	9	10
6	C	0.000000				
7	C	1.538244	0.000000			
8	H	2.856933	3.439672	0.000000		
9	H	4.663465	5.250119	2.760667	0.000000	
10	H	1.089508	2.160944	3.831019	5.331138	0.000000
11	H	1.090980	2.187871	2.718289	4.972905	1.772210
12	H	2.174007	1.094440	3.000572	5.002613	3.067235
13	H	2.151847	1.093562	3.947524	5.208978	2.502771
14	Br	3.961543	3.771977	5.784144	5.870949	3.615216
15	H	2.799738	3.484798	4.233439	4.243922	2.524392
16	C	4.865770	5.494589	4.631642	2.860339	4.998528
17	C	6.001237	6.666929	5.270038	2.919757	6.203808
18	H	4.998966	5.505239	5.306573	3.845616	4.956016
19	H	6.931675	7.541787	6.336365	3.940857	7.052585
20	H	6.202171	6.935565	4.988676	2.414513	6.531658
21	O	2.407382	1.419904	4.601047	6.633685	2.634255
22	H	2.869569	1.948291	5.320707	7.107089	2.774118

		11	12	13	14	15
11	H	0.000000				
12	H	2.501603	0.000000			
13	H	3.070310	1.789021	0.000000		
14	Br	5.045147	4.563478	2.827911	0.000000	
15	H	3.744021	4.191880	3.032197	2.289823	0.000000
16	C	5.601243	5.763485	5.018901	4.185279	2.765260
17	C	6.627758	6.817287	6.242133	5.463560	4.065320
18	H	5.867700	5.923913	4.868569	3.451423	2.477737
19	H	7.614917	7.736473	7.019798	5.881592	4.750065
20	H	6.679271	6.955780	6.651995	6.268739	4.676490

21	O	2.710931	2.042949	2.086490	4.462127	4.502401
22	H	3.372991	2.769377	2.155861	4.001136	4.431266

		16	17	18	19	20
16	C	0.000000				
17	C	1.326299	0.000000			
18	H	1.084278	2.132360	0.000000		
19	H	2.081105	1.081010	2.463577	0.000000	
20	H	2.123175	1.083206	3.105548	1.849697	0.000000
21	O	6.792236	8.004219	6.709023	8.856350	8.301616
22	H	6.889076	8.159127	6.653782	8.933817	8.572225

		21	22
21	O	0.000000	
22	H	0.963159	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.072802	-2.336072	-0.265389
2	6	0	-2.203911	-1.617084	-0.473879
3	7	0	-1.994246	-0.363581	0.092361
4	6	0	-0.762499	-0.333953	0.633524
5	7	0	-0.188615	-1.522520	0.429165
6	6	0	1.228693	-1.801006	0.711354
7	6	0	2.102824	-1.530793	-0.525204
8	1	0	-0.820194	-3.343754	-0.547241
9	1	0	-3.116217	-1.873608	-0.981098
10	1	0	1.533069	-1.140206	1.522356
11	1	0	1.320934	-2.834577	1.048192
12	1	0	1.861209	-2.241822	-1.321356
13	1	0	1.910226	-0.511224	-0.870550
14	35	0	1.123568	2.082522	-0.063873
15	1	0	-0.244227	0.565727	0.971386
16	6	0	-2.849633	0.773814	0.068488
17	6	0	-4.163461	0.705374	-0.099559
18	1	0	-2.298250	1.701103	0.176974
19	1	0	-4.739164	1.619144	-0.146186
20	1	0	-4.701709	-0.229440	-0.198284

```
      21                8                0            3.466106      -1.713688      -0.172869
      22                1                0            3.845366      -0.849076       0.017611
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.7661359           0.5470077           0.3315570
 Standard basis: 6-311++G(d,p) (5D, 7F)
 There are     358 symmetry adapted cartesian basis functions of A      symmetry.
 There are     345 symmetry adapted basis functions of A      symmetry.
    345 basis functions,      553 primitive gaussians,      358 cartesian basis functions
     55 alpha electrons             55 beta electrons
          nuclear repulsion energy             850.1627746966 Hartrees.
 NAtoms=       22 NActive=       22 NUniq=       22 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      345 RedAO= T EigKep=    6.05D-06    NBF=      345
 NBsUse=      345 1.00D-06 EigRej= -1.00D+00 NBFU=      345
 Lowest energy guess from the checkpoint file:    "."
 B after Tr=          0.000000        0.000000        0.000000
             Rot=        0.999997        0.001025       -0.000409       -0.002244 Ang=      0.29 deg.
 B after Tr=          0.000000        0.000000        0.000000
             Rot=        0.999983       -0.002330        0.000918        0.005218 Ang=     -0.66 deg.
 Keep R1 ints in memory in canonical form, NReq=1804729152.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                    energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3032.33895077         A.U. after        9 cycles
                  NFock=    9    Conv=0.29D-08         -V/T= 2.0016
 Calling FoFJK, ICntrl=            2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 ---------------------------------------------------------------------
 Center         Atomic                             Forces (Hartrees/Bohr)
 Number         Number                       X                   Y                   Z
 ---------------------------------------------------------------------
        1              6                0.000437587      -0.000268199       0.000647813
        2              6               -0.000939602      -0.000138899       0.000108728
        3              7               -0.000243330      -0.000421729       0.000251803
        4              6                0.000247865       0.000390985      -0.003601008
        5              7               -0.000232490      -0.000463807       0.000203889
        6              6                0.000316218       0.000012575       0.000158939
        7              6                0.000388703      -0.000075093       0.001415577
```

8	1	-0.000151425	0.000057605	-0.000062022
9	1	0.000133306	-0.000087416	-0.000054951
10	1	-0.000007785	-0.000075762	0.000043398
11	1	-0.000074767	-0.000059099	-0.000056421
12	1	0.000461916	0.000121837	0.000167863
13	1	-0.000259102	0.000240150	-0.000891150
14	35	0.000222627	-0.000068998	0.000346545
15	1	0.000291154	0.000618138	0.002435435
16	6	0.000026731	-0.000067546	-0.000498248
17	6	-0.000068475	0.000342221	-0.000246857
18	1	-0.000076801	-0.000125472	0.000164612
19	1	-0.000264528	-0.000049044	0.000173618
20	1	0.000006317	0.000000256	0.000069668
21	8	-0.000107435	-0.000010433	-0.000941903
22	1	-0.000106685	0.000127729	0.000164671

Cartesian Forces: Max 0.003601008 RMS 0.000640174

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.002208657 RMS 0.000381984

Search for a local minimum.

Step number 44 out of a maximum of 116

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 32 33 38 37 40
39 41 43 42 44

ITU= 0 -1 1 0 -1 0 -1 0 0 1 -1 0 1 1 1 1 1 1 0 -1

ITU= 1 1 1 1 1 0 -1 1 1 1 1 1 1 1 1 1 1 1 1 0

ITU= 0 -1 0 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00122	0.00179	0.00208	0.00493	0.00761
Eigenvalues ---	0.01102	0.01386	0.01693	0.01800	0.02096
Eigenvalues ---	0.02180	0.02375	0.03064	0.03167	0.03804
Eigenvalues ---	0.04583	0.04957	0.05429	0.06246	0.06624
Eigenvalues ---	0.08431	0.09285	0.12632	0.13824	0.14639
Eigenvalues ---	0.15330	0.15892	0.15948	0.16079	0.16436
Eigenvalues ---	0.16933	0.17273	0.21082	0.22533	0.22906
Eigenvalues ---	0.23941	0.24883	0.25827	0.29388	0.32843
Eigenvalues ---	0.33542	0.33863	0.33885	0.34052	0.34232
Eigenvalues ---	0.34669	0.34761	0.36132	0.36298	0.36475
Eigenvalues ---	0.39126	0.43132	0.44560	0.46830	0.49202

Eigenvalues --- 0.53704 0.54823 0.58648 0.61302 1.43475

RFO step: Lambda=-1.97064072D-04 EMin= 1.22136016D-03

Quartic linear search produced a step of -0.02955.

Iteration 1 RMS(Cart)= 0.04201713 RMS(Int)= 0.00096850

Iteration 2 RMS(Cart)= 0.00118739 RMS(Int)= 0.00002166

Iteration 3 RMS(Cart)= 0.00000119 RMS(Int)= 0.00002164

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00002164

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56322	0.00058	-0.00004	0.00123	0.00117	2.56440
R2	2.62261	-0.00007	0.00005	-0.00086	-0.00080	2.62181
R3	2.03413	-0.00009	0.00002	0.00013	0.00015	2.03428
R4	2.62927	-0.00016	0.00004	-0.00062	-0.00059	2.62868
R5	2.03124	-0.00003	0.00000	0.00007	0.00008	2.03132
R6	2.54302	0.00059	0.00007	0.00106	0.00115	2.54417
R7	2.68974	0.00031	-0.00004	-0.00090	-0.00094	2.68880
R8	2.52390	0.00013	-0.00003	-0.00022	-0.00023	2.52366
R9	2.06333	0.00221	-0.00006	0.01496	0.01490	2.07824
R10	2.78114	0.00093	-0.00009	-0.00142	-0.00151	2.77963
R11	2.90686	0.00041	0.00010	0.00047	0.00057	2.90743
R12	2.05887	0.00002	0.00002	-0.00014	-0.00012	2.05875
R13	2.06165	0.00003	0.00002	0.00022	0.00024	2.06189
R14	2.06819	-0.00015	-0.00003	-0.00102	-0.00105	2.06714
R15	2.06653	0.00014	0.00015	-0.00149	-0.00134	2.06520
R16	2.68323	-0.00050	-0.00005	0.00025	0.00020	2.68343
R17	5.34398	0.00002	-0.00023	0.07369	0.07347	5.41744
R18	2.50634	0.00022	0.00003	-0.00014	-0.00012	2.50623
R19	2.04899	-0.00002	0.00003	-0.00050	-0.00047	2.04852
R20	2.04281	0.00021	0.00004	-0.00005	-0.00001	2.04280
R21	2.04696	-0.00004	0.00003	0.00003	0.00007	2.04703
R22	1.82011	0.00020	0.00004	-0.00012	-0.00008	1.82003
A1	1.87285	0.00034	0.00002	-0.00011	-0.00007	1.87278
A2	2.28058	-0.00032	0.00002	0.00061	0.00062	2.28120
A3	2.12976	-0.00002	-0.00005	-0.00050	-0.00056	2.12920
A4	1.86433	-0.00011	0.00002	-0.00084	-0.00083	1.86350
A5	2.28340	-0.00011	-0.00001	0.00009	0.00007	2.28347
A6	2.13524	0.00022	0.00000	0.00081	0.00081	2.13605
A7	1.89803	-0.00019	-0.00005	0.00123	0.00119	1.89922
A8	2.24278	-0.00002	0.00005	0.00126	0.00127	2.24405
A9	2.14031	0.00020	-0.00002	-0.00171	-0.00177	2.13855
A10	1.88828	0.00034	0.00003	-0.00154	-0.00150	1.88677
A11	2.18590	0.00030	0.00008	0.00123	0.00122	2.18712
A12	2.18544	-0.00049	-0.00004	-0.00377	-0.00389	2.18155
A13	1.90128	-0.00038	-0.00002	0.00127	0.00122	1.90250

A14	2.21253	0.00001	-0.00003	0.00090	0.00076	2.21329
A15	2.15659	0.00038	0.00000	0.00141	0.00130	2.15789
A16	1.93894	0.00021	0.00017	0.00332	0.00349	1.94243
A17	1.87235	0.00015	0.00002	0.00227	0.00229	1.87464
A18	1.89641	-0.00036	-0.00009	-0.00042	-0.00051	1.89590
A19	1.91037	-0.00022	-0.00007	-0.00128	-0.00136	1.90901
A20	1.94612	0.00020	0.00004	-0.00392	-0.00388	1.94223
A21	1.89774	0.00002	-0.00007	0.00022	0.00015	1.89789
A22	1.92325	0.00001	-0.00010	0.00185	0.00175	1.92500
A23	1.89395	-0.00033	0.00014	0.00436	0.00450	1.89845
A24	1.90023	0.00086	0.00009	0.00375	0.00385	1.90408
A25	1.91464	0.00029	0.00010	0.00029	0.00037	1.91501
A26	1.88471	-0.00051	-0.00024	-0.00539	-0.00564	1.87907
A27	1.94717	-0.00031	0.00000	-0.00481	-0.00483	1.94234
A28	2.52188	-0.00155	0.00019	-0.03977	-0.03959	2.48229
A29	2.16061	0.00046	0.00019	0.00200	0.00218	2.16279
A30	1.95639	-0.00019	0.00006	0.00180	0.00185	1.95824
A31	2.16585	-0.00026	-0.00025	-0.00362	-0.00387	2.16198
A32	2.08220	0.00013	-0.00007	0.00029	0.00022	2.08241
A33	2.15114	-0.00008	0.00008	0.00059	0.00067	2.15181
A34	2.04984	-0.00005	-0.00001	-0.00088	-0.00089	2.04895
A35	1.88758	-0.00017	-0.00008	0.00001	-0.00008	1.88750
D1	0.00540	0.00006	0.00009	-0.00058	-0.00048	0.00492
D2	3.12474	0.00010	0.00013	0.00239	0.00253	3.12727
D3	-3.13507	-0.00007	-0.00001	0.00365	0.00363	-3.13144
D4	-0.01573	-0.00003	0.00003	0.00662	0.00665	-0.00908
D5	-0.00562	-0.00017	-0.00026	0.00238	0.00212	-0.00350
D6	-2.97964	-0.00025	0.00008	-0.02097	-0.02090	-3.00053
D7	3.13497	-0.00005	-0.00016	-0.00141	-0.00156	3.13341
D8	0.16095	-0.00014	0.00018	-0.02475	-0.02457	0.13638
D9	-0.00339	0.00006	0.00010	-0.00140	-0.00130	-0.00469
D10	3.06976	0.00008	-0.00024	0.01152	0.01129	3.08105
D11	-3.12505	0.00004	0.00006	-0.00405	-0.00399	-3.12905
D12	-0.05190	0.00006	-0.00027	0.00886	0.00860	-0.04330
D13	-0.00009	-0.00016	-0.00026	0.00289	0.00263	0.00255
D14	2.91920	0.00047	0.00010	-0.01664	-0.01657	2.90263
D15	-3.07809	-0.00017	0.00005	-0.00924	-0.00917	-3.08727
D16	-0.15881	0.00046	0.00040	-0.02877	-0.02838	-0.18718
D17	0.42094	-0.00007	0.00025	-0.03517	-0.03491	0.38603
D18	-2.69398	-0.00022	0.00028	-0.04251	-0.04223	-2.73621
D19	-2.79762	-0.00007	-0.00013	-0.02052	-0.02065	-2.81826
D20	0.37065	-0.00021	-0.00009	-0.02787	-0.02797	0.34267
D21	0.00350	0.00020	0.00032	-0.00326	-0.00293	0.00056
D22	2.98405	0.00024	-0.00001	0.01912	0.01912	3.00317

D23	-2.91586	-0.00056	-0.00006	0.01547	0.01538	-2.90048
D24	0.06469	-0.00052	-0.00039	0.03785	0.03744	0.10213
D25	1.36502	0.00032	-0.00035	0.03648	0.03614	1.40116
D26	-2.83085	0.00027	-0.00032	0.03824	0.03793	-2.79292
D27	-0.78207	0.00018	-0.00044	0.03951	0.03908	-0.74299
D28	-1.58609	0.00030	0.00004	0.00996	0.01000	-1.57609
D29	0.50122	0.00025	0.00007	0.01173	0.01179	0.51301
D30	2.55001	0.00016	-0.00005	0.01300	0.01294	2.56295
D31	-1.15538	0.00018	-0.00061	0.01747	0.01686	-1.13852
D32	0.94129	0.00034	-0.00045	0.02164	0.02118	0.96247
D33	3.06379	0.00029	-0.00031	0.02069	0.02038	3.08417
D34	3.06333	0.00001	-0.00069	0.01345	0.01277	3.07609
D35	-1.12319	0.00017	-0.00053	0.01762	0.01709	-1.10610
D36	0.99931	0.00011	-0.00039	0.01667	0.01629	1.01560
D37	0.96284	0.00000	-0.00058	0.01654	0.01595	0.97879
D38	3.05951	0.00016	-0.00043	0.02070	0.02027	3.07979
D39	-1.10117	0.00011	-0.00029	0.01976	0.01947	-1.08170
D40	0.49445	0.00055	0.00067	0.02613	0.02679	0.52125
D41	2.59648	0.00054	0.00070	0.03123	0.03193	2.62840
D42	-1.59901	-0.00011	0.00046	0.02162	0.02209	-1.57693
D43	-1.70656	0.00013	-0.00142	0.07758	0.07616	-1.63041
D44	2.48849	-0.00007	-0.00122	0.07635	0.07515	2.56364
D45	0.38320	0.00009	-0.00119	0.08244	0.08124	0.46444
D46	-3.09823	-0.00028	-0.00006	-0.00437	-0.00443	-3.10266
D47	0.03907	-0.00004	-0.00003	-0.00397	-0.00399	0.03508
D48	0.01352	-0.00012	-0.00010	0.00394	0.00384	0.01736
D49	-3.13237	0.00013	-0.00006	0.00435	0.00428	-3.12809

Item	Value	Threshold	Converged?
Maximum Force	0.002209	0.000450	NO
RMS Force	0.000382	0.000300	NO
Maximum Displacement	0.278347	0.001800	NO
RMS Displacement	0.042662	0.001200	NO

Predicted change in Energy=-1.015134D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.507275	-2.163006	-1.257311
2	6	0	-1.798965	-1.783241	-1.427062
3	7	0	-2.096411	-0.899346	-0.394955
4	6	0	-1.006298	-0.756436	0.382090

5	7	0	-0.032317	-1.516111	-0.125574
6	6	0	1.357169	-1.489040	0.356288
7	6	0	2.195634	-0.454367	-0.414136
8	1	0	0.111602	-2.825870	-1.837354
9	1	0	-2.514944	-2.045640	-2.184682
10	1	0	1.331009	-1.219592	1.411559
11	1	0	1.778800	-2.490832	0.260618
12	1	0	2.287411	-0.746509	-1.464285
13	1	0	1.704214	0.519229	-0.343778
14	35	0	0.027971	2.092934	1.368567
15	1	0	-0.864488	0.027334	1.140416
16	6	0	-3.298224	-0.172165	-0.168329
17	6	0	-4.478649	-0.521140	-0.662009
18	1	0	-3.134346	0.710899	0.438681
19	1	0	-5.338117	0.106505	-0.472413
20	1	0	-4.634042	-1.412492	-1.257622
21	8	0	3.503501	-0.412774	0.137391
22	1	0	3.527117	0.284784	0.801053

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357020	0.000000			
3	N	2.205867	1.391039	0.000000		
4	C	2.217003	2.226137	1.346317	0.000000	
5	N	1.387403	2.210492	2.171048	1.335465	0.000000
6	C	2.556185	3.637042	3.583200	2.474541	1.470916
7	C	3.306979	4.329983	4.315093	3.313245	2.484821
8	H	1.076497	2.214877	3.266088	3.233913	2.160179
9	H	2.214617	1.074926	2.166168	3.244438	3.268603
10	H	3.375231	4.262888	3.887578	2.595635	2.075899
11	H	2.763642	4.018626	4.240267	3.283239	2.092695
12	H	3.139995	4.216002	4.514944	3.775939	2.786677
13	H	3.594386	4.329797	4.057059	3.082382	2.684355
14	Br	5.029389	5.116442	4.071456	3.187751	3.906571
15	H	3.267153	3.277709	2.175715	1.099756	2.162744
16	C	3.597045	2.535301	1.422851	2.428427	3.531879
17	C	4.338424	3.059234	2.426812	3.633556	4.587766
18	H	4.247026	3.388949	2.089293	2.585510	3.860122
19	H	5.394793	4.124087	3.395054	4.498833	5.559199
20	H	4.194459	2.864232	2.728934	4.034798	4.740057
21	O	4.592911	5.695775	5.646164	4.529489	3.713289
22	H	5.148287	6.132568	5.869981	4.670281	4.095294

	6	7	8	9	10

6	C	0.000000				
7	C	1.538546	0.000000			
8	H	2.854929	3.463058	0.000000		
9	H	4.664717	5.277928	2.761908	0.000000	
10	H	1.089442	2.160164	3.823940	5.329789	0.000000
11	H	1.091107	2.185460	2.700609	4.961242	1.772353
12	H	2.175129	1.093884	3.032667	5.026860	3.067408
13	H	2.154919	1.092855	3.994605	5.269608	2.498798
14	Br	3.952469	3.790189	5.871930	6.018288	3.559858
15	H	2.801786	3.465980	4.238000	4.251765	2.539399
16	C	4.866422	5.506590	4.631922	2.861663	5.002294
17	C	6.002544	6.679218	5.269119	2.915266	6.208030
18	H	5.002022	5.522122	5.312744	3.855412	4.961117
19	H	6.932486	7.554825	6.337296	3.941307	7.055857
20	H	6.205254	6.947946	4.985465	2.398102	6.537857
21	O	2.411018	1.420010	4.607345	6.654319	2.644652
22	H	2.837771	1.948301	5.320067	7.131058	2.731073

		11	12	13	14	15
11	H	0.000000				
12	H	2.505322	0.000000			
13	H	3.071046	1.788224	0.000000		
14	Br	5.030295	4.603537	2.866787	0.000000	
15	H	3.755287	4.161462	3.007162	2.261690	0.000000
16	C	5.597891	5.762698	5.053038	4.307702	2.770503
17	C	6.624696	6.817184	6.277853	5.591623	4.075748
18	H	5.867009	5.927964	4.905165	3.574207	2.472236
19	H	7.611439	7.736932	7.055588	6.010825	4.756138
20	H	6.677755	6.956490	6.688808	6.396816	4.693956
21	O	2.703351	2.038534	2.082687	4.457991	4.503231
22	H	3.324565	2.780682	2.165313	3.979385	4.412216

		16	17	18	19	20
16	C	0.000000				
17	C	1.326238	0.000000			
18	H	1.084029	2.129927	0.000000		
19	H	2.081175	1.081004	2.460080	0.000000	
20	H	2.123530	1.083241	3.104082	1.849223	0.000000
21	O	6.812843	8.022812	6.739023	8.877822	8.316556
22	H	6.908964	8.178164	6.684907	8.958007	8.586234

		21	22
21	O	0.000000	
22	H	0.963116	0.000000

Stoichiometry C7H11BrN2O

Framework group C1[X(C7H11BrN2O)]

Deg. of freedom 60

Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.244348	-2.293509	-0.196812
2	6	0	-2.342558	-1.526367	-0.413445
3	7	0	-2.049129	-0.257950	0.076460
4	6	0	-0.801551	-0.265768	0.582480
5	7	0	-0.297877	-1.492653	0.425852
6	6	0	1.103870	-1.839806	0.705467
7	6	0	1.983284	-1.662959	-0.544526
8	1	0	-1.052037	-3.326341	-0.431590
9	1	0	-3.283198	-1.760811	-0.877880
10	1	0	1.454492	-1.171959	1.491551
11	1	0	1.141849	-2.865925	1.074455
12	1	0	1.686410	-2.373993	-1.320978
13	1	0	1.866062	-0.641662	-0.915394
14	35	0	1.313333	2.034426	-0.048498
15	1	0	-0.216119	0.627656	0.844258
16	6	0	-2.846833	0.919164	0.025690
17	6	0	-4.164408	0.914310	-0.125571
18	1	0	-2.251186	1.821345	0.105639
19	1	0	-4.693130	1.854943	-0.190628
20	1	0	-4.751871	0.006654	-0.192342
21	8	0	3.334617	-1.935944	-0.204221
22	1	0	3.759443	-1.103433	0.028245

Rotational constants (GHZ): 0.7636795 0.5313754 0.3244201
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 358 symmetry adapted cartesian basis functions of A symmetry.
There are 345 symmetry adapted basis functions of A symmetry.
345 basis functions, 553 primitive gaussians, 358 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 845.6798846037 Hartrees.
NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 5.94D-06 NBF= 345
NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345
Initial guess from the checkpoint file: "."
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999498 0.002268 -0.000093 0.031592 Ang= 3.63 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.33910416 A.U. after 12 cycles
NFock= 12 Conv=0.97D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000265187	-0.000108994	0.000544853
2	6	-0.000685183	-0.000329283	0.000187833
3	7	0.000321225	-0.000339530	0.000365977
4	6	0.000121743	0.002166339	-0.003257027
5	7	-0.000939766	-0.000403212	0.000367611
6	6	0.001580491	0.000263934	0.000167625
7	6	0.001257728	0.000164747	0.001414817
8	1	-0.000305297	-0.000119307	0.000026363
9	1	0.000227475	-0.000097121	-0.000088395
10	1	-0.000339808	-0.000075505	0.000139861
11	1	-0.000258935	-0.000008649	-0.000110777
12	1	0.000362696	-0.000025770	0.000044739
13	1	-0.000897941	0.000462112	-0.000842754

14	35	0.000042279	-0.001058158	0.000145340
15	1	0.000625791	-0.000323339	0.001892377
16	6	-0.000350785	0.000025595	-0.000291599
17	6	-0.000164392	0.000208690	-0.000449053
18	1	0.000011295	-0.000206561	0.000160911
19	1	-0.000224519	-0.000042548	0.000209200
20	1	0.000049406	0.000059592	0.000065583
21	8	-0.000544751	-0.000834568	-0.000958537
22	1	-0.000153939	0.000621537	0.000265052

Cartesian Forces: Max 0.003257027 RMS 0.000723812

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.004811456 RMS 0.000752898
Search for a local minimum.
Step number 45 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 33 38 37 40 39
41 43 42 44 45
DE= -1.53D-04 DEPred=-1.02D-04 R= 1.51D+00
TightC=F SS= 1.41D+00 RLast= 2.10D-01 DXNew= 1.8507D-01 6.2955D-01
Trust test= 1.51D+00 RLast= 2.10D-01 DXMaxT set to 1.85D-01
ITU= 1 0 -1 1 0 -1 0 -1 0 0 1 -1 0 1 1 1 1 1 1 0
ITU= -1 1 1 1 1 1 0 -1 1 1 1 1 1 1 1 1 1 1 1 1
ITU= 0 0 -1 0 0

Eigenvalues ---	0.00085	0.00154	0.00232	0.00527	0.00822
Eigenvalues ---	0.01180	0.01376	0.01476	0.01757	0.02142
Eigenvalues ---	0.02243	0.02381	0.03065	0.03169	0.03835
Eigenvalues ---	0.04528	0.04990	0.05465	0.06141	0.06496
Eigenvalues ---	0.08644	0.09326	0.12232	0.13835	0.14678
Eigenvalues ---	0.15560	0.15927	0.15986	0.16193	0.16378
Eigenvalues ---	0.17053	0.17880	0.21148	0.22629	0.22945
Eigenvalues ---	0.24446	0.25020	0.25630	0.29321	0.33068
Eigenvalues ---	0.33734	0.33862	0.33887	0.34101	0.34248
Eigenvalues ---	0.34723	0.34961	0.36282	0.36309	0.36935
Eigenvalues ---	0.37268	0.43161	0.44591	0.46620	0.49479
Eigenvalues ---	0.53736	0.54863	0.58427	0.61208	1.60711

En-DIIS/RFO-DIIS IScMMF= 0 using points: 45 44
RFO step: Lambda=-8.42040326D-05.

DidBck=F Rises=F RFO-DIIS coefs: 2.03979 -1.03979
Maximum step size (0.185) exceeded in Quadratic search.
-- Step size scaled by 0.526
Iteration 1 RMS(Cart)= 0.08583596 RMS(Int)= 0.00295146
Iteration 2 RMS(Cart)= 0.00478196 RMS(Int)= 0.00012216
Iteration 3 RMS(Cart)= 0.00001481 RMS(Int)= 0.00012173
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00012173

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56440	0.00025	0.00064	0.00083	0.00139	2.56579
R2	2.62181	-0.00020	-0.00044	-0.00152	-0.00193	2.61988
R3	2.03428	-0.00012	0.00008	0.00001	0.00010	2.03438
R4	2.62868	0.00010	-0.00032	-0.00090	-0.00130	2.62739
R5	2.03132	-0.00007	0.00004	-0.00011	-0.00007	2.03125
R6	2.54417	0.00038	0.00063	0.00129	0.00195	2.54613
R7	2.68880	0.00055	-0.00051	-0.00173	-0.00225	2.68655
R8	2.52366	0.00009	-0.00013	-0.00075	-0.00078	2.52289
R9	2.07824	0.00116	0.00815	0.02006	0.02822	2.10645
R10	2.77963	0.00106	-0.00083	0.00005	-0.00077	2.77886
R11	2.90743	-0.00044	0.00031	-0.00122	-0.00091	2.90652
R12	2.05875	0.00012	-0.00007	-0.00025	-0.00032	2.05843
R13	2.06189	-0.00008	0.00013	0.00000	0.00013	2.06202
R14	2.06714	0.00000	-0.00057	-0.00011	-0.00068	2.06646
R15	2.06520	-0.00019	-0.00073	-0.00194	-0.00267	2.06252
R16	2.68343	-0.00092	0.00011	0.00070	0.00081	2.68424
R17	5.41744	-0.00052	0.04019	0.11689	0.15707	5.57451
R18	2.50623	0.00030	-0.00006	-0.00010	-0.00016	2.50607
R19	2.04852	-0.00007	-0.00026	-0.00155	-0.00180	2.04672
R20	2.04280	0.00019	-0.00001	-0.00035	-0.00035	2.04245
R21	2.04703	-0.00010	0.00004	-0.00041	-0.00037	2.04666
R22	1.82003	0.00062	-0.00004	-0.00039	-0.00043	1.81959
A1	1.87278	0.00013	-0.00004	-0.00046	-0.00038	1.87240
A2	2.28120	-0.00031	0.00034	0.00015	0.00042	2.28162
A3	2.12920	0.00018	-0.00031	0.00030	-0.00008	2.12912
A4	1.86350	0.00001	-0.00045	-0.00133	-0.00176	1.86175
A5	2.28347	-0.00025	0.00004	-0.00118	-0.00117	2.28230
A6	2.13605	0.00025	0.00044	0.00263	0.00304	2.13909
A7	1.89922	-0.00021	0.00065	0.00235	0.00291	1.90213
A8	2.24405	-0.00015	0.00070	0.00177	0.00214	2.24620
A9	2.13855	0.00037	-0.00097	-0.00250	-0.00380	2.13475
A10	1.88677	0.00013	-0.00082	-0.00325	-0.00395	1.88282
A11	2.18712	0.00094	0.00066	0.00730	0.00756	2.19467
A12	2.18155	-0.00088	-0.00213	-0.00876	-0.01117	2.17038
A13	1.90250	-0.00007	0.00067	0.00270	0.00315	1.90565

A14	2.21329	0.00080	0.00041	0.00154	0.00131	2.21460
A15	2.15789	-0.00075	0.00071	0.00130	0.00137	2.15926
A16	1.94243	-0.00129	0.00191	0.00480	0.00671	1.94914
A17	1.87464	-0.00002	0.00125	0.00174	0.00298	1.87761
A18	1.89590	0.00044	-0.00028	-0.00241	-0.00268	1.89323
A19	1.90901	0.00004	-0.00075	-0.00020	-0.00098	1.90803
A20	1.94223	0.00095	-0.00212	-0.00495	-0.00708	1.93516
A21	1.89789	-0.00014	0.00008	0.00120	0.00128	1.89916
A22	1.92500	0.00090	0.00096	0.00170	0.00265	1.92766
A23	1.89845	-0.00329	0.00246	0.00386	0.00631	1.90476
A24	1.90408	0.00107	0.00211	-0.00073	0.00139	1.90546
A25	1.91501	0.00082	0.00020	0.00008	0.00024	1.91525
A26	1.87907	-0.00074	-0.00309	-0.00066	-0.00376	1.87532
A27	1.94234	0.00132	-0.00264	-0.00429	-0.00695	1.93539
A28	2.48229	-0.00481	-0.02166	-0.06166	-0.08332	2.39897
A29	2.16279	0.00037	0.00119	0.00380	0.00496	2.16775
A30	1.95824	-0.00025	0.00101	0.00182	0.00280	1.96104
A31	2.16198	-0.00012	-0.00212	-0.00544	-0.00759	2.15439
A32	2.08241	0.00008	0.00012	0.00006	0.00018	2.08259
A33	2.15181	-0.00008	0.00037	0.00159	0.00196	2.15377
A34	2.04895	0.00000	-0.00049	-0.00165	-0.00214	2.04682
A35	1.88750	-0.00041	-0.00004	0.00023	0.00018	1.88768
D1	0.00492	0.00010	-0.00026	-0.00133	-0.00154	0.00338
D2	3.12727	0.00014	0.00139	0.00571	0.00712	3.13439
D3	-3.13144	-0.00012	0.00199	0.00235	0.00434	-3.12710
D4	-0.00908	-0.00008	0.00364	0.00938	0.01300	0.00391
D5	-0.00350	-0.00023	0.00116	0.00407	0.00520	0.00169
D6	-3.00053	-0.00004	-0.01143	-0.03786	-0.04936	-3.04989
D7	3.13341	-0.00004	-0.00085	0.00079	-0.00005	3.13335
D8	0.13638	0.00015	-0.01344	-0.04114	-0.05461	0.08177
D9	-0.00469	0.00006	-0.00071	-0.00184	-0.00259	-0.00729
D10	3.08105	0.00014	0.00617	0.03108	0.03730	3.11835
D11	-3.12905	0.00003	-0.00219	-0.00810	-0.01032	-3.13937
D12	-0.04330	0.00011	0.00470	0.02482	0.02957	-0.01374
D13	0.00255	-0.00021	0.00144	0.00440	0.00584	0.00838
D14	2.90263	0.00047	-0.00906	-0.01730	-0.02655	2.87607
D15	-3.08727	-0.00026	-0.00502	-0.02628	-0.03121	-3.11848
D16	-0.18718	0.00042	-0.01552	-0.04798	-0.06360	-0.25078
D17	0.38603	-0.00019	-0.01910	-0.09577	-0.11480	0.27124
D18	-2.73621	-0.00031	-0.02310	-0.10624	-0.12933	-2.86555
D19	-2.81826	-0.00012	-0.01129	-0.05864	-0.06994	-2.88821
D20	0.34267	-0.00024	-0.01530	-0.06911	-0.08448	0.25819
D21	0.00056	0.00027	-0.00161	-0.00523	-0.00681	-0.00624
D22	3.00317	0.00024	0.01046	0.03510	0.04564	3.04881

D23	-2.90048	-0.00072	0.00841	0.01360	0.02180	-2.87868
D24	0.10213	-0.00075	0.02048	0.05394	0.07425	0.17637
D25	1.40116	0.00089	0.01977	0.06060	0.08037	1.48153
D26	-2.79292	0.00018	0.02075	0.06424	0.08501	-2.70791
D27	-0.74299	0.00023	0.02138	0.06533	0.08672	-0.65627
D28	-1.57609	0.00103	0.00547	0.01282	0.01827	-1.55782
D29	0.51301	0.00032	0.00645	0.01646	0.02291	0.53592
D30	2.56295	0.00037	0.00708	0.01755	0.02461	2.58756
D31	-1.13852	-0.00027	0.00922	0.03679	0.04601	-1.09251
D32	0.96247	-0.00078	0.01159	0.04035	0.05194	1.01441
D33	3.08417	-0.00054	0.01115	0.03702	0.04818	3.13235
D34	3.07609	0.00052	0.00698	0.03183	0.03881	3.11490
D35	-1.10610	0.00000	0.00935	0.03539	0.04474	-1.06136
D36	1.01560	0.00025	0.00891	0.03207	0.04098	1.05658
D37	0.97879	0.00006	0.00873	0.03360	0.04231	1.02110
D38	3.07979	-0.00045	0.01109	0.03716	0.04824	3.12803
D39	-1.08170	-0.00021	0.01065	0.03383	0.04448	-1.03722
D40	0.52125	-0.00018	0.01466	0.00351	0.01815	0.53940
D41	2.62840	-0.00062	0.01746	0.00803	0.02550	2.65390
D42	-1.57693	-0.00019	0.01208	0.00458	0.01668	-1.56025
D43	-1.63041	0.00117	0.04166	0.03123	0.07289	-1.55751
D44	2.56364	-0.00008	0.04111	0.02999	0.07111	2.63475
D45	0.46444	-0.00140	0.04444	0.03287	0.07728	0.54172
D46	-3.10266	-0.00029	-0.00242	-0.00811	-0.01051	-3.11316
D47	0.03508	-0.00005	-0.00218	-0.00790	-0.01006	0.02502
D48	0.01736	-0.00015	0.00210	0.00366	0.00574	0.02310
D49	-3.12809	0.00008	0.00234	0.00387	0.00618	-3.12190

Item	Value	Threshold	Converged?
Maximum Force	0.004811	0.000450	NO
RMS Force	0.000753	0.000300	NO
Maximum Displacement	0.557394	0.001800	NO
RMS Displacement	0.088260	0.001200	NO

Predicted change in Energy=-2.503763D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.526547	-2.197555	-1.225135
2	6	0	-1.824783	-1.838724	-1.396387
3	7	0	-2.108479	-0.890133	-0.420287
4	6	0	-1.006759	-0.689041	0.328801

5	7	0	-0.036980	-1.471603	-0.150254
6	6	0	1.349403	-1.445766	0.339306
7	6	0	2.204971	-0.425735	-0.430878
8	1	0	0.088600	-2.891003	-1.772565
9	1	0	-2.553134	-2.162313	-2.117623
10	1	0	1.321223	-1.170167	1.392760
11	1	0	1.766640	-2.449995	0.249322
12	1	0	2.268029	-0.700403	-1.487464
13	1	0	1.755578	0.564123	-0.333577
14	35	0	0.165143	2.041971	1.663527
15	1	0	-0.839314	0.165806	1.024306
16	6	0	-3.321905	-0.185554	-0.191625
17	6	0	-4.494114	-0.533587	-0.704931
18	1	0	-3.183266	0.676631	0.449055
19	1	0	-5.363348	0.075272	-0.500269
20	1	0	-4.635435	-1.405846	-1.331171
21	8	0	3.525878	-0.435848	0.091369
22	1	0	3.568947	0.202592	0.810875

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357757	0.000000			
3	N	2.204460	1.390353	0.000000		
4	C	2.218318	2.228723	1.347351	0.000000	
5	N	1.386381	2.209947	2.168440	1.335054	0.000000
6	C	2.555749	3.639025	3.583665	2.474721	1.470508
7	C	3.351325	4.378089	4.338390	3.310839	2.489766
8	H	1.076548	2.215815	3.264858	3.234840	2.159250
9	H	2.214685	1.074889	2.167282	3.247583	3.267821
10	H	3.364990	4.257190	3.889526	2.604418	2.077612
11	H	2.737966	3.997540	4.230614	3.286186	2.090444
12	H	3.181185	4.249139	4.508734	3.744754	2.774157
13	H	3.691861	4.440971	4.129566	3.104782	2.718649
14	Br	5.176523	5.327540	4.255452	3.257802	3.959275
15	H	3.277695	3.293789	2.193772	1.114688	2.168972
16	C	3.595876	2.534916	1.421661	2.425746	3.527941
17	C	4.333704	3.050708	2.428868	3.640660	4.588418
18	H	4.256995	3.402667	2.089418	2.572294	3.856578
19	H	5.393127	4.121632	3.395965	4.500155	5.557475
20	H	4.185810	2.844539	2.735174	4.054208	4.748124
21	O	4.610742	5.728093	5.675751	4.545908	3.718216
22	H	5.165183	6.175055	5.911258	4.686629	4.090160

	6	7	8	9	10

6	C	0.000000				
7	C	1.538064	0.000000			
8	H	2.852777	3.515209	0.000000		
9	H	4.666876	5.338574	2.762031	0.000000	
10	H	1.089272	2.158898	3.807875	5.321446	0.000000
11	H	1.091174	2.180007	2.664269	4.934130	1.773078
12	H	2.176357	1.093523	3.103211	5.077193	3.068030
13	H	2.158101	1.091440	4.097243	5.401969	2.485289
14	Br	3.914121	3.825834	6.012223	6.273924	3.424568
15	H	2.803011	3.425661	4.245891	4.269547	2.566808
16	C	4.867355	5.537264	4.631455	2.864970	5.003836
17	C	6.005763	6.705555	5.262938	2.901008	6.214796
18	H	5.006166	5.569792	5.326229	3.878724	4.958998
19	H	6.933936	7.585201	6.335714	3.939534	7.058198
20	H	6.213725	6.968666	4.971623	2.350899	6.554168
21	O	2.412146	1.420436	4.617024	6.694379	2.663334
22	H	2.804609	1.948634	5.325157	7.186706	2.697280

		11	12	13	14	15
11	H	0.000000				
12	H	2.515728	0.000000			
13	H	3.069983	1.786921	0.000000		
14	Br	4.974186	4.676696	2.949906	0.000000	
15	H	3.772799	4.088384	2.955667	2.222056	0.000000
16	C	5.587076	5.761218	5.134492	4.534640	2.786611
17	C	6.616665	6.809314	6.356219	5.826815	4.103288
18	H	5.858092	5.946674	5.001735	3.814570	2.466975
19	H	7.601025	7.733960	7.137638	6.254129	4.774872
20	H	6.676434	6.941174	6.761733	6.625799	4.735916
21	O	2.678928	2.035900	2.077133	4.461593	4.504138
22	H	3.255744	2.791084	2.174576	3.961844	4.413578

		16	17	18	19	20
16	C	0.000000				
17	C	1.326154	0.000000			
18	H	1.083075	2.124766	0.000000		
19	H	2.081053	1.080817	2.452673	0.000000	
20	H	2.124392	1.083044	3.100760	1.847692	0.000000
21	O	6.858197	8.060020	6.810151	8.923543	8.340956
22	H	6.974203	8.237267	6.778495	9.028909	8.630604

		21	22
21	O	0.000000	
22	H	0.962886	0.000000

Stoichiometry C7H11BrN2O

Framework group C1[X(C7H11BrN2O)]

Deg. of freedom 60

Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.503309	-2.201757	-0.048762
2	6	0	-2.556304	-1.375523	-0.276891
3	7	0	-2.131708	-0.090740	0.042690
4	6	0	-0.852797	-0.143716	0.463328
5	7	0	-0.455865	-1.417234	0.408880
6	6	0	0.920361	-1.855775	0.684702
7	6	0	1.785342	-1.846236	-0.587052
8	1	0	-1.404421	-3.265854	-0.178660
9	1	0	-3.546541	-1.584180	-0.639215
10	1	0	1.344921	-1.167565	1.414517
11	1	0	0.883784	-2.854558	1.122601
12	1	0	1.390410	-2.552116	-1.322956
13	1	0	1.791092	-0.839367	-1.008267
14	35	0	1.611454	1.932676	-0.015565
15	1	0	-0.163124	0.726441	0.561847
16	6	0	-2.851767	1.131707	-0.048198
17	6	0	-4.168226	1.212968	-0.186094
18	1	0	-2.202526	1.997102	0.003076
19	1	0	-4.632230	2.185148	-0.274018
20	1	0	-4.818743	0.347699	-0.219604
21	8	0	3.102207	-2.265456	-0.258782
22	1	0	3.612038	-1.486953	-0.011488

Rotational constants (GHZ): 0.7676239 0.5015114 0.3123818
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 358 symmetry adapted cartesian basis functions of A symmetry.
There are 345 symmetry adapted basis functions of A symmetry.
345 basis functions, 553 primitive gaussians, 358 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 838.4540754159 Hartrees.
NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 5.50D-06 NBF= 345
NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345
Initial guess from the checkpoint file: "."
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.998858 0.004401 -0.000663 0.047571 Ang= 5.48 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.33910719 A.U. after 13 cycles
NFock= 13 Conv=0.78D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000030261	0.000238877	0.000257610
2	6	-0.000253639	-0.000435850	0.000395452
3	7	-0.000004595	-0.000582141	0.001060620
4	6	0.000515951	0.006470255	-0.004472704
5	7	-0.001196661	-0.000846942	0.001404577
6	6	0.003136204	0.000496100	-0.000056613
7	6	0.002476494	0.000192438	0.001611098
8	1	-0.000392617	-0.000392842	0.000239204
9	1	0.000302216	-0.000171449	-0.000099286
10	1	-0.000723845	0.000226064	0.000277431
11	1	-0.000442737	0.000032392	-0.000287622
12	1	0.000343728	-0.000191332	-0.000046238
13	1	-0.002200872	0.000907862	-0.000688589

14	35	-0.000144812	-0.002438098	-0.000927495
15	1	0.000774738	-0.003193868	0.002752849
16	6	-0.000936637	-0.000027096	-0.000349264
17	6	-0.000257550	0.000038197	-0.000702537
18	1	0.000400143	0.000058058	0.000090220
19	1	-0.000243739	0.000016575	0.000319951
20	1	0.000003257	0.000121367	0.000018385
21	8	-0.001048338	-0.001642189	-0.001398528
22	1	-0.000136949	0.001123619	0.000601477

Cartesian Forces: Max 0.006470255 RMS 0.001399914

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.007669806 RMS 0.001497889

Search for a local minimum.

Step number 46 out of a maximum of 116

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 43 44 45 46

DE= -3.03D-06 DEPred=-2.50D-04 R= 1.21D-02

Trust test= 1.21D-02 RLast= 3.95D-01 DXMaxT set to 9.25D-02

ITU= -1 1 0 -1 1 0 -1 0 -1 0 0 1 -1 0 1 1 1 1 1 1

ITU= 0 -1 1 1 1 1 1 0 -1 1 1 1 1 1 1 1 1 1 1 1

ITU= 1 0 0 -1 0 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00126	0.00220	0.00378	0.00570	0.00902
Eigenvalues ---	0.01184	0.01387	0.01497	0.01729	0.02130
Eigenvalues ---	0.02274	0.02468	0.03061	0.03158	0.03756
Eigenvalues ---	0.04232	0.04943	0.05528	0.06091	0.06197
Eigenvalues ---	0.08535	0.09324	0.11981	0.13523	0.14253
Eigenvalues ---	0.15505	0.15945	0.16009	0.16089	0.16447
Eigenvalues ---	0.17064	0.18212	0.20307	0.22548	0.22946
Eigenvalues ---	0.24619	0.25073	0.25679	0.29040	0.32614
Eigenvalues ---	0.33732	0.33857	0.33888	0.34127	0.34250
Eigenvalues ---	0.34614	0.34829	0.36283	0.36292	0.36859
Eigenvalues ---	0.37280	0.43034	0.44366	0.46616	0.49222
Eigenvalues ---	0.53369	0.54890	0.57904	0.60785	1.75188

RFO step: Lambda=-4.44843362D-04 EMin= 1.25518781D-03

Quartic linear search produced a step of -0.45213.

Maximum step size (0.093) exceeded in Quadratic search.

-- Step size scaled by 0.725

Iteration 1 RMS(Cart)= 0.02476752 RMS(Int)= 0.00054247
Iteration 2 RMS(Cart)= 0.00052065 RMS(Int)= 0.00017993
Iteration 3 RMS(Cart)= 0.00000015 RMS(Int)= 0.00017993

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56579	0.00016	-0.00063	0.00117	0.00037	2.56616
R2	2.61988	-0.00046	0.00087	-0.00012	0.00068	2.62056
R3	2.03438	-0.00009	-0.00004	-0.00001	-0.00005	2.03433
R4	2.62739	0.00060	0.00059	0.00006	0.00062	2.62800
R5	2.03125	-0.00009	0.00003	-0.00004	-0.00001	2.03123
R6	2.54613	0.00063	-0.00088	0.00197	0.00124	2.54736
R7	2.68655	0.00088	0.00102	-0.00172	-0.00071	2.68584
R8	2.52289	0.00043	0.00035	-0.00060	-0.00012	2.52276
R9	2.10645	-0.00062	-0.01276	0.01070	-0.00206	2.10440
R10	2.77886	0.00086	0.00035	-0.00213	-0.00178	2.77707
R11	2.90652	-0.00134	0.00041	0.00216	0.00257	2.90909
R12	2.05843	0.00035	0.00015	0.00003	0.00017	2.05860
R13	2.06202	-0.00018	-0.00006	0.00085	0.00079	2.06281
R14	2.06646	0.00011	0.00031	-0.00185	-0.00154	2.06492
R15	2.06252	-0.00057	0.00121	-0.00003	0.00117	2.06370
R16	2.68424	-0.00139	-0.00036	0.00033	-0.00003	2.68421
R17	5.57451	-0.00177	-0.07102	0.07310	0.00208	5.57660
R18	2.50607	0.00054	0.00007	0.00031	0.00038	2.50644
R19	2.04672	0.00015	0.00081	-0.00034	0.00048	2.04720
R20	2.04245	0.00027	0.00016	0.00067	0.00083	2.04328
R21	2.04666	-0.00011	0.00017	0.00044	0.00061	2.04727
R22	1.81959	0.00119	0.00020	-0.00041	-0.00021	1.81938
A1	1.87240	-0.00013	0.00017	0.00127	0.00133	1.87373
A2	2.28162	-0.00018	-0.00019	-0.00048	-0.00062	2.28099
A3	2.12912	0.00031	0.00004	-0.00087	-0.00079	2.12833
A4	1.86175	0.00039	0.00079	-0.00018	0.00056	1.86231
A5	2.28230	-0.00055	0.00053	-0.00110	-0.00054	2.28176
A6	2.13909	0.00016	-0.00137	0.00126	-0.00008	2.13901
A7	1.90213	-0.00056	-0.00132	-0.00139	-0.00239	1.89973
A8	2.24620	-0.00013	-0.00097	0.00066	-0.00035	2.24584
A9	2.13475	0.00070	0.00172	0.00078	0.00245	2.13720
A10	1.88282	-0.00001	0.00179	0.00186	0.00308	1.88590
A11	2.19467	0.00218	-0.00342	0.01371	0.00920	2.20387
A12	2.17038	-0.00169	0.00505	0.00145	0.00532	2.17570
A13	1.90565	0.00031	-0.00143	-0.00150	-0.00255	1.90310
A14	2.21460	0.00224	-0.00059	-0.00149	-0.00197	2.21263
A15	2.15926	-0.00259	-0.00062	0.00465	0.00415	2.16341
A16	1.94914	-0.00319	-0.00303	0.00466	0.00163	1.95077
A17	1.87761	-0.00061	-0.00135	0.00356	0.00222	1.87984

A18	1.89323	0.00190	0.00121	-0.00160	-0.00040	1.89283
A19	1.90803	0.00063	0.00044	-0.00220	-0.00175	1.90628
A20	1.93516	0.00150	0.00320	-0.00436	-0.00116	1.93400
A21	1.89916	-0.00023	-0.00058	0.00009	-0.00048	1.89868
A22	1.92766	0.00220	-0.00120	0.00122	0.00004	1.92770
A23	1.90476	-0.00677	-0.00285	0.00744	0.00456	1.90932
A24	1.90546	0.00111	-0.00063	0.00897	0.00833	1.91379
A25	1.91525	0.00101	-0.00011	-0.00137	-0.00148	1.91377
A26	1.87532	-0.00113	0.00170	-0.01336	-0.01166	1.86366
A27	1.93539	0.00375	0.00314	-0.00312	-0.00004	1.93536
A28	2.39897	-0.00767	0.03767	-0.04331	-0.00564	2.39334
A29	2.16775	0.00066	-0.00224	0.00523	0.00300	2.17075
A30	1.96104	-0.00072	-0.00126	0.00105	-0.00020	1.96083
A31	2.15439	0.00006	0.00343	-0.00625	-0.00281	2.15158
A32	2.08259	-0.00008	-0.00008	0.00083	0.00074	2.08334
A33	2.15377	0.00006	-0.00089	0.00115	0.00026	2.15403
A34	2.04682	0.00002	0.00097	-0.00197	-0.00100	2.04582
A35	1.88768	-0.00054	-0.00008	0.00027	0.00019	1.88787
D1	0.00338	0.00008	0.00070	0.00024	0.00090	0.00428
D2	3.13439	0.00016	-0.00322	-0.00150	-0.00471	3.12968
D3	-3.12710	-0.00020	-0.00196	0.00978	0.00780	-3.11930
D4	0.00391	-0.00013	-0.00588	0.00804	0.00219	0.00611
D5	0.00169	-0.00022	-0.00235	-0.00421	-0.00655	-0.00486
D6	-3.04989	0.00028	0.02232	-0.02470	-0.00235	-3.05224
D7	3.13335	0.00003	0.00002	-0.01273	-0.01271	3.12064
D8	0.08177	0.00053	0.02469	-0.03322	-0.00851	0.07325
D9	-0.00729	0.00008	0.00117	0.00378	0.00500	-0.00229
D10	3.11835	0.00011	-0.01686	0.00728	-0.00955	3.10880
D11	-3.13937	0.00002	0.00467	0.00536	0.01004	-3.12933
D12	-0.01374	0.00005	-0.01337	0.00885	-0.00450	-0.01824
D13	0.00838	-0.00022	-0.00264	-0.00640	-0.00910	-0.00071
D14	2.87607	0.00125	0.01201	0.05790	0.07014	2.94621
D15	-3.11848	-0.00024	0.01411	-0.00963	0.00439	-3.11409
D16	-0.25078	0.00123	0.02875	0.05467	0.08362	-0.16716
D17	0.27124	-0.00022	0.05190	-0.03825	0.01362	0.28486
D18	-2.86555	-0.00018	0.05848	-0.04277	0.01570	-2.84984
D19	-2.88821	-0.00020	0.03162	-0.03436	-0.00273	-2.89094
D20	0.25819	-0.00016	0.03820	-0.03888	-0.00065	0.25754
D21	-0.00624	0.00027	0.00308	0.00655	0.00966	0.00342
D22	3.04881	0.00008	-0.02063	0.02589	0.00524	3.05405
D23	-2.87868	-0.00193	-0.00986	-0.05903	-0.06875	-2.94743
D24	0.17637	-0.00211	-0.03357	-0.03969	-0.07317	0.10320
D25	1.48153	0.00106	-0.03634	0.00999	-0.02636	1.45517
D26	-2.70791	-0.00045	-0.03844	0.01234	-0.02611	-2.73401

D27	-0.65627	-0.00004	-0.03921	0.01353	-0.02568	-0.68195
D28	-1.55782	0.00144	-0.00826	-0.01294	-0.02118	-1.57901
D29	0.53592	-0.00007	-0.01036	-0.01058	-0.02093	0.51499
D30	2.58756	0.00034	-0.01113	-0.00939	-0.02051	2.56705
D31	-1.09251	-0.00131	-0.02080	0.02472	0.00392	-1.08859
D32	1.01441	-0.00302	-0.02348	0.02855	0.00505	1.01946
D33	3.13235	-0.00192	-0.02178	0.03486	0.01309	-3.13774
D34	3.11490	0.00101	-0.01755	0.01883	0.00128	3.11619
D35	-1.06136	-0.00069	-0.02023	0.02265	0.00241	-1.05895
D36	1.05658	0.00041	-0.01853	0.02897	0.01045	1.06703
D37	1.02110	-0.00004	-0.01913	0.02285	0.00372	1.02482
D38	3.12803	-0.00174	-0.02181	0.02667	0.00485	3.13287
D39	-1.03722	-0.00064	-0.02011	0.03299	0.01289	-1.02433
D40	0.53940	-0.00160	-0.00821	-0.02881	-0.03701	0.50239
D41	2.65390	-0.00251	-0.01153	-0.02348	-0.03501	2.61889
D42	-1.56025	-0.00096	-0.00754	-0.04277	-0.05032	-1.61057
D43	-1.55751	0.00243	-0.03296	0.07763	0.04466	-1.51286
D44	2.63475	-0.00018	-0.03215	0.07889	0.04676	2.68151
D45	0.54172	-0.00289	-0.03494	0.09069	0.05574	0.59746
D46	-3.11316	-0.00024	0.00475	-0.00549	-0.00075	-3.11391
D47	0.02502	-0.00002	0.00455	-0.00350	0.00104	0.02606
D48	0.02310	-0.00029	-0.00259	-0.00046	-0.00304	0.02006
D49	-3.12190	-0.00007	-0.00280	0.00153	-0.00126	-3.12316

Item	Value	Threshold	Converged?
Maximum Force	0.007670	0.000450	NO
RMS Force	0.001498	0.000300	NO
Maximum Displacement	0.116624	0.001800	NO
RMS Displacement	0.024926	0.001200	NO

Predicted change in Energy=-3.104254D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.519526	-2.178561	-1.228627
2	6	0	-1.820044	-1.827061	-1.399316
3	7	0	-2.113582	-0.890576	-0.414014
4	6	0	-1.011521	-0.686479	0.334935
5	7	0	-0.036243	-1.462047	-0.144146
6	6	0	1.348483	-1.437165	0.347315
7	6	0	2.213751	-0.432010	-0.434222
8	1	0	0.103081	-2.857198	-1.786039

9	1	0	-2.542673	-2.145098	-2.128721
10	1	0	1.322297	-1.147614	1.397166
11	1	0	1.760394	-2.445161	0.270827
12	1	0	2.274851	-0.718451	-1.486945
13	1	0	1.776804	0.565255	-0.349738
14	35	0	0.141962	2.051540	1.606456
15	1	0	-0.865940	0.122706	1.086021
16	6	0	-3.329494	-0.190059	-0.188423
17	6	0	-4.501067	-0.538338	-0.703526
18	1	0	-3.194706	0.673490	0.451670
19	1	0	-5.371883	0.069059	-0.498916
20	1	0	-4.641595	-1.410679	-1.330387
21	8	0	3.540485	-0.448238	0.072836
22	1	0	3.586516	0.165806	0.812946

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357952	0.000000			
3	N	2.205338	1.390679	0.000000		
4	C	2.216551	2.227614	1.348006	0.000000	
5	N	1.386742	2.211478	2.171347	1.334988	0.000000
6	C	2.553962	3.638998	3.586681	2.476551	1.469564
7	C	3.339510	4.375966	4.351610	3.325468	2.491504
8	H	1.076520	2.215659	3.265524	3.233093	2.159090
9	H	2.214591	1.074882	2.167524	3.246783	3.269142
10	H	3.368969	4.261017	3.892520	2.605319	2.078495
11	H	2.741801	3.998870	4.230063	3.283380	2.089645
12	H	3.163415	4.243213	4.520968	3.757727	2.774383
13	H	3.684305	4.445459	4.154357	3.132151	2.727519
14	Br	5.135077	5.284664	4.222064	3.231723	3.929587
15	H	3.282290	3.299819	2.198513	1.113599	2.170979
16	C	3.596121	2.534655	1.421287	2.427619	3.530640
17	C	4.338057	3.054966	2.430632	3.643800	4.593561
18	H	4.256075	3.401264	2.089148	2.574769	3.858938
19	H	5.397188	4.125718	3.397739	4.503210	5.562302
20	H	4.194216	2.852941	2.738812	4.058965	4.755951
21	O	4.601252	5.727448	5.692202	4.565766	3.723960
22	H	5.150112	6.172237	5.925579	4.700726	4.085377

		6	7	8	9	10
6	C	0.000000				
7	C	1.539423	0.000000			
8	H	2.849336	3.487674	0.000000		
9	H	4.666157	5.331939	2.761256	0.000000	

10	H	1.089364	2.158880	3.813391	5.325866	0.000000
11	H	1.091593	2.180688	2.673417	4.936016	1.773188
12	H	2.176974	1.092707	3.062724	5.065149	3.067513
13	H	2.163106	1.092061	4.071546	5.400803	2.488408
14	Br	3.900281	3.824224	5.967096	6.226603	3.416369
15	H	2.807589	3.478986	4.250594	4.276556	2.549295
16	C	4.870910	5.553965	4.631261	2.864615	5.007011
17	C	6.010774	6.721058	5.267554	2.906573	6.220586
18	H	5.010621	5.590916	5.324330	3.876596	4.961219
19	H	6.938886	7.602440	6.339944	3.945019	7.063106
20	H	6.220645	6.982598	4.981163	2.362664	6.563288
21	O	2.420369	1.420421	4.590670	6.688124	2.676441
22	H	2.791974	1.948664	5.294108	7.180573	2.681991

		11	12	13	14	15
11	H	0.000000				
12	H	2.517133	0.000000			
13	H	3.073755	1.785830	0.000000		
14	Br	4.962211	4.668103	2.951007	0.000000	
15	H	3.762460	4.146356	3.039958	2.237659	0.000000
16	C	5.585996	5.777027	5.164378	4.505260	2.791259
17	C	6.617494	6.823434	6.383945	5.796655	4.105315
18	H	5.857618	5.967560	5.036852	3.790239	2.475665
19	H	7.601524	7.750413	7.167439	6.226180	4.776864
20	H	6.679782	6.952763	6.786886	6.595030	4.737707
21	O	2.682467	2.026761	2.077573	4.488968	4.557313
22	H	3.231990	2.791392	2.187796	4.006320	4.461030

		16	17	18	19	20
16	C	0.000000				
17	C	1.326353	0.000000			
18	H	1.083329	2.123578	0.000000		
19	H	2.082042	1.081256	2.451336	0.000000	
20	H	2.124995	1.083366	3.100479	1.847779	0.000000
21	O	6.879791	8.079445	6.838464	8.945658	8.357138
22	H	6.997183	8.258602	6.809789	9.054460	8.647600

		21	22
21	O	0.000000	
22	H	0.962772	0.000000

Stoichiometry C7H11BrN2O

Framework group C1[X(C7H11BrN2O)]

Deg. of freedom 60

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.427602	-2.225265	-0.073543
2	6	0	-2.503347	-1.427085	-0.296510
3	7	0	-2.121881	-0.135796	0.051405
4	6	0	-0.843220	-0.159375	0.477538
5	7	0	-0.407980	-1.419645	0.410607
6	6	0	0.975619	-1.826280	0.693306
7	6	0	1.847251	-1.806002	-0.575422
8	1	0	-1.293583	-3.282082	-0.228691
9	1	0	-3.481683	-1.658537	-0.676854
10	1	0	1.384691	-1.126091	1.420704
11	1	0	0.958879	-2.823753	1.136413
12	1	0	1.469143	-2.521321	-1.309834
13	1	0	1.840653	-0.801552	-1.003950
14	35	0	1.539209	1.965753	-0.024359
15	1	0	-0.193296	0.726192	0.660501
16	6	0	-2.875346	1.066322	-0.033797
17	6	0	-4.192651	1.115667	-0.180381
18	1	0	-2.250636	1.949246	0.027721
19	1	0	-4.681441	2.076667	-0.262106
20	1	0	-4.821363	0.234555	-0.225589
21	8	0	3.170137	-2.210224	-0.252668
22	1	0	3.660013	-1.432680	0.034346

Rotational constants (GHZ): 0.7658861 0.5059747 0.3140008
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 358 symmetry adapted cartesian basis functions of A symmetry.
There are 345 symmetry adapted basis functions of A symmetry.
345 basis functions, 553 primitive gaussians, 358 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 839.4412417077 Hartrees.
NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F
Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 345 RedAO= T EigKep= 5.50D-06 NBF= 345
NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345
Initial guess from the checkpoint file: "."
B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999916 0.000355 0.000144 -0.012988 Ang= 1.49 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.33929518 A.U. after 12 cycles
NFock= 12 Conv=0.29D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000324867	0.000233101	-0.000344003
2	6	0.000531230	-0.000501501	0.000125837
3	7	0.001591008	0.000296779	0.000781536
4	6	-0.000850546	0.003954028	0.000917313
5	7	-0.002042538	0.000377185	0.000498316
6	6	0.004339753	0.000780596	0.000198845
7	6	0.002813959	0.000571193	0.000362501
8	1	-0.000439628	-0.000501125	0.000278785
9	1	0.000268016	-0.000071840	-0.000117311
10	1	-0.001084596	0.000130608	0.000304464
11	1	-0.000478234	0.000263743	-0.000300200
12	1	-0.000399008	-0.000369960	-0.000564304
13	1	-0.002403068	0.000322415	-0.000339972
14	35	-0.000012508	-0.001976424	-0.000241713
15	1	0.000776069	-0.002890985	-0.001841974
16	6	-0.001294257	0.000504573	0.000326484
17	6	-0.000231632	-0.000431652	-0.000831462

18	1	0.000503981	-0.000075237	0.000033640
19	1	0.000112678	-0.000032448	0.000263904
20	1	0.000112565	0.000234241	0.000096603
21	8	-0.001529286	-0.002175036	-0.000246935
22	1	0.000040909	0.001357746	0.000639645

Cartesian Forces: Max 0.004339753 RMS 0.001178503

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.007993782 RMS 0.001416651
Search for a local minimum.
Step number 47 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 43 44 45 46 47
DE= -1.88D-04 DEPred=-3.10D-04 R= 6.06D-01
TightC=F SS= 1.41D+00 RLast= 2.00D-01 DXNew= 1.5563D-01 6.0038D-01
Trust test= 6.06D-01 RLast= 2.00D-01 DXMaxT set to 1.56D-01
ITU= 1 -1 1 0 -1 1 0 -1 0 -1 0 0 1 -1 0 1 1 1 1 1
ITU= 1 0 -1 1 1 1 1 1 0 -1 1 1 1 1 1 1 1 1 1 1
ITU= 1 1 0 0 -1 0 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00147	0.00236	0.00337	0.00555	0.00941
Eigenvalues ---	0.01255	0.01380	0.01714	0.01893	0.02147
Eigenvalues ---	0.02343	0.02499	0.03057	0.03146	0.03847
Eigenvalues ---	0.04307	0.04965	0.05531	0.06085	0.06147
Eigenvalues ---	0.09121	0.09318	0.11776	0.13643	0.14405
Eigenvalues ---	0.15538	0.15930	0.16005	0.16081	0.16629
Eigenvalues ---	0.17098	0.18539	0.20452	0.22513	0.22946
Eigenvalues ---	0.24602	0.25152	0.25740	0.29206	0.32668
Eigenvalues ---	0.33830	0.33876	0.33922	0.34145	0.34287
Eigenvalues ---	0.34544	0.34862	0.36266	0.36303	0.36763
Eigenvalues ---	0.39872	0.43059	0.44293	0.46552	0.49215
Eigenvalues ---	0.53401	0.55668	0.57845	0.60756	2.11317

RFO step: Lambda=-1.72971349D-04 EMin= 1.47492071D-03
Quartic linear search produced a step of -0.19867.
Iteration 1 RMS(Cart)= 0.01893176 RMS(Int)= 0.00016209
Iteration 2 RMS(Cart)= 0.00016851 RMS(Int)= 0.00003796
Iteration 3 RMS(Cart)= 0.00000003 RMS(Int)= 0.00003796

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X

R1	2.56616	-0.00069	-0.00007	0.00005	0.00001	2.56617
R2	2.62056	-0.00013	-0.00014	-0.00036	-0.00048	2.62008
R3	2.03433	-0.00008	0.00001	-0.00014	-0.00013	2.03420
R4	2.62800	0.00072	-0.00012	0.00040	0.00028	2.62829
R5	2.03123	-0.00008	0.00000	-0.00013	-0.00013	2.03111
R6	2.54736	-0.00088	-0.00025	-0.00053	-0.00081	2.54655
R7	2.68584	0.00077	0.00014	0.00118	0.00132	2.68717
R8	2.52276	-0.00029	0.00002	-0.00043	-0.00044	2.52232
R9	2.10440	-0.00324	0.00041	0.00002	0.00043	2.10483
R10	2.77707	0.00114	0.00035	0.00241	0.00277	2.77984
R11	2.90909	-0.00213	-0.00051	-0.00124	-0.00175	2.90734
R12	2.05860	0.00036	-0.00003	0.00019	0.00015	2.05875
R13	2.06281	-0.00040	-0.00016	-0.00037	-0.00053	2.06229
R14	2.06492	0.00062	0.00031	0.00090	0.00121	2.06613
R15	2.06370	-0.00059	-0.00023	0.00008	-0.00016	2.06354
R16	2.68421	-0.00124	0.00001	-0.00048	-0.00048	2.68373
R17	5.57660	-0.00115	-0.00041	0.01328	0.01287	5.58947
R18	2.50644	0.00025	-0.00007	0.00008	0.00000	2.50645
R19	2.04720	0.00002	-0.00010	-0.00012	-0.00022	2.04698
R20	2.04328	-0.00006	-0.00017	-0.00003	-0.00019	2.04308
R21	2.04727	-0.00026	-0.00012	-0.00042	-0.00055	2.04672
R22	1.81938	0.00136	0.00004	0.00036	0.00040	1.81978
A1	1.87373	-0.00045	-0.00026	-0.00005	-0.00030	1.87343
A2	2.28099	-0.00005	0.00012	-0.00087	-0.00075	2.28024
A3	2.12833	0.00051	0.00016	0.00095	0.00110	2.12942
A4	1.86231	0.00022	-0.00011	-0.00008	-0.00018	1.86212
A5	2.28176	-0.00039	0.00011	-0.00130	-0.00119	2.28056
A6	2.13901	0.00017	0.00002	0.00139	0.00140	2.14041
A7	1.89973	-0.00017	0.00048	-0.00025	0.00016	1.89990
A8	2.24584	-0.00017	0.00007	-0.00005	0.00005	2.24589
A9	2.13720	0.00034	-0.00049	0.00038	-0.00008	2.13713
A10	1.88590	-0.00009	-0.00061	0.00034	-0.00017	1.88573
A11	2.20387	0.00139	-0.00183	0.00602	0.00443	2.20830
A12	2.17570	-0.00130	-0.00106	-0.00412	-0.00492	2.17078
A13	1.90310	0.00049	0.00051	0.00005	0.00050	1.90359
A14	2.21263	0.00159	0.00039	0.00088	0.00129	2.21392
A15	2.16341	-0.00211	-0.00082	-0.00025	-0.00106	2.16234
A16	1.95077	-0.00303	-0.00032	0.00016	-0.00016	1.95061
A17	1.87984	-0.00042	-0.00044	-0.00186	-0.00230	1.87754
A18	1.89283	0.00141	0.00008	-0.00180	-0.00172	1.89111
A19	1.90628	0.00062	0.00035	0.00138	0.00173	1.90801
A20	1.93400	0.00163	0.00023	0.00009	0.00031	1.93431
A21	1.89868	-0.00021	0.00010	0.00202	0.00211	1.90079
A22	1.92770	0.00177	-0.00001	0.00015	0.00014	1.92784

A23	1.90932	-0.00636	-0.00091	-0.00126	-0.00217	1.90715
A24	1.91379	0.00023	-0.00165	-0.00315	-0.00480	1.90899
A25	1.91377	0.00137	0.00029	0.00026	0.00055	1.91432
A26	1.86366	-0.00027	0.00232	0.00292	0.00523	1.86889
A27	1.93536	0.00350	0.00001	0.00118	0.00118	1.93654
A28	2.39334	-0.00799	0.00112	-0.00910	-0.00798	2.38535
A29	2.17075	-0.00012	-0.00060	0.00065	0.00005	2.17080
A30	1.96083	-0.00046	0.00004	-0.00190	-0.00186	1.95898
A31	2.15158	0.00058	0.00056	0.00126	0.00182	2.15340
A32	2.08334	-0.00021	-0.00015	-0.00004	-0.00019	2.08314
A33	2.15403	0.00004	-0.00005	0.00025	0.00019	2.15423
A34	2.04582	0.00017	0.00020	-0.00020	0.00000	2.04581
A35	1.88787	-0.00033	-0.00004	0.00075	0.00071	1.88858
D1	0.00428	0.00007	-0.00018	-0.00064	-0.00081	0.00346
D2	3.12968	0.00000	0.00094	0.00012	0.00105	3.13073
D3	-3.11930	-0.00012	-0.00155	-0.00266	-0.00421	-3.12351
D4	0.00611	-0.00019	-0.00044	-0.00190	-0.00235	0.00376
D5	-0.00486	0.00000	0.00130	0.00203	0.00333	-0.00152
D6	-3.05224	0.00048	0.00047	-0.00586	-0.00541	-3.05765
D7	3.12064	0.00016	0.00253	0.00382	0.00635	3.12699
D8	0.07325	0.00064	0.00169	-0.00408	-0.00239	0.07086
D9	-0.00229	-0.00011	-0.00099	-0.00095	-0.00195	-0.00424
D10	3.10880	-0.00008	0.00190	0.00192	0.00380	3.11260
D11	-3.12933	-0.00004	-0.00200	-0.00160	-0.00360	-3.13293
D12	-0.01824	-0.00001	0.00089	0.00127	0.00215	-0.01609
D13	-0.00071	0.00010	0.00181	0.00222	0.00404	0.00332
D14	2.94621	-0.00011	-0.01393	0.01375	-0.00023	2.94598
D15	-3.11409	0.00009	-0.00087	-0.00042	-0.00128	-3.11537
D16	-0.16716	-0.00012	-0.01661	0.01110	-0.00555	-0.17271
D17	0.28486	-0.00020	-0.00271	-0.02968	-0.03238	0.25248
D18	-2.84984	-0.00015	-0.00312	-0.03140	-0.03451	-2.88436
D19	-2.89094	-0.00018	0.00054	-0.02647	-0.02593	-2.91687
D20	0.25754	-0.00013	0.00013	-0.02819	-0.02806	0.22948
D21	0.00342	-0.00006	-0.00192	-0.00263	-0.00455	-0.00113
D22	3.05405	-0.00029	-0.00104	0.00507	0.00403	3.05807
D23	-2.94743	-0.00023	0.01366	-0.01532	-0.00168	-2.94911
D24	0.10320	-0.00045	0.01454	-0.00762	0.00690	0.11010
D25	1.45517	0.00130	0.00524	0.01360	0.01883	1.47401
D26	-2.73401	-0.00003	0.00519	0.01420	0.01938	-2.71463
D27	-0.68195	0.00025	0.00510	0.01461	0.01972	-0.66223
D28	-1.57901	0.00168	0.00421	0.00456	0.00877	-1.57024
D29	0.51499	0.00035	0.00416	0.00517	0.00932	0.52431
D30	2.56705	0.00062	0.00407	0.00558	0.00966	2.57671
D31	-1.08859	-0.00072	-0.00078	0.00873	0.00795	-1.08064

D32	1.01946	-0.00199	-0.00100	0.00833	0.00732	1.02678
D33	-3.13774	-0.00158	-0.00260	0.00697	0.00437	-3.13337
D34	3.11619	0.00129	-0.00026	0.01004	0.00978	3.12597
D35	-1.05895	0.00001	-0.00048	0.00964	0.00916	-1.04979
D36	1.06703	0.00043	-0.00208	0.00828	0.00621	1.07324
D37	1.02482	0.00015	-0.00074	0.00660	0.00586	1.03069
D38	3.13287	-0.00113	-0.00096	0.00620	0.00524	3.13811
D39	-1.02433	-0.00072	-0.00256	0.00485	0.00229	-1.02204
D40	0.50239	-0.00119	0.00735	-0.00172	0.00564	0.50802
D41	2.61889	-0.00217	0.00696	-0.00216	0.00479	2.62368
D42	-1.61057	0.00046	0.01000	0.00229	0.01229	-1.59828
D43	-1.51286	0.00219	-0.00887	-0.03178	-0.04065	-1.55351
D44	2.68151	0.00011	-0.00929	-0.03193	-0.04122	2.64029
D45	0.59746	-0.00335	-0.01107	-0.03468	-0.04575	0.55171
D46	-3.11391	-0.00015	0.00015	-0.00493	-0.00479	-3.11870
D47	0.02606	-0.00004	-0.00021	-0.00203	-0.00223	0.02382
D48	0.02006	-0.00021	0.00060	-0.00304	-0.00244	0.01762
D49	-3.12316	-0.00009	0.00025	-0.00014	0.00011	-3.12305

Item	Value	Threshold	Converged?
Maximum Force	0.007994	0.000450	NO
RMS Force	0.001417	0.000300	NO
Maximum Displacement	0.097460	0.001800	NO
RMS Displacement	0.018949	0.001200	NO

Predicted change in Energy=-9.713877D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.524597	-2.192093	-1.218932
2	6	0	-1.825638	-1.842047	-1.388670
3	7	0	-2.114260	-0.892550	-0.414216
4	6	0	-1.009953	-0.681292	0.328638
5	7	0	-0.036479	-1.460986	-0.146754
6	6	0	1.349934	-1.433638	0.344201
7	6	0	2.211517	-0.425646	-0.435927
8	1	0	0.093642	-2.880977	-1.768446
9	1	0	-2.551037	-2.170980	-2.110353
10	1	0	1.321307	-1.146316	1.394686
11	1	0	1.762737	-2.440689	0.264146
12	1	0	2.265909	-0.705752	-1.491385
13	1	0	1.774605	0.570687	-0.341874

14	35	0	0.156559	2.030480	1.658030
15	1	0	-0.855942	0.135581	1.069995
16	6	0	-3.330564	-0.190963	-0.189649
17	6	0	-4.498564	-0.528178	-0.720006
18	1	0	-3.197306	0.661387	0.465404
19	1	0	-5.369968	0.076688	-0.510996
20	1	0	-4.635976	-1.389810	-1.361695
21	8	0	3.538108	-0.448388	0.070548
22	1	0	3.596316	0.188601	0.790409

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357959	0.000000			
3	N	2.205314	1.390829	0.000000		
4	C	2.216543	2.227519	1.347575	0.000000	
5	N	1.386486	2.211031	2.170676	1.334755	0.000000
6	C	2.555877	3.640591	3.587285	2.476960	1.471028
7	C	3.349590	4.383210	4.350956	3.320811	2.491793
8	H	1.076451	2.215230	3.265365	3.233311	2.159443
9	H	2.213941	1.074815	2.168418	3.246967	3.268458
10	H	3.366305	4.258448	3.890970	2.605279	2.078133
11	H	2.737374	3.995824	4.229423	3.284425	2.089457
12	H	3.173383	4.247644	4.514540	3.747580	2.771173
13	H	3.699799	4.458567	4.155667	3.125828	2.728698
14	Br	5.154707	5.311116	4.242044	3.237552	3.935078
15	H	3.281317	3.300963	2.200750	1.113827	2.168184
16	C	3.596859	2.535455	1.421988	2.427814	3.530693
17	C	4.337045	3.052523	2.431292	3.646026	4.594448
18	H	4.257077	3.403857	2.088406	2.570215	3.856168
19	H	5.396866	4.124818	3.398297	4.504359	5.562663
20	H	4.191358	2.846620	2.739349	4.062914	4.757786
21	O	4.605306	5.730740	5.690479	4.561328	3.721592
22	H	5.165954	6.186235	5.935545	4.710378	4.098366

		6	7	8	9	10
6	C	0.000000				
7	C	1.538497	0.000000			
8	H	2.852427	3.505660	0.000000		
9	H	4.667557	5.341518	2.759587	0.000000	
10	H	1.089445	2.159394	3.810724	5.322620	0.000000
11	H	1.091315	2.179887	2.666676	4.931494	1.774368
12	H	2.176742	1.093347	3.086602	5.072769	3.068513
13	H	2.160640	1.091978	4.095696	5.418066	2.483791
14	Br	3.892352	3.826233	5.988915	6.259717	3.393821

15	H	2.802698	3.462959	4.249480	4.278807	2.547371
16	C	4.871991	5.552512	4.631842	2.866573	5.006268
17	C	6.013096	6.716874	5.265287	2.902539	6.222935
18	H	5.008114	5.590116	5.326233	3.882589	4.954716
19	H	6.940427	7.598479	6.338769	3.944151	7.064030
20	H	6.224397	6.976734	4.975773	2.348976	6.568573
21	O	2.415308	1.420169	4.600406	6.693381	2.674818
22	H	2.806598	1.949069	5.314017	7.195276	2.706071

		11	12	13	14	15
11	H	0.000000				
12	H	2.518944	0.000000			
13	H	3.071773	1.786631	0.000000		
14	Br	4.951169	4.674948	2.957818	0.000000	
15	H	3.760856	4.124859	3.017030	2.227462	0.000000
16	C	5.586493	5.768885	5.163916	4.528659	2.795905
17	C	6.620434	6.810628	6.379901	5.819962	4.112587
18	H	5.853665	5.961946	5.037839	3.813814	2.474668
19	H	7.603519	7.738216	7.163627	6.250158	4.783244
20	H	6.685150	6.936914	6.780791	6.617062	4.746429
21	O	2.675573	2.030852	2.078112	4.483276	4.543963
22	H	3.248405	2.788625	2.178689	3.997151	4.461343

		16	17	18	19	20
16	C	0.000000				
17	C	1.326355	0.000000			
18	H	1.083214	2.124508	0.000000		
19	H	2.081843	1.081153	2.452690	0.000000	
20	H	2.124859	1.083078	3.100882	1.847444	0.000000
21	O	6.878417	8.075856	6.837639	8.942467	8.351841
22	H	7.006158	8.265725	6.817804	9.060928	8.654107

		21	22
21	O	0.000000	
22	H	0.962986	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.463177	-2.214202	-0.042319

2	6	0	-2.532504	-1.407599	-0.265884
3	7	0	-2.130172	-0.114191	0.049762
4	6	0	-0.846826	-0.145101	0.459671
5	7	0	-0.426975	-1.411088	0.408943
6	6	0	0.956128	-1.828376	0.686111
7	6	0	1.818813	-1.825887	-0.587758
8	1	0	-1.345992	-3.276047	-0.174605
9	1	0	-3.519202	-1.636204	-0.625599
10	1	0	1.373931	-1.125216	1.405763
11	1	0	0.931540	-2.822268	1.136156
12	1	0	1.424549	-2.538064	-1.317667
13	1	0	1.822981	-0.822356	-1.018252
14	35	0	1.575394	1.949622	-0.016491
15	1	0	-0.179696	0.732912	0.616648
16	6	0	-2.871865	1.095327	-0.045141
17	6	0	-4.187262	1.156738	-0.203814
18	1	0	-2.238162	1.971240	0.022305
19	1	0	-4.666490	2.122239	-0.287716
20	1	0	-4.823597	0.281784	-0.254702
21	8	0	3.136624	-2.245669	-0.265210
22	1	0	3.648532	-1.467878	-0.019577

Rotational constants (GHZ): 0.7673294 0.5028156 0.3128935

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 838.8681765319 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 5.32D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Initial guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999982 0.000405 -0.000224 0.006060 Ang= 0.70 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.33945663 A.U. after 12 cycles
NFock= 12 Conv=0.23D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000385310	0.000342206	-0.000363804
2	6	0.000554693	-0.000387611	0.000135986
3	7	0.000714474	0.000133021	0.000616661
4	6	-0.000263443	0.004003978	-0.000022775
5	7	-0.001545843	-0.000168555	0.000840948
6	6	0.003117740	0.000590096	0.000070690
7	6	0.002431673	0.000385884	0.000673104
8	1	-0.000312390	-0.000435567	0.000239822
9	1	0.000195187	-0.000068173	-0.000081750
10	1	-0.000725646	0.000148327	0.000203036
11	1	-0.000348820	0.000161671	-0.000220174
12	1	-0.000197641	-0.000279959	-0.000241157
13	1	-0.002208893	0.000436746	-0.000484583
14	35	0.000100775	-0.001911173	-0.000364973
15	1	0.000476949	-0.002412095	-0.000972249
16	6	-0.000720717	0.000085899	0.000288494
17	6	-0.000163830	-0.000274009	-0.000502694
18	1	0.000309400	0.000020935	-0.000038225
19	1	0.000072641	0.000046773	0.000191027
20	1	0.000055287	0.000150770	-0.000006103
21	8	-0.001061917	-0.001516109	-0.000485728
22	1	-0.000094369	0.000946945	0.000524446

Cartesian Forces: Max 0.004003978 RMS 0.000961539

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.007408910 RMS 0.001259645

Search for a local minimum.

Step number 48 out of a maximum of 116

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 43 45 46 47 48

DE= -1.61D-04 DEPred=-9.71D-05 R= 1.66D+00

TightC=F SS= 1.41D+00 RLast= 1.09D-01 DXNew= 2.6173D-01 3.2648D-01

Trust test= 1.66D+00 RLast= 1.09D-01 DXMaxT set to 2.62D-01

ITU= 1 1 -1 1 0 -1 1 0 -1 0 -1 0 0 1 -1 0 1 1 1 1

ITU= 1 1 0 -1 1 1 1 1 1 0 -1 1 1 1 1 1 1 1 1 1

ITU= 1 1 1 0 0 -1 0 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00130	0.00222	0.00345	0.00586	0.00938
Eigenvalues ---	0.01144	0.01370	0.01727	0.01859	0.02147
Eigenvalues ---	0.02336	0.02504	0.03046	0.03173	0.03887
Eigenvalues ---	0.04455	0.04983	0.05506	0.06039	0.06349
Eigenvalues ---	0.08732	0.09303	0.11733	0.13822	0.14553
Eigenvalues ---	0.15240	0.15821	0.15969	0.16089	0.16642
Eigenvalues ---	0.17098	0.17469	0.20846	0.22433	0.22949
Eigenvalues ---	0.24585	0.25031	0.25885	0.29273	0.32612
Eigenvalues ---	0.33225	0.33864	0.33892	0.34001	0.34239
Eigenvalues ---	0.34508	0.34766	0.35392	0.36301	0.36355
Eigenvalues ---	0.38600	0.43164	0.44214	0.46516	0.49267
Eigenvalues ---	0.53593	0.55114	0.57848	0.60803	1.41558

RFO step: Lambda=-3.93506163D-04 EMin= 1.29603952D-03

Quartic linear search produced a step of 2.00000.

Iteration 1 RMS(Cart)= 0.09435127 RMS(Int)= 0.00388873

Iteration 2 RMS(Cart)= 0.00483470 RMS(Int)= 0.00021403

Iteration 3 RMS(Cart)= 0.00001279 RMS(Int)= 0.00021394

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00021394

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56617	-0.00056	0.00003	-0.00074	-0.00083	2.56534
R2	2.62008	-0.00009	-0.00097	-0.00056	-0.00154	2.61854
R3	2.03420	-0.00002	-0.00026	0.00028	0.00002	2.03422
R4	2.62829	0.00058	0.00057	0.00135	0.00186	2.63015

R5	2.03111	-0.00006	-0.00025	-0.00043	-0.00068	2.03042
R6	2.54655	-0.00046	-0.00163	-0.00020	-0.00175	2.54480
R7	2.68717	0.00039	0.00265	-0.00117	0.00148	2.68865
R8	2.52232	-0.00002	-0.00088	-0.00114	-0.00190	2.52042
R9	2.10483	-0.00235	0.00086	0.00593	0.00679	2.11162
R10	2.77984	0.00083	0.00553	0.00568	0.01121	2.79105
R11	2.90734	-0.00167	-0.00350	-0.00010	-0.00360	2.90374
R12	2.05875	0.00026	0.00031	0.00048	0.00079	2.05954
R13	2.06229	-0.00026	-0.00105	-0.00049	-0.00155	2.06074
R14	2.06613	0.00029	0.00242	-0.00113	0.00130	2.06742
R15	2.06354	-0.00058	-0.00031	0.00088	0.00057	2.06411
R16	2.68373	-0.00105	-0.00095	-0.00229	-0.00324	2.68049
R17	5.58947	-0.00125	0.02574	0.04507	0.07081	5.66027
R18	2.50645	0.00018	0.00001	0.00017	0.00017	2.50662
R19	2.04698	0.00003	-0.00044	-0.00109	-0.00153	2.04545
R20	2.04308	0.00000	-0.00039	-0.00015	-0.00054	2.04255
R21	2.04672	-0.00012	-0.00109	-0.00063	-0.00172	2.04500
R22	1.81978	0.00101	0.00081	0.00127	0.00208	1.82186
A1	1.87343	-0.00030	-0.00060	0.00002	-0.00054	1.87289
A2	2.28024	-0.00004	-0.00150	-0.00192	-0.00346	2.27678
A3	2.12942	0.00035	0.00219	0.00194	0.00408	2.13351
A4	1.86212	0.00025	-0.00037	-0.00014	-0.00051	1.86161
A5	2.28056	-0.00034	-0.00239	-0.00440	-0.00681	2.27375
A6	2.14041	0.00009	0.00280	0.00461	0.00740	2.14781
A7	1.89990	-0.00018	0.00033	-0.00054	-0.00016	1.89974
A8	2.24589	-0.00002	0.00010	0.00279	0.00264	2.24854
A9	2.13713	0.00020	-0.00015	-0.00184	-0.00223	2.13490
A10	1.88573	-0.00011	-0.00034	0.00016	-0.00029	1.88544
A11	2.20830	0.00111	0.00886	0.02290	0.03129	2.23960
A12	2.17078	-0.00095	-0.00985	-0.01167	-0.02234	2.14843
A13	1.90359	0.00035	0.00099	0.00052	0.00149	1.90508
A14	2.21392	0.00139	0.00258	-0.00005	0.00206	2.21598
A15	2.16234	-0.00177	-0.00212	0.00153	-0.00104	2.16131
A16	1.95061	-0.00279	-0.00032	0.00389	0.00358	1.95419
A17	1.87754	-0.00022	-0.00460	-0.00462	-0.00923	1.86830
A18	1.89111	0.00134	-0.00344	-0.00553	-0.00897	1.88214
A19	1.90801	0.00040	0.00346	0.00078	0.00424	1.91225
A20	1.93431	0.00148	0.00063	-0.00096	-0.00034	1.93397
A21	1.90079	-0.00021	0.00423	0.00644	0.01062	1.91141
A22	1.92784	0.00162	0.00029	0.00094	0.00125	1.92909
A23	1.90715	-0.00582	-0.00434	-0.00206	-0.00641	1.90074
A24	1.90899	0.00060	-0.00960	0.00290	-0.00672	1.90228
A25	1.91432	0.00122	0.00110	0.00394	0.00502	1.91934
A26	1.86889	-0.00046	0.01047	-0.00555	0.00490	1.87379

A27	1.93654	0.00302	0.00236	-0.00017	0.00211	1.93865
A28	2.38535	-0.00741	-0.01596	-0.06417	-0.08014	2.30522
A29	2.17080	0.00009	0.00010	0.00717	0.00727	2.17807
A30	1.95898	-0.00035	-0.00371	-0.00352	-0.00723	1.95175
A31	2.15340	0.00025	0.00364	-0.00366	-0.00003	2.15337
A32	2.08314	-0.00023	-0.00038	-0.00214	-0.00252	2.08062
A33	2.15423	0.00009	0.00039	0.00344	0.00382	2.15805
A34	2.04581	0.00013	0.00000	-0.00129	-0.00130	2.04451
A35	1.88858	-0.00044	0.00142	-0.00285	-0.00143	1.88715
D1	0.00346	0.00008	-0.00163	-0.00184	-0.00363	-0.00017
D2	3.13073	0.00006	0.00210	0.00325	0.00530	3.13603
D3	-3.12351	-0.00013	-0.00842	-0.00507	-0.01348	-3.13699
D4	0.00376	-0.00015	-0.00469	0.00001	-0.00456	-0.00080
D5	-0.00152	-0.00011	0.00667	-0.00134	0.00547	0.00394
D6	-3.05765	0.00037	-0.01082	-0.02702	-0.03764	-3.09529
D7	3.12699	0.00008	0.01270	0.00152	0.01426	3.14125
D8	0.07086	0.00056	-0.00478	-0.02416	-0.02885	0.04201
D9	-0.00424	-0.00002	-0.00390	0.00437	0.00061	-0.00362
D10	3.11260	-0.00003	0.00760	0.02353	0.03146	-3.13912
D11	-3.13293	0.00000	-0.00720	-0.00012	-0.00737	-3.14030
D12	-0.01609	0.00000	0.00430	0.01904	0.02347	0.00738
D13	0.00332	-0.00005	0.00808	-0.00524	0.00278	0.00610
D14	2.94598	0.00009	-0.00046	0.05369	0.05411	3.00009
D15	-3.11537	-0.00004	-0.00257	-0.02304	-0.02573	-3.14111
D16	-0.17271	0.00010	-0.01111	0.03588	0.02560	-0.14712
D17	0.25248	-0.00017	-0.06476	-0.11647	-0.18132	0.07116
D18	-2.88436	-0.00006	-0.06903	-0.11401	-0.18311	-3.06747
D19	-2.91687	-0.00018	-0.05186	-0.09496	-0.14674	-3.06361
D20	0.22948	-0.00007	-0.05612	-0.09250	-0.14854	0.08095
D21	-0.00113	0.00010	-0.00910	0.00407	-0.00508	-0.00622
D22	3.05807	-0.00018	0.00805	0.02873	0.03656	3.09463
D23	-2.94911	-0.00032	-0.00336	-0.05812	-0.06053	-3.00964
D24	0.11010	-0.00061	0.01380	-0.03346	-0.01889	0.09121
D25	1.47401	0.00115	0.03767	0.04385	0.08146	1.55546
D26	-2.71463	-0.00016	0.03877	0.04415	0.08284	-2.63179
D27	-0.66223	0.00018	0.03944	0.04632	0.08570	-0.57653
D28	-1.57024	0.00157	0.01754	0.01467	0.03228	-1.53795
D29	0.52431	0.00026	0.01865	0.01497	0.03367	0.55798
D30	2.57671	0.00060	0.01932	0.01714	0.03653	2.61324
D31	-1.08064	-0.00067	0.01589	0.02783	0.04372	-1.03692
D32	1.02678	-0.00187	0.01465	0.03198	0.04661	1.07339
D33	-3.13337	-0.00143	0.00875	0.03230	0.04107	-3.09230
D34	3.12597	0.00108	0.01957	0.03065	0.05023	-3.10699
D35	-1.04979	-0.00012	0.01832	0.03481	0.05311	-0.99668

D36	1.07324	0.00032	0.01242	0.03513	0.04757	1.12082
D37	1.03069	0.00016	0.01173	0.02277	0.03449	1.06518
D38	3.13811	-0.00104	0.01048	0.02692	0.03737	-3.10770
D39	-1.02204	-0.00060	0.00458	0.02724	0.03184	-0.99020
D40	0.50802	-0.00097	0.01127	0.02382	0.03509	0.54312
D41	2.62368	-0.00187	0.00958	0.02615	0.03572	2.65940
D42	-1.59828	0.00017	0.02457	0.02167	0.04626	-1.55203
D43	-1.55351	0.00214	-0.08131	0.07489	-0.00643	-1.55994
D44	2.64029	0.00013	-0.08244	0.07538	-0.00702	2.63327
D45	0.55171	-0.00279	-0.09150	0.07411	-0.01741	0.53429
D46	-3.11870	-0.00004	-0.00957	-0.00385	-0.01343	-3.13212
D47	0.02382	-0.00003	-0.00447	-0.00795	-0.01242	0.01140
D48	0.01762	-0.00015	-0.00487	-0.00658	-0.01145	0.00617
D49	-3.12305	-0.00015	0.00023	-0.01067	-0.01044	-3.13349

Item	Value	Threshold	Converged?
Maximum Force	0.007409	0.000450	NO
RMS Force	0.001260	0.000300	NO
Maximum Displacement	0.504918	0.001800	NO
RMS Displacement	0.095927	0.001200	NO

Predicted change in Energy=-3.493850D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.544221	-2.244090	-1.165649
2	6	0	-1.850647	-1.915566	-1.333510
3	7	0	-2.126748	-0.899426	-0.423361
4	6	0	-1.009682	-0.628431	0.278199
5	7	0	-0.040308	-1.431352	-0.162844
6	6	0	1.351514	-1.387413	0.329415
7	6	0	2.208945	-0.385810	-0.459716
8	1	0	0.062540	-2.975459	-1.671329
9	1	0	-2.584335	-2.309773	-2.012297
10	1	0	1.310767	-1.087516	1.376410
11	1	0	1.764253	-2.394007	0.254588
12	1	0	2.231735	-0.652497	-1.520501
13	1	0	1.788677	0.614705	-0.335546
14	35	0	0.304257	1.902016	1.925221
15	1	0	-0.830133	0.205305	1.000194
16	6	0	-3.351989	-0.212176	-0.198078
17	6	0	-4.500188	-0.495286	-0.798868

18	1	0	-3.240007	0.582541	0.528206
19	1	0	-5.376627	0.092667	-0.565536
20	1	0	-4.618718	-1.293310	-1.520118
21	8	0	3.542801	-0.441880	0.019542
22	1	0	3.628462	0.189881	0.742732

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357518	0.000000			
3	N	2.205336	1.391813	0.000000		
4	C	2.216237	2.227452	1.346649	0.000000	
5	N	1.385673	2.209581	2.168882	1.333749	0.000000
6	C	2.561820	3.646656	3.592090	2.480710	1.476962
7	C	3.395801	4.425376	4.366161	3.311033	2.498085
8	H	1.076462	2.213093	3.265015	3.234016	2.161104
9	H	2.209795	1.074454	2.173288	3.248510	3.265605
10	H	3.352717	4.245452	3.884722	2.607932	2.076759
11	H	2.714516	3.977242	4.222946	3.288241	2.087436
12	H	3.219475	4.277400	4.501230	3.707113	2.758990
13	H	3.782088	4.543443	4.198912	3.122960	2.749793
14	Br	5.240572	5.462314	4.390183	3.292762	3.948428
15	H	3.282097	3.314470	2.219944	1.117421	2.157574
16	C	3.598393	2.538655	1.422772	2.426213	3.529145
17	C	4.340798	3.053376	2.436709	3.655330	4.601226
18	H	4.257494	3.411282	2.083519	2.550158	3.843356
19	H	5.401178	4.129809	3.400908	4.505783	5.564270
20	H	4.198947	2.843280	2.750987	4.086704	4.777351
21	O	4.621297	5.752546	5.705200	4.563640	3.721692
22	H	5.193979	6.226100	5.972337	4.732632	4.111975

		6	7	8	9	10
6	C	0.000000				
7	C	1.536595	0.000000			
8	H	2.861175	3.575100	0.000000		
9	H	4.671753	5.393299	2.750518	0.000000	
10	H	1.089861	2.161128	3.796197	5.305570	0.000000
11	H	1.090497	2.177346	2.634970	4.904700	1.780745
12	H	2.176484	1.094033	3.181872	5.116929	3.070752
13	H	2.154475	1.092279	4.201564	5.521531	2.461046
14	Br	3.803116	3.814434	6.064929	6.448813	3.201806
15	H	2.783214	3.422973	4.248666	4.298598	2.529106
16	C	4.876717	5.569792	4.633056	2.877602	4.998652
17	C	6.025889	6.718592	5.266017	2.904353	6.232959
18	H	5.000230	5.621812	5.329553	3.905066	4.921187

19	H	6.946903	7.601384	6.341981	3.957490	7.062947
20	H	6.250864	6.968858	4.976612	2.326832	6.602349
21	O	2.406615	1.418452	4.624964	6.720060	2.690709
22	H	2.800568	1.947391	5.344424	7.241361	2.721213

		11	12	13	14	15
11	H	0.000000				
12	H	2.530284	0.000000			
13	H	3.066137	1.790592	0.000000		
14	Br	4.835123	4.702522	2.995286	0.000000	
15	H	3.747424	4.057680	2.968160	2.240836	0.000000
16	C	5.580432	5.755055	5.208558	4.727192	2.823102
17	C	6.630093	6.772316	6.402857	6.020832	4.146898
18	H	5.829006	5.971807	5.102427	4.031684	2.484466
19	H	7.605808	7.704181	7.187976	6.461429	4.809866
20	H	6.715908	6.880360	6.789583	6.805597	4.790740
21	O	2.651280	2.033467	2.078319	4.428728	4.528033
22	H	3.223358	2.789744	2.174389	3.921737	4.466049

		16	17	18	19	20
16	C	0.000000				
17	C	1.326447	0.000000			
18	H	1.082406	2.123887	0.000000		
19	H	2.080172	1.080869	2.449774	0.000000	
20	H	2.126321	1.082170	3.100853	1.845694	0.000000
21	O	6.902047	8.084697	6.878565	8.954567	8.349005
22	H	7.055031	8.301864	6.883027	9.100146	8.679650

		21	22
21	O	0.000000	
22	H	0.964087	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.630236	-2.129387	0.127839
2	6	0	-2.679552	-1.298529	-0.099020
3	7	0	-2.196702	-0.000063	0.035089
4	6	0	-0.886214	-0.052639	0.340570
5	7	0	-0.526399	-1.335751	0.395746

6	6	0	0.855133	-1.792226	0.649556
7	6	0	1.668469	-1.912230	-0.648600
8	1	0	-1.575705	-3.204418	0.117516
9	1	0	-3.701957	-1.521427	-0.342855
10	1	0	1.319793	-1.055428	1.304549
11	1	0	0.800578	-2.752883	1.162727
12	1	0	1.195913	-2.622904	-1.333100
13	1	0	1.732568	-0.928182	-1.118295
14	35	0	1.788883	1.840767	0.022532
15	1	0	-0.153969	0.789435	0.398525
16	6	0	-2.897145	1.230783	-0.101580
17	6	0	-4.201424	1.339541	-0.317197
18	1	0	-2.235400	2.082578	-0.011353
19	1	0	-4.639639	2.322685	-0.415551
20	1	0	-4.868116	0.491245	-0.400910
21	8	0	2.958386	-2.415313	-0.340335
22	1	0	3.535452	-1.666213	-0.152435

Rotational constants (GHZ): 0.7884949 0.4770122 0.3058497

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 835.1180000502 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 4.57D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Initial guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999503 0.003372 -0.001207 0.031329 Ang= 3.61 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid=

0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Keep R1 ints in memory in canonical form, NReq=1804729152.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

EnCoef did 2 forward-backward iterations

SCF Done: E(RB3LYP) = -3032.33981254 A.U. after 13 cycles

NFock= 13 Conv=0.51D-08 -V/T= 2.0017

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000310937	0.000847571	-0.000429723
2	6	0.000514745	0.000182495	0.000301880
3	7	-0.001484453	-0.000206699	0.000263656
4	6	0.002318401	0.004135831	0.000215643
5	7	0.000711350	-0.000903150	0.001595009
6	6	-0.000259590	-0.000097892	-0.000507425
7	6	0.001106575	-0.000156708	0.001162562
8	1	0.000085874	-0.000110144	0.000292426
9	1	-0.000469512	0.000059709	0.000235619
10	1	0.000453807	0.000216449	0.000117437
11	1	0.000104447	-0.000102772	-0.000005411
12	1	-0.000062398	-0.000017181	0.000094121
13	1	-0.001593465	0.000587535	-0.001021518
14	35	-0.000168700	-0.002717717	-0.001344497
15	1	-0.001001668	-0.002243075	-0.000822299
16	6	0.000363070	-0.000105640	-0.000267081
17	6	0.000255571	-0.000052653	0.000216456
18	1	-0.000288957	0.000507140	-0.000059944
19	1	-0.000086504	0.000160335	0.000164734
20	1	0.000111955	-0.000198223	-0.000328970
21	8	-0.000119442	0.000094189	-0.000031576
22	1	-0.000180170	0.000120598	0.000158899

Cartesian Forces: Max 0.004135831 RMS 0.000909289

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.008953541 RMS 0.001586299
Search for a local minimum.
Step number 49 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 46 47 48 49
DE= -3.56D-04 DEPred=-3.49D-04 R= 1.02D+00
TightC=F SS= 1.41D+00 RLast= 4.30D-01 DXNew= 4.4018D-01 1.2896D+00
Trust test= 1.02D+00 RLast= 4.30D-01 DXMaxT set to 4.40D-01
ITU= 1 1 1 -1 1 0 -1 1 0 -1 0 -1 0 0 1 -1 0 1 1 1
ITU= 1 1 1 0 -1 1 1 1 1 1 0 -1 1 1 1 1 1 1 1 1
ITU= 1 1 1 1 0 0 -1 0 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00160	0.00245	0.00309	0.00588	0.00946
Eigenvalues ---	0.01063	0.01442	0.01729	0.01915	0.02159
Eigenvalues ---	0.02313	0.02409	0.03019	0.03160	0.03745
Eigenvalues ---	0.04417	0.05055	0.05422	0.06065	0.06531
Eigenvalues ---	0.08698	0.09319	0.11560	0.13807	0.14608
Eigenvalues ---	0.14763	0.15905	0.15988	0.16096	0.16574
Eigenvalues ---	0.17011	0.17272	0.20933	0.22510	0.23037
Eigenvalues ---	0.24427	0.25063	0.25904	0.29304	0.31618
Eigenvalues ---	0.33151	0.33863	0.33889	0.33993	0.34239
Eigenvalues ---	0.34479	0.34749	0.35299	0.36303	0.36356
Eigenvalues ---	0.38933	0.43256	0.44300	0.46436	0.49232
Eigenvalues ---	0.53597	0.55125	0.57721	0.60769	1.24024

RFO step: Lambda=-6.14406414D-04 EMin= 1.59878524D-03
Quartic linear search produced a step of -0.04975.
Iteration 1 RMS(Cart)= 0.02964369 RMS(Int)= 0.00046843
Iteration 2 RMS(Cart)= 0.00056666 RMS(Int)= 0.00013359
Iteration 3 RMS(Cart)= 0.00000025 RMS(Int)= 0.00013359

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56534	0.00038	0.00004	-0.00194	-0.00201	2.56332
R2	2.61854	-0.00038	0.00008	0.00082	0.00086	2.61941
R3	2.03422	-0.00001	0.00000	0.00004	0.00004	2.03426
R4	2.63015	-0.00017	-0.00009	0.00147	0.00134	2.63149
R5	2.03042	0.00015	0.00003	-0.00011	-0.00008	2.03035
R6	2.54480	0.00040	0.00009	-0.00072	-0.00054	2.54426
R7	2.68865	-0.00020	-0.00007	0.00157	0.00149	2.69014
R8	2.52042	0.00070	0.00009	-0.00066	-0.00047	2.51995

R9	2.11162	-0.00237	-0.00034	-0.01571	-0.01605	2.09557
R10	2.79105	-0.00119	-0.00056	0.00685	0.00629	2.79735
R11	2.90374	-0.00145	0.00018	-0.00058	-0.00040	2.90334
R12	2.05954	0.00016	-0.00004	0.00145	0.00141	2.06095
R13	2.06074	0.00014	0.00008	-0.00059	-0.00052	2.06022
R14	2.06742	-0.00009	-0.00006	0.00076	0.00070	2.06812
R15	2.06411	-0.00155	-0.00003	0.00371	0.00369	2.06779
R16	2.68049	-0.00024	0.00016	-0.00305	-0.00288	2.67760
R17	5.66027	-0.00210	-0.00352	-0.04554	-0.04907	5.61121
R18	2.50662	-0.00025	-0.00001	0.00017	0.00016	2.50678
R19	2.04545	0.00030	0.00008	0.00064	0.00071	2.04617
R20	2.04255	0.00019	0.00003	0.00058	0.00061	2.04316
R21	2.04500	0.00035	0.00009	0.00005	0.00014	2.04514
R22	1.82186	0.00018	-0.00010	0.00230	0.00219	1.82405
A1	1.87289	-0.00014	0.00003	0.00091	0.00089	1.87378
A2	2.27678	0.00028	0.00017	-0.00207	-0.00192	2.27486
A3	2.13351	-0.00013	-0.00020	0.00122	0.00099	2.13450
A4	1.86161	0.00046	0.00003	0.00076	0.00077	1.86238
A5	2.27375	0.00022	0.00034	-0.00168	-0.00134	2.27242
A6	2.14781	-0.00068	-0.00037	0.00094	0.00058	2.14838
A7	1.89974	-0.00039	0.00001	-0.00227	-0.00210	1.89764
A8	2.24854	-0.00022	-0.00013	-0.00043	-0.00067	2.24787
A9	2.13490	0.00061	0.00011	0.00276	0.00277	2.13766
A10	1.88544	0.00008	0.00001	0.00272	0.00243	1.88787
A11	2.23960	-0.00042	-0.00156	0.01435	0.01209	2.25169
A12	2.14843	0.00040	0.00111	-0.00824	-0.00791	2.14052
A13	1.90508	0.00000	-0.00007	-0.00210	-0.00198	1.90310
A14	2.21598	0.00248	-0.00010	0.00073	0.00054	2.21652
A15	2.16131	-0.00250	0.00005	0.00159	0.00157	2.16288
A16	1.95419	-0.00367	-0.00018	0.00664	0.00647	1.96065
A17	1.86830	0.00013	0.00046	-0.00532	-0.00487	1.86343
A18	1.88214	0.00247	0.00045	-0.00727	-0.00683	1.87531
A19	1.91225	-0.00006	-0.00021	0.00114	0.00094	1.91319
A20	1.93397	0.00158	0.00002	0.00027	0.00030	1.93427
A21	1.91141	-0.00044	-0.00053	0.00432	0.00378	1.91519
A22	1.92909	0.00251	-0.00006	-0.00143	-0.00149	1.92760
A23	1.90074	-0.00688	0.00032	-0.00079	-0.00047	1.90027
A24	1.90228	0.00101	0.00033	-0.00664	-0.00631	1.89596
A25	1.91934	0.00082	-0.00025	0.00449	0.00424	1.92358
A26	1.87379	-0.00076	-0.00024	0.00320	0.00295	1.87674
A27	1.93865	0.00350	-0.00011	0.00110	0.00098	1.93963
A28	2.30522	-0.00895	0.00399	-0.02641	-0.02243	2.28279
A29	2.17807	-0.00051	-0.00036	0.00143	0.00107	2.17913
A30	1.95175	0.00067	0.00036	-0.00296	-0.00260	1.94915

A31	2.15337	-0.00015	0.00000	0.00151	0.00151	2.15487
A32	2.08062	-0.00012	0.00013	-0.00273	-0.00260	2.07802
A33	2.15805	-0.00006	-0.00019	0.00141	0.00122	2.15927
A34	2.04451	0.00018	0.00006	0.00131	0.00138	2.04589
A35	1.88715	-0.00034	0.00007	-0.00277	-0.00270	1.88445
D1	-0.00017	0.00026	0.00018	0.00058	0.00070	0.00053
D2	3.13603	0.00018	-0.00026	0.00518	0.00491	3.14094
D3	-3.13699	0.00005	0.00067	-0.01444	-0.01376	3.13243
D4	-0.00080	-0.00003	0.00023	-0.00984	-0.00955	-0.01034
D5	0.00394	-0.00030	-0.00027	-0.00321	-0.00343	0.00052
D6	-3.09529	0.00036	0.00187	-0.00907	-0.00709	-3.10238
D7	3.14125	-0.00011	-0.00071	0.01029	0.00960	-3.13234
D8	0.04201	0.00055	0.00144	0.00443	0.00594	0.04795
D9	-0.00362	-0.00013	-0.00003	0.00222	0.00223	-0.00139
D10	-3.13912	-0.00023	-0.00156	-0.00757	-0.00902	3.13504
D11	-3.14030	-0.00007	0.00037	-0.00196	-0.00160	3.14128
D12	0.00738	-0.00017	-0.00117	-0.01175	-0.01285	-0.00547
D13	0.00610	-0.00005	-0.00014	-0.00422	-0.00438	0.00172
D14	3.00009	0.00041	-0.00269	0.06145	0.05913	3.05922
D15	-3.14111	0.00004	0.00128	0.00479	0.00601	-3.13510
D16	-0.14712	0.00050	-0.00127	0.07046	0.06952	-0.07760
D17	0.07116	0.00008	0.00902	-0.05476	-0.04576	0.02540
D18	-3.06747	0.00019	0.00911	-0.04960	-0.04052	-3.10799
D19	-3.06361	-0.00003	0.00730	-0.06570	-0.05837	-3.12199
D20	0.08095	0.00008	0.00739	-0.06055	-0.05314	0.02781
D21	-0.00622	0.00021	0.00025	0.00459	0.00482	-0.00139
D22	3.09463	-0.00028	-0.00182	0.01020	0.00832	3.10296
D23	-3.00964	-0.00014	0.00301	-0.05915	-0.05576	-3.06540
D24	0.09121	-0.00063	0.00094	-0.05353	-0.05226	0.03895
D25	1.55546	0.00130	-0.00405	0.01896	0.01488	1.57035
D26	-2.63179	-0.00086	-0.00412	0.02084	0.01668	-2.61511
D27	-0.57653	-0.00003	-0.00426	0.01935	0.01508	-0.56145
D28	-1.53795	0.00197	-0.00161	0.01238	0.01079	-1.52716
D29	0.55798	-0.00019	-0.00167	0.01426	0.01260	0.57057
D30	2.61324	0.00064	-0.00182	0.01277	0.01099	2.62423
D31	-1.03692	-0.00139	-0.00218	-0.00168	-0.00385	-1.04077
D32	1.07339	-0.00322	-0.00232	0.00247	0.00015	1.07354
D33	-3.09230	-0.00254	-0.00204	-0.00073	-0.00277	-3.09507
D34	-3.10699	0.00079	-0.00250	0.00006	-0.00244	-3.10943
D35	-0.99668	-0.00104	-0.00264	0.00421	0.00156	-0.99512
D36	1.12082	-0.00036	-0.00237	0.00101	-0.00136	1.11946
D37	1.06518	0.00037	-0.00172	-0.00626	-0.00797	1.05721
D38	-3.10770	-0.00147	-0.00186	-0.00210	-0.00396	-3.11166
D39	-0.99020	-0.00079	-0.00158	-0.00530	-0.00689	-0.99709

D40	0.54312	-0.00222	-0.00175	-0.03001	-0.03176	0.51136
D41	2.65940	-0.00298	-0.00178	-0.02949	-0.03127	2.62813
D42	-1.55203	-0.00121	-0.00230	-0.02196	-0.02426	-1.57628
D43	-1.55994	0.00298	0.00032	-0.04480	-0.04449	-1.60442
D44	2.63327	-0.00014	0.00035	-0.04123	-0.04088	2.59239
D45	0.53429	-0.00272	0.00087	-0.04938	-0.04852	0.48577
D46	-3.13212	0.00003	0.00067	-0.00849	-0.00782	-3.13994
D47	0.01140	-0.00007	0.00062	-0.00702	-0.00640	0.00500
D48	0.00617	-0.00009	0.00057	-0.01423	-0.01366	-0.00749
D49	-3.13349	-0.00019	0.00052	-0.01275	-0.01224	3.13746

Item	Value	Threshold	Converged?
Maximum Force	0.008954	0.000450	NO
RMS Force	0.001586	0.000300	NO
Maximum Displacement	0.153332	0.001800	NO
RMS Displacement	0.029622	0.001200	NO

Predicted change in Energy=-3.178955D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.549520	-2.253318	-1.150605
2	6	0	-1.857773	-1.932446	-1.310221
3	7	0	-2.130727	-0.905408	-0.410325
4	6	0	-1.006935	-0.620458	0.274215
5	7	0	-0.038592	-1.426796	-0.162086
6	6	0	1.358980	-1.377322	0.323310
7	6	0	2.215916	-0.375299	-0.465413
8	1	0	0.051078	-2.996776	-1.645955
9	1	0	-2.595985	-2.341402	-1.975174
10	1	0	1.317639	-1.078447	1.371353
11	1	0	1.768526	-2.384554	0.243667
12	1	0	2.239742	-0.644360	-1.525956
13	1	0	1.795176	0.626863	-0.338980
14	35	0	0.270123	1.820876	1.911668
15	1	0	-0.827163	0.182253	1.017893
16	6	0	-3.355704	-0.214290	-0.190520
17	6	0	-4.494191	-0.469953	-0.821527
18	1	0	-3.248518	0.561854	0.556830
19	1	0	-5.370684	0.115831	-0.581544
20	1	0	-4.604981	-1.242109	-1.571695
21	8	0	3.545610	-0.436103	0.020278

22 1 0 3.638333 0.224482 0.717942

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.356452	0.000000			
3	N	2.205695	1.392524	0.000000		
4	C	2.214852	2.226134	1.346365	0.000000	
5	N	1.386130	2.209822	2.170368	1.333502	0.000000
6	C	2.565574	3.650218	3.597080	2.484514	1.480293
7	C	3.412342	4.442223	4.379196	3.315708	2.506084
8	H	1.076485	2.211160	3.265099	3.233161	2.162116
9	H	2.208097	1.074413	2.174234	3.247533	3.265585
10	H	3.350653	4.243041	3.885299	2.610960	2.076571
11	H	2.708238	3.971022	4.221345	3.288792	2.085093
12	H	3.241853	4.300621	4.518161	3.712425	2.768240
13	H	3.801549	4.564802	4.214934	3.127883	2.758897
14	Br	5.162208	5.384788	4.311422	3.205034	3.865635
15	H	3.272840	3.309717	2.218580	1.108928	2.145515
16	C	3.599176	2.539604	1.423562	2.428511	3.531885
17	C	4.341556	3.054244	2.438169	3.658449	4.604646
18	H	4.257361	3.411977	2.082716	2.549985	3.843851
19	H	5.401881	4.131217	3.401406	4.507410	5.566583
20	H	4.200789	2.844659	2.753921	4.091426	4.782574
21	O	4.630693	5.762449	5.711958	4.563347	3.723067
22	H	5.212396	6.242834	5.985959	4.742293	4.125645

		6	7	8	9	10
6	C	0.000000				
7	C	1.536382	0.000000			
8	H	2.865528	3.598937	0.000000		
9	H	4.674851	5.412885	2.746787	0.000000	
10	H	1.090609	2.162181	3.793193	5.301957	0.000000
11	H	1.090224	2.177167	2.625856	4.896333	1.783505
12	H	2.175491	1.094401	3.215356	5.144511	3.071336
13	H	2.155378	1.094229	4.228573	5.547073	2.461984
14	Br	3.733224	3.776217	5.992866	6.375474	3.129745
15	H	2.773796	3.430946	4.239531	4.296047	2.512862
16	C	4.883126	5.580720	4.633215	2.878675	5.002634
17	C	6.032709	6.720216	5.265357	2.904550	6.241502
18	H	5.004395	5.637665	5.329488	3.907140	4.919738
19	H	6.952456	7.603367	6.341671	3.959691	7.069212
20	H	6.259247	6.964184	4.976269	2.325362	6.615568
21	O	2.399806	1.416926	4.641674	6.732843	2.683629
22	H	2.813709	1.945080	5.369629	7.259708	2.740473

		11	12	13	14	15
11	H	0.000000				
12	H	2.526239	0.000000			
13	H	3.067380	1.795148	0.000000		
14	Br	4.765825	4.666267	2.969322	0.000000	
15	H	3.731693	4.069443	2.985875	2.165168	0.000000
16	C	5.581783	5.768653	5.221221	4.659154	2.830376
17	C	6.634905	6.772923	6.402499	5.951213	4.154026
18	H	5.826673	5.992824	5.123041	3.975116	2.493919
19	H	7.609285	7.706386	7.188153	6.398592	4.817281
20	H	6.724754	6.870926	6.780462	6.729215	4.796528
21	O	2.646581	2.034577	2.079178	4.404557	4.527553
22	H	3.244716	2.783167	2.162457	3.913860	4.475758

		16	17	18	19	20
16	C	0.000000				
17	C	1.326531	0.000000			
18	H	1.082784	2.125134	0.000000		
19	H	2.078947	1.081191	2.449168	0.000000	
20	H	2.127145	1.082243	3.102401	1.846808	0.000000
21	O	6.908094	8.083821	6.887958	8.953609	8.343630
22	H	7.066426	8.306031	6.896992	9.102904	8.680182

		21	22
21	O	0.000000	
22	H	0.965248	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.542691	-2.164208	0.155189
2	6	0	-2.621088	-1.370656	-0.062292
3	7	0	-2.178085	-0.054872	0.045334
4	6	0	-0.860798	-0.063669	0.323502
5	7	0	-0.458916	-1.333293	0.392607
6	6	0	0.942376	-1.744244	0.635021
7	6	0	1.754236	-1.846283	-0.665341
8	1	0	-1.458544	-3.237315	0.168577
9	1	0	-3.640609	-1.630430	-0.280141

10	1	0	1.384352	-0.987506	1.284201
11	1	0	0.916854	-2.703589	1.152314
12	1	0	1.303050	-2.579386	-1.341139
13	1	0	1.784953	-0.861669	-1.141711
14	35	0	1.682459	1.864591	0.030413
15	1	0	-0.159531	0.791174	0.408302
16	6	0	-2.919748	1.150975	-0.104314
17	6	0	-4.220463	1.214617	-0.356852
18	1	0	-2.289361	2.024483	0.005303
19	1	0	-4.689771	2.183773	-0.454128
20	1	0	-4.853584	0.344320	-0.470834
21	8	0	3.058268	-2.302228	-0.350233
22	1	0	3.618032	-1.528758	-0.208418

Rotational constants (GHZ): 0.8002457 0.4856124 0.3113346

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 839.9974408583 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 4.43D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Initial guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999851 0.000159 0.000043 -0.017242 Ang= 1.98 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.33982289 A.U. after 12 cycles
NFock= 12 Conv=0.30D-08 -V/T= 2.0016
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000472785	0.000123446	-0.000294609
2	6	-0.000335334	0.000371374	-0.000175113
3	7	-0.001276799	-0.000087322	-0.001003200
4	6	0.000642862	-0.003232209	-0.000555716
5	7	0.001375998	-0.000465123	0.000148222
6	6	-0.002733607	-0.000575202	-0.000056563
7	6	-0.000976076	0.000005656	0.001008355
8	1	0.000268032	0.000210138	0.000021780
9	1	-0.000511286	0.000134873	0.000164576
10	1	0.000972487	0.000028276	-0.000425640
11	1	0.000613416	-0.000099259	0.000243786
12	1	-0.000178170	0.000401374	0.000123800
13	1	-0.001120099	-0.000825520	-0.001568602
14	35	0.001707221	0.001077193	0.001181237
15	1	-0.001395650	0.002459994	0.000389093
16	6	0.001476026	-0.000253616	0.000006711
17	6	0.000117308	0.000046422	0.000655651
18	1	-0.000579816	0.000216302	-0.000110246
19	1	0.000035815	0.000096211	-0.000188006
20	1	0.000115005	-0.000194093	-0.000139650
21	8	0.001336880	0.001832759	0.001115383
22	1	-0.000027000	-0.001271673	-0.000541247

Cartesian Forces: Max 0.003232209 RMS 0.000937854

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.004040697 RMS 0.001167585

Search for a local minimum.
Step number 50 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 48 49 50
DE= -1.04D-05 DEPred=-3.18D-04 R= 3.26D-02
Trust test= 3.26D-02 RLast= 1.98D-01 DXMaxT set to 2.20D-01
ITU= -1 1 1 1 -1 1 0 -1 1 0 -1 0 -1 0 0 1 -1 0 1 1
ITU= 1 1 1 1 0 -1 1 1 1 1 1 0 -1 1 1 1 1 1 1 1
ITU= 1 1 1 1 1 0 0 -1 0 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00124	0.00182	0.00365	0.00611	0.00854
Eigenvalues ---	0.00999	0.01440	0.01733	0.02014	0.02157
Eigenvalues ---	0.02333	0.02883	0.03074	0.03230	0.03822
Eigenvalues ---	0.04401	0.05114	0.05621	0.05986	0.06723
Eigenvalues ---	0.08780	0.09461	0.11350	0.13885	0.14627
Eigenvalues ---	0.15478	0.15977	0.16046	0.16106	0.16985
Eigenvalues ---	0.17231	0.19461	0.21380	0.22548	0.23318
Eigenvalues ---	0.24784	0.25102	0.28213	0.29308	0.33071
Eigenvalues ---	0.33608	0.33863	0.33888	0.34012	0.34250
Eigenvalues ---	0.34686	0.34890	0.35231	0.36305	0.36358
Eigenvalues ---	0.38822	0.43373	0.44690	0.46449	0.49192
Eigenvalues ---	0.53607	0.55634	0.57726	0.60799	1.26180

RFO step: Lambda=-4.80335386D-04 EMin= 1.23516983D-03
Quartic linear search produced a step of -0.48356.
Iteration 1 RMS(Cart)= 0.07302310 RMS(Int)= 0.00341690
Iteration 2 RMS(Cart)= 0.00444945 RMS(Int)= 0.00004253
Iteration 3 RMS(Cart)= 0.00002453 RMS(Int)= 0.00004076
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00004076

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56332	0.00038	0.00097	-0.00021	0.00075	2.56408
R2	2.61941	0.00045	-0.00042	-0.00157	-0.00198	2.61742
R3	2.03426	-0.00001	-0.00002	-0.00035	-0.00037	2.03389
R4	2.63149	-0.00104	-0.00065	0.00011	-0.00055	2.63094
R5	2.03035	0.00020	0.00004	-0.00012	-0.00008	2.03027
R6	2.54426	0.00046	0.00026	-0.00275	-0.00249	2.54178
R7	2.69014	-0.00101	-0.00072	0.00458	0.00386	2.69400
R8	2.51995	0.00073	0.00023	0.00112	0.00136	2.52132
R9	2.09557	0.00181	0.00776	-0.01092	-0.00316	2.09241
R10	2.79735	0.00000	-0.00304	0.01321	0.01017	2.80752
R11	2.90334	0.00051	0.00019	-0.00312	-0.00292	2.90042
R12	2.06095	-0.00044	-0.00068	0.00121	0.00053	2.06148
R13	2.06022	0.00030	0.00025	-0.00142	-0.00117	2.05905

R14	2.06812	-0.00023	-0.00034	0.00100	0.00067	2.06878
R15	2.06779	-0.00004	-0.00178	0.00051	-0.00127	2.06652
R16	2.67760	0.00141	0.00139	-0.00416	-0.00277	2.67483
R17	5.61121	0.00045	0.02373	-0.07862	-0.05490	5.55631
R18	2.50678	-0.00037	-0.00008	-0.00077	-0.00085	2.50593
R19	2.04617	0.00002	-0.00035	0.00003	-0.00032	2.04585
R20	2.04316	-0.00002	-0.00029	-0.00015	-0.00044	2.04271
R21	2.04514	0.00023	-0.00007	-0.00065	-0.00072	2.04443
R22	1.82405	-0.00126	-0.00106	0.00256	0.00150	1.82556
A1	1.87378	0.00065	-0.00043	0.00080	0.00036	1.87414
A2	2.27486	-0.00004	0.00093	-0.00369	-0.00279	2.27208
A3	2.13450	-0.00061	-0.00048	0.00271	0.00220	2.13671
A4	1.86238	-0.00031	-0.00037	-0.00009	-0.00046	1.86193
A5	2.27242	0.00065	0.00065	-0.00197	-0.00133	2.27109
A6	2.14838	-0.00035	-0.00028	0.00206	0.00178	2.15016
A7	1.89764	0.00048	0.00101	-0.00075	0.00028	1.89792
A8	2.24787	-0.00027	0.00032	-0.00268	-0.00238	2.24549
A9	2.13766	-0.00021	-0.00134	0.00346	0.00209	2.13976
A10	1.88787	0.00007	-0.00118	0.00167	0.00046	1.88833
A11	2.25169	-0.00216	-0.00585	0.01893	0.01299	2.26468
A12	2.14052	0.00204	0.00383	-0.01457	-0.01085	2.12967
A13	1.90310	-0.00089	0.00096	-0.00163	-0.00066	1.90244
A14	2.21652	-0.00316	-0.00026	0.00095	0.00064	2.21716
A15	2.16288	0.00404	-0.00076	0.00121	0.00040	2.16329
A16	1.96065	-0.00102	-0.00313	-0.00420	-0.00734	1.95331
A17	1.86343	0.00232	0.00235	-0.00597	-0.00363	1.85980
A18	1.87531	-0.00072	0.00330	-0.00654	-0.00322	1.87209
A19	1.91319	-0.00032	-0.00045	0.00035	-0.00015	1.91304
A20	1.93427	0.00002	-0.00014	0.00596	0.00579	1.94006
A21	1.91519	-0.00021	-0.00183	0.01026	0.00843	1.92361
A22	1.92760	-0.00215	0.00072	0.00305	0.00378	1.93138
A23	1.90027	0.00335	0.00023	-0.01269	-0.01248	1.88779
A24	1.89596	0.00108	0.00305	-0.00462	-0.00161	1.89435
A25	1.92358	0.00009	-0.00205	0.00695	0.00491	1.92849
A26	1.87674	0.00049	-0.00143	0.00912	0.00770	1.88444
A27	1.93963	-0.00295	-0.00048	-0.00165	-0.00218	1.93745
A28	2.28279	0.00125	0.01084	-0.05020	-0.03935	2.24344
A29	2.17913	-0.00070	-0.00052	-0.00329	-0.00381	2.17533
A30	1.94915	0.00099	0.00126	-0.00457	-0.00331	1.94584
A31	2.15487	-0.00029	-0.00073	0.00785	0.00713	2.16200
A32	2.07802	0.00018	0.00126	-0.00048	0.00078	2.07879
A33	2.15927	-0.00024	-0.00059	-0.00067	-0.00126	2.15801
A34	2.04589	0.00006	-0.00067	0.00115	0.00049	2.04638
A35	1.88445	0.00045	0.00130	-0.00351	-0.00220	1.88224

D1	0.00053	0.00012	-0.00034	-0.00006	-0.00043	0.00010
D2	3.14094	0.00001	-0.00237	0.00581	0.00342	-3.13883
D3	3.13243	0.00018	0.00665	-0.02223	-0.01556	3.11687
D4	-0.01034	0.00007	0.00462	-0.01636	-0.01171	-0.02206
D5	0.00052	-0.00005	0.00166	0.00133	0.00302	0.00354
D6	-3.10238	0.00010	0.00343	-0.01347	-0.01000	-3.11237
D7	-3.13234	-0.00011	-0.00464	0.02137	0.01675	-3.11559
D8	0.04795	0.00005	-0.00287	0.00657	0.00373	0.05168
D9	-0.00139	-0.00015	-0.00108	-0.00123	-0.00228	-0.00367
D10	3.13504	-0.00023	0.00436	0.00547	0.00986	-3.13828
D11	3.14128	-0.00005	0.00077	-0.00657	-0.00579	3.13549
D12	-0.00547	-0.00012	0.00621	0.00012	0.00635	0.00088
D13	0.00172	0.00012	0.00212	0.00207	0.00418	0.00590
D14	3.05922	-0.00035	-0.02859	0.08255	0.05414	3.11337
D15	-3.13510	0.00019	-0.00290	-0.00410	-0.00706	3.14103
D16	-0.07760	-0.00028	-0.03362	0.07638	0.04291	-0.03469
D17	0.02540	0.00016	0.02213	-0.12732	-0.10522	-0.07982
D18	-3.10799	0.00020	0.01960	-0.12629	-0.10671	3.06848
D19	-3.12199	0.00008	0.02823	-0.11982	-0.09158	3.06962
D20	0.02781	0.00012	0.02570	-0.11879	-0.09307	-0.06526
D21	-0.00139	-0.00004	-0.00233	-0.00211	-0.00445	-0.00585
D22	3.10296	-0.00038	-0.00402	0.01214	0.00808	3.11103
D23	-3.06540	0.00063	0.02696	-0.07825	-0.05109	-3.11650
D24	0.03895	0.00029	0.02527	-0.06400	-0.03856	0.00038
D25	1.57035	-0.00064	-0.00720	0.07012	0.06291	1.63326
D26	-2.61511	-0.00012	-0.00807	0.06420	0.05614	-2.55897
D27	-0.56145	0.00047	-0.00729	0.06977	0.06246	-0.49900
D28	-1.52716	-0.00033	-0.00522	0.05331	0.04810	-1.47906
D29	0.57057	0.00019	-0.00609	0.04739	0.04133	0.61190
D30	2.62423	0.00078	-0.00531	0.05296	0.04764	2.67187
D31	-1.04077	0.00198	0.00186	-0.01120	-0.00933	-1.05010
D32	1.07354	0.00291	-0.00007	-0.00885	-0.00893	1.06462
D33	-3.09507	0.00199	0.00134	-0.02126	-0.01990	-3.11497
D34	-3.10943	-0.00007	0.00118	-0.00132	-0.00013	-3.10956
D35	-0.99512	0.00085	-0.00076	0.00103	0.00027	-0.99485
D36	1.11946	-0.00007	0.00066	-0.01138	-0.01071	1.10875
D37	1.05721	0.00038	0.00385	-0.01825	-0.01441	1.04280
D38	-3.11166	0.00131	0.00192	-0.01590	-0.01401	-3.12567
D39	-0.99709	0.00039	0.00333	-0.02831	-0.02499	-1.02207
D40	0.51136	0.00394	0.01536	0.10724	0.12262	0.63398
D41	2.62813	0.00348	0.01512	0.10724	0.12236	2.75049
D42	-1.57628	0.00227	0.01173	0.12207	0.13377	-1.44251
D43	-1.60442	-0.00127	0.02151	0.00482	0.02634	-1.57809
D44	2.59239	0.00041	0.01977	-0.00143	0.01834	2.61073

D45	0.48577	0.00175	0.02346	-0.01478	0.00867	0.49445
D46	-3.13994	0.00021	0.00378	-0.01319	-0.00941	3.13383
D47	0.00500	0.00001	0.00309	-0.01272	-0.00963	-0.00463
D48	-0.00749	0.00017	0.00661	-0.01440	-0.00779	-0.01528
D49	3.13746	-0.00003	0.00592	-0.01394	-0.00802	3.12944

Item	Value	Threshold	Converged?
Maximum Force	0.004041	0.000450	NO
RMS Force	0.001168	0.000300	NO
Maximum Displacement	0.389251	0.001800	NO
RMS Displacement	0.072498	0.001200	NO

Predicted change in Energy=-4.028604D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.566967	-2.296527	-1.111802
2	6	0	-1.877118	-1.980336	-1.268556
3	7	0	-2.136364	-0.914567	-0.411091
4	6	0	-1.005139	-0.604418	0.247162
5	7	0	-0.042000	-1.428994	-0.168274
6	6	0	1.364335	-1.368132	0.306851
7	6	0	2.192266	-0.345502	-0.483389
8	1	0	0.020578	-3.070955	-1.573806
9	1	0	-2.624187	-2.419540	-1.903583
10	1	0	1.325354	-1.074690	1.356808
11	1	0	1.781603	-2.370115	0.211194
12	1	0	2.215547	-0.606098	-1.546418
13	1	0	1.742059	0.640822	-0.340747
14	35	0	0.476105	1.745117	2.072362
15	1	0	-0.813821	0.195575	0.988391
16	6	0	-3.363115	-0.219781	-0.199664
17	6	0	-4.480194	-0.438641	-0.879907
18	1	0	-3.269967	0.519357	0.585864
19	1	0	-5.363300	0.136634	-0.639804
20	1	0	-4.566135	-1.170862	-1.671676
21	8	0	3.521711	-0.371452	0.001823
22	1	0	3.589096	0.276226	0.715415

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				

2	C	1.356851	0.000000			
3	N	2.205405	1.392234	0.000000		
4	C	2.214048	2.225061	1.345050	0.000000	
5	N	1.385081	2.209583	2.170243	1.334222	0.000000
6	C	2.569907	3.655642	3.602229	2.490226	1.485674
7	C	3.437262	4.455228	4.366474	3.290006	2.503037
8	H	1.076289	2.209950	3.264094	3.232928	2.162284
9	H	2.207759	1.074370	2.174958	3.246796	3.264991
10	H	3.341826	4.238933	3.890321	2.623674	2.078716
11	H	2.696575	3.965833	4.225674	3.299229	2.086919
12	H	3.284635	4.326158	4.508131	3.686428	2.770010
13	H	3.814990	4.563961	4.179276	3.073004	2.738020
14	Br	5.249932	5.529773	4.479560	3.323516	3.919677
15	H	3.268381	3.310437	2.222630	1.107254	2.138412
16	C	3.600460	2.539738	1.425605	2.430566	3.534542
17	C	4.338071	3.050225	2.437178	3.657017	4.602694
18	H	4.256463	3.409892	2.082094	2.550890	3.845071
19	H	5.398876	4.126785	3.401537	4.508818	5.566846
20	H	4.192126	2.836999	2.749281	4.084543	4.774374
21	O	4.654392	5.774922	5.699060	4.539475	3.721205
22	H	5.218299	6.237604	5.955493	4.701254	4.107741

		6	7	8	9	10
6	C	0.000000				
7	C	1.534835	0.000000			
8	H	2.870917	3.651484	0.000000		
9	H	4.679721	5.432937	2.743697	0.000000	
10	H	1.090889	2.160921	3.778361	5.295058	0.000000
11	H	1.089602	2.179483	2.603577	4.887301	1.788497
12	H	2.177122	1.094753	3.300629	5.180652	3.072580
13	H	2.144284	1.093558	4.273315	5.556291	2.449146
14	Br	3.687587	3.721258	6.057772	6.539443	3.030603
15	H	2.766593	3.390495	4.234536	4.298809	2.515029
16	C	4.891222	5.564042	4.633232	2.878940	5.013503
17	C	6.035799	6.684880	5.259993	2.901144	6.253946
18	H	5.011708	5.632697	5.327495	3.905316	4.924664
19	H	6.958560	7.572549	6.336176	3.953973	7.084621
20	H	6.254915	6.911529	4.965669	2.320375	6.624998
21	O	2.395972	1.415460	4.693384	6.752577	2.674793
22	H	2.796497	1.942887	5.401710	7.261624	2.713096

		11	12	13	14	15
11	H	0.000000				
12	H	2.527698	0.000000			
13	H	3.061363	1.797956	0.000000		
14	Br	4.701426	4.652896	2.940272	0.000000	

15	H	3.731357	4.030509	2.915025	2.289101	0.000000
16	C	5.591142	5.751909	5.179126	4.874684	2.843043
17	C	6.643132	6.730915	6.338167	6.168435	4.163539
18	H	5.831620	5.992006	5.098408	4.212508	2.509884
19	H	7.619556	7.668932	7.129500	6.636394	4.832417
20	H	6.728833	6.806310	6.696781	6.924229	4.798225
21	O	2.658282	2.039160	2.075865	4.247671	4.482374
22	H	3.244131	2.789448	2.158693	3.699955	4.412108

		16	17	18	19	20
16	C	0.000000				
17	C	1.326083	0.000000			
18	H	1.082615	2.128590	0.000000		
19	H	2.078821	1.080957	2.455765	0.000000	
20	H	2.125707	1.081865	3.103768	1.846558	0.000000
21	O	6.889444	8.050618	6.874703	8.922627	8.297765
22	H	7.029697	8.256484	6.864594	9.055469	8.619748

		21	22
21	O	0.000000	
22	H	0.966043	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.714427	-2.061846	0.260933
2	6	0	-2.760701	-1.226233	0.041605
3	7	0	-2.246158	0.067427	0.043513
4	6	0	-0.920796	0.005072	0.264169
5	7	0	-0.580000	-1.278356	0.393859
6	6	0	0.812290	-1.749211	0.610768
7	6	0	1.578690	-1.899312	-0.710527
8	1	0	-1.689267	-3.133961	0.352221
9	1	0	-3.801710	-1.444990	-0.109121
10	1	0	1.300684	-0.998892	1.234090
11	1	0	0.753429	-2.699078	1.141354
12	1	0	1.084161	-2.625606	-1.363537
13	1	0	1.622463	-0.918672	-1.192501
14	35	0	1.915000	1.726041	0.058544

15	1	0	-0.171582	0.819037	0.310543
16	6	0	-2.937048	1.300863	-0.139945
17	6	0	-4.225214	1.406333	-0.436594
18	1	0	-2.275653	2.148539	-0.013231
19	1	0	-4.660148	2.389542	-0.548844
20	1	0	-4.880424	0.556329	-0.573059
21	8	0	2.877989	-2.382707	-0.424730
22	1	0	3.455483	-1.619533	-0.293175

Rotational constants (GHZ): 0.8362919 0.4573123 0.3053511

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 836.2959513495 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 4.53D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Initial guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999460 0.000069 -0.001263 0.032824 Ang= 3.76 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Keep R1 ints in memory in canonical form, NReq=1804729152.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3032.33999200 A.U. after 13 cycles
NFock= 13 Conv=0.45D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000063085	0.000396740	0.000024326
2	6	0.000194685	0.000837442	-0.000186190
3	7	-0.003378490	0.000277081	-0.000638937
4	6	0.004612783	-0.001328696	0.001528839
5	7	0.002356308	-0.000714105	0.001365457
6	6	-0.005242036	-0.001238772	-0.000911981
7	6	-0.001058478	0.000153439	0.002308611
8	1	0.000711829	0.000535306	-0.000222746
9	1	-0.000734042	0.000217683	0.000426576
10	1	0.001477836	0.000136982	-0.000360248
11	1	0.000645531	-0.000393340	0.000370995
12	1	0.000348653	0.000338476	0.000471628
13	1	-0.000566399	0.000211695	-0.002192193
14	35	-0.000550028	-0.002584920	-0.001295690
15	1	-0.001367252	0.002654683	-0.000740016
16	6	0.002867848	-0.000975586	-0.000184602
17	6	-0.000092716	0.000359117	0.001147909
18	1	-0.001309367	0.000475197	-0.000327747
19	1	-0.000087404	0.000261867	-0.000208106
20	1	0.000048666	-0.000318180	-0.000286650
21	8	0.001476484	0.001804225	0.000324281
22	1	-0.000417494	-0.001106336	-0.000413515

Cartesian Forces: Max 0.005242036 RMS 0.001408843

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.008198160 RMS 0.001690350
Search for a local minimum.
Step number 51 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 49 50 51

DE= -1.69D-04 DEPred=-4.03D-04 R= 4.20D-01

Trust test= 4.20D-01 RLast= 3.51D-01 DXMaxT set to 2.20D-01

ITU= 0 -1 1 1 1 -1 1 0 -1 1 0 -1 0 -1 0 0 1 -1 0 1

ITU= 1 1 1 1 1 0 -1 1 1 1 1 1 0 -1 1 1 1 1 1 1

ITU= 1 1 1 1 1 1 0 0 -1 0 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00170	0.00188	0.00384	0.00596	0.00904
Eigenvalues ---	0.01002	0.01531	0.01774	0.02096	0.02201
Eigenvalues ---	0.02345	0.02884	0.03076	0.03237	0.03800
Eigenvalues ---	0.04375	0.05267	0.05693	0.05937	0.07091
Eigenvalues ---	0.08899	0.09442	0.11127	0.13994	0.14643
Eigenvalues ---	0.15522	0.15971	0.16064	0.16295	0.17045
Eigenvalues ---	0.17404	0.19623	0.20970	0.22529	0.23375
Eigenvalues ---	0.24631	0.25101	0.27286	0.29471	0.33093
Eigenvalues ---	0.33855	0.33888	0.33906	0.34014	0.34251
Eigenvalues ---	0.34581	0.34932	0.35347	0.36304	0.36337
Eigenvalues ---	0.38903	0.43235	0.44461	0.46460	0.49216
Eigenvalues ---	0.53673	0.55709	0.57688	0.60802	1.27672

RFO step: Lambda=-3.01081879D-04 EMin= 1.69895647D-03

Quartic linear search produced a step of -0.35419.

Iteration 1 RMS(Cart)= 0.02193571 RMS(Int)= 0.00018535

Iteration 2 RMS(Cart)= 0.00023014 RMS(Int)= 0.00001186

Iteration 3 RMS(Cart)= 0.00000003 RMS(Int)= 0.00001186

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56408	0.00126	-0.00027	0.00064	0.00038	2.56445
R2	2.61742	-0.00063	0.00070	-0.00024	0.00047	2.61789
R3	2.03389	0.00010	0.00013	0.00011	0.00024	2.03413
R4	2.63094	-0.00043	0.00019	-0.00084	-0.00064	2.63030
R5	2.03027	0.00017	0.00003	0.00024	0.00027	2.03054
R6	2.54178	0.00109	0.00088	0.00112	0.00199	2.54377
R7	2.69400	-0.00129	-0.00137	-0.00102	-0.00239	2.69161
R8	2.52132	-0.00002	-0.00048	0.00060	0.00011	2.52143
R9	2.09241	0.00119	0.00112	-0.00102	0.00010	2.09251
R10	2.80752	-0.00433	-0.00360	-0.00133	-0.00494	2.80258
R11	2.90042	-0.00079	0.00104	0.00103	0.00206	2.90248
R12	2.06148	-0.00036	-0.00019	0.00011	-0.00007	2.06141
R13	2.05905	0.00058	0.00042	0.00027	0.00068	2.05973
R14	2.06878	-0.00053	-0.00024	-0.00090	-0.00113	2.06765
R15	2.06652	-0.00214	0.00045	0.00021	0.00066	2.06718
R16	2.67483	0.00095	0.00098	-0.00047	0.00052	2.67535
R17	5.55631	-0.00180	0.01944	-0.06827	-0.04883	5.50748
R18	2.50593	-0.00028	0.00030	-0.00003	0.00027	2.50620
R19	2.04585	-0.00002	0.00011	0.00000	0.00012	2.04596

R20	2.04271	0.00017	0.00016	0.00017	0.00033	2.04304
R21	2.04443	0.00042	0.00025	0.00042	0.00067	2.04510
R22	1.82556	-0.00108	-0.00053	0.00040	-0.00013	1.82542
A1	1.87414	-0.00035	-0.00013	0.00025	0.00013	1.87427
A2	2.27208	0.00079	0.00099	0.00124	0.00224	2.27431
A3	2.13671	-0.00045	-0.00078	-0.00158	-0.00235	2.13436
A4	1.86193	0.00027	0.00016	0.00016	0.00032	1.86224
A5	2.27109	0.00067	0.00047	0.00226	0.00273	2.27382
A6	2.15016	-0.00093	-0.00063	-0.00242	-0.00305	2.14711
A7	1.89792	-0.00031	-0.00010	-0.00009	-0.00020	1.89772
A8	2.24549	0.00024	0.00084	-0.00087	-0.00002	2.24547
A9	2.13976	0.00008	-0.00074	0.00097	0.00024	2.14000
A10	1.88833	-0.00008	-0.00016	-0.00003	-0.00017	1.88816
A11	2.26468	-0.00219	-0.00460	-0.00397	-0.00850	2.25618
A12	2.12967	0.00225	0.00384	0.00385	0.00776	2.13743
A13	1.90244	0.00048	0.00023	-0.00027	-0.00006	1.90238
A14	2.21716	0.00297	-0.00023	-0.00003	-0.00025	2.21691
A15	2.16329	-0.00346	-0.00014	0.00025	0.00011	2.16340
A16	1.95331	-0.00372	0.00260	-0.00120	0.00140	1.95471
A17	1.85980	0.00066	0.00129	0.00200	0.00330	1.86310
A18	1.87209	0.00284	0.00114	0.00114	0.00227	1.87436
A19	1.91304	-0.00085	0.00005	-0.00451	-0.00444	1.90860
A20	1.94006	0.00168	-0.00205	0.00254	0.00049	1.94054
A21	1.92361	-0.00060	-0.00298	0.00013	-0.00286	1.92076
A22	1.93138	0.00285	-0.00134	0.00178	0.00044	1.93182
A23	1.88779	-0.00615	0.00442	-0.00005	0.00437	1.89216
A24	1.89435	0.00123	0.00057	0.00170	0.00230	1.89664
A25	1.92849	0.00031	-0.00174	0.00179	0.00004	1.92852
A26	1.88444	-0.00112	-0.00273	-0.00152	-0.00424	1.88019
A27	1.93745	0.00302	0.00077	-0.00370	-0.00291	1.93454
A28	2.24344	-0.00820	0.01394	-0.00593	0.00801	2.25145
A29	2.17533	-0.00010	0.00135	-0.00131	0.00004	2.17536
A30	1.94584	0.00150	0.00117	0.00343	0.00460	1.95044
A31	2.16200	-0.00140	-0.00252	-0.00213	-0.00465	2.15735
A32	2.07879	0.00014	-0.00027	0.00008	-0.00020	2.07860
A33	2.15801	-0.00016	0.00045	-0.00078	-0.00033	2.15768
A34	2.04638	0.00002	-0.00017	0.00071	0.00053	2.04691
A35	1.88224	-0.00035	0.00078	-0.00297	-0.00219	1.88005
D1	0.00010	0.00043	0.00015	0.00209	0.00225	0.00235
D2	-3.13883	0.00017	-0.00121	0.00428	0.00307	-3.13575
D3	3.11687	0.00046	0.00551	-0.00233	0.00317	3.12004
D4	-0.02206	0.00020	0.00415	-0.00015	0.00399	-0.01806
D5	0.00354	-0.00052	-0.00107	-0.00299	-0.00406	-0.00053
D6	-3.11237	0.00020	0.00354	-0.00044	0.00310	-3.10927

D7	-3.11559	-0.00057	-0.00593	0.00097	-0.00497	-3.12056
D8	0.05168	0.00015	-0.00132	0.00353	0.00219	0.05388
D9	-0.00367	-0.00019	0.00081	-0.00051	0.00029	-0.00338
D10	-3.13828	-0.00046	-0.00349	-0.00211	-0.00561	3.13930
D11	3.13549	0.00005	0.00205	-0.00250	-0.00045	3.13504
D12	0.00088	-0.00023	-0.00225	-0.00410	-0.00634	-0.00547
D13	0.00590	-0.00014	-0.00148	-0.00135	-0.00283	0.00308
D14	3.11337	-0.00086	-0.01918	-0.00644	-0.02564	3.08773
D15	3.14103	0.00012	0.00250	0.00013	0.00264	-3.13952
D16	-0.03469	-0.00060	-0.01520	-0.00496	-0.02017	-0.05486
D17	-0.07982	0.00036	0.03727	-0.01402	0.02325	-0.05657
D18	3.06848	0.00044	0.03780	-0.01258	0.02521	3.09370
D19	3.06962	0.00005	0.03244	-0.01582	0.01661	3.08624
D20	-0.06526	0.00014	0.03296	-0.01438	0.01858	-0.04668
D21	-0.00585	0.00040	0.00158	0.00268	0.00425	-0.00159
D22	3.11103	-0.00017	-0.00286	0.00021	-0.00265	3.10838
D23	-3.11650	0.00116	0.01810	0.00747	0.02555	-3.09095
D24	0.00038	0.00058	0.01366	0.00500	0.01865	0.01903
D25	1.63326	0.00170	-0.02228	0.02390	0.00162	1.63487
D26	-2.55897	-0.00105	-0.01988	0.01898	-0.00091	-2.55988
D27	-0.49900	0.00002	-0.02212	0.02073	-0.00139	-0.50039
D28	-1.47906	0.00245	-0.01704	0.02682	0.00979	-1.46927
D29	0.61190	-0.00031	-0.01464	0.02190	0.00726	0.61916
D30	2.67187	0.00076	-0.01687	0.02365	0.00678	2.67865
D31	-1.05010	-0.00168	0.00330	-0.03536	-0.03206	-1.08216
D32	1.06462	-0.00348	0.00316	-0.03210	-0.02894	1.03568
D33	-3.11497	-0.00273	0.00705	-0.03559	-0.02855	3.13967
D34	-3.10956	0.00035	0.00005	-0.03420	-0.03415	3.13947
D35	-0.99485	-0.00145	-0.00009	-0.03094	-0.03103	-1.02588
D36	1.10875	-0.00070	0.00379	-0.03443	-0.03064	1.07811
D37	1.04280	0.00057	0.00510	-0.03298	-0.02787	1.01492
D38	-3.12567	-0.00123	0.00496	-0.02972	-0.02475	3.13276
D39	-1.02207	-0.00048	0.00885	-0.03321	-0.02436	-1.04643
D40	0.63398	-0.00272	-0.04343	0.05596	0.01252	0.64650
D41	2.75049	-0.00294	-0.04334	0.05921	0.01588	2.76636
D42	-1.44251	-0.00217	-0.04738	0.05608	0.00871	-1.43379
D43	-1.57809	0.00317	-0.00933	0.03462	0.02529	-1.55280
D44	2.61073	-0.00030	-0.00649	0.03239	0.02590	2.63663
D45	0.49445	-0.00181	-0.00307	0.03342	0.03034	0.52479
D46	3.13383	0.00031	0.00333	0.00079	0.00412	3.13795
D47	-0.00463	0.00005	0.00341	-0.00172	0.00169	-0.00295
D48	-0.01528	0.00023	0.00276	-0.00080	0.00196	-0.01332
D49	3.12944	-0.00003	0.00284	-0.00331	-0.00047	3.12897

Item	Value	Threshold	Converged?

Maximum Force	0.008198	0.000450	NO
RMS Force	0.001690	0.000300	NO
Maximum Displacement	0.115822	0.001800	NO
RMS Displacement	0.021950	0.001200	NO

Predicted change in Energy=-2.356462D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.566678	-2.294507	-1.121227
2	6	0	-1.876545	-1.974124	-1.273509
3	7	0	-2.132354	-0.914517	-0.407963
4	6	0	-0.998476	-0.611313	0.251113
5	7	0	-0.038702	-1.437165	-0.169735
6	6	0	1.366704	-1.381827	0.300632
7	6	0	2.193994	-0.348852	-0.478869
8	1	0	0.020995	-3.064491	-1.590734
9	1	0	-2.627862	-2.405422	-1.909185
10	1	0	1.334823	-1.099150	1.353737
11	1	0	1.785339	-2.382612	0.194837
12	1	0	2.242005	-0.613049	-1.539562
13	1	0	1.730704	0.633614	-0.349441
14	35	0	0.442611	1.757324	2.011072
15	1	0	-0.807368	0.199188	0.980973
16	6	0	-3.354800	-0.215418	-0.194350
17	6	0	-4.478184	-0.439730	-0.862603
18	1	0	-3.257772	0.535134	0.579889
19	1	0	-5.357049	0.142977	-0.624087
20	1	0	-4.572424	-1.182168	-1.644338
21	8	0	3.516410	-0.352660	0.026603
22	1	0	3.554978	0.281890	0.753901

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357051	0.000000			
3	N	2.205553	1.391897	0.000000		
4	C	2.214252	2.225474	1.346103	0.000000	
5	N	1.385328	2.210047	2.171011	1.334282	0.000000
6	C	2.567612	3.653409	3.600540	2.488015	1.483062
7	C	3.437951	4.454464	4.363747	3.285365	2.502982

8	H	1.076415	2.211377	3.264697	3.232616	2.161248
9	H	2.209448	1.074513	2.173015	3.246631	3.266031
10	H	3.342160	4.240387	3.893455	2.626413	2.078892
11	H	2.696622	3.966396	4.226936	3.300044	2.086602
12	H	3.300152	4.345775	4.528400	3.702328	2.785178
13	H	3.800988	4.546036	4.162132	3.059236	2.729691
14	Br	5.219895	5.485496	4.429549	3.283996	3.897735
15	H	3.270428	3.308945	2.219250	1.107308	2.143041
16	C	3.599352	2.538281	1.424340	2.430521	3.534087
17	C	4.336700	3.048234	2.436193	3.657618	4.602601
18	H	4.259420	3.411634	2.084204	2.554771	3.848936
19	H	5.397790	4.125261	3.400539	4.509112	5.566696
20	H	4.190102	2.834162	2.748491	4.085550	4.774318
21	O	4.664749	5.779567	5.693247	4.527858	3.722032
22	H	5.209796	6.221047	5.926808	4.667392	4.089351

		6	7	8	9	10
6	C	0.000000				
7	C	1.535926	0.000000			
8	H	2.866977	3.651419	0.000000		
9	H	4.678418	5.433744	2.748131	0.000000	
10	H	1.090849	2.158603	3.776059	5.296780	0.000000
11	H	1.089963	2.181068	2.601179	4.889148	1.786977
12	H	2.177955	1.094154	3.308334	5.202386	3.070904
13	H	2.148742	1.093906	4.259095	5.537656	2.461708
14	Br	3.692400	3.701774	6.033297	6.490353	3.063915
15	H	2.772915	3.382257	4.236917	4.295487	2.532512
16	C	4.888569	5.557686	4.632828	2.874929	5.016983
17	C	6.033521	6.683821	5.259482	2.895336	6.256041
18	H	5.013830	5.623536	5.330967	3.903735	4.935752
19	H	6.956219	7.568437	6.336057	3.948959	7.087723
20	H	6.252681	6.916441	4.964425	2.312535	6.625022
21	O	2.399065	1.415733	4.710385	6.761152	2.660423
22	H	2.786028	1.941607	5.402279	7.248530	2.682566

		11	12	13	14	15
11	H	0.000000				
12	H	2.519532	0.000000			
13	H	3.065427	1.797772	0.000000		
14	Br	4.716004	4.632870	2.914435	0.000000	
15	H	3.742437	4.038750	2.898368	2.247518	0.000000
16	C	5.591889	5.769915	5.158222	4.814138	2.835964
17	C	6.642641	6.756422	6.321842	6.107314	4.157148
18	H	5.839047	6.004826	5.075257	4.151490	2.505635
19	H	7.619905	7.691248	7.110021	6.571624	4.824829
20	H	6.726424	6.838956	6.686048	6.866820	4.793334

21	O	2.673128	2.035874	2.074341	4.223552	4.462109
22	H	3.247113	2.790123	2.160799	3.666635	4.369035

		16	17	18	19	20
16	C	0.000000				
17	C	1.326224	0.000000			
18	H	1.082677	2.126158	0.000000		
19	H	2.078972	1.081130	2.451594	0.000000	
20	H	2.125954	1.082222	3.102357	1.847311	0.000000
21	O	6.876131	8.044364	6.854476	8.911079	8.301167
22	H	6.992247	8.225905	6.819675	9.019001	8.599400

		21	22
21	O	0.000000	
22	H	0.965973	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.684456	-2.085044	0.230660
2	6	0	-2.734361	-1.252635	0.015298
3	7	0	-2.229525	0.044117	0.046166
4	6	0	-0.905067	-0.013074	0.279687
5	7	0	-0.557259	-1.296236	0.392968
6	6	0	0.833730	-1.761073	0.613306
7	6	0	1.617683	-1.874373	-0.702616
8	1	0	-1.649925	-3.158635	0.300517
9	1	0	-3.772970	-1.472867	-0.150139
10	1	0	1.313479	-1.022989	1.257529
11	1	0	0.778941	-2.722846	1.123216
12	1	0	1.155516	-2.612003	-1.365547
13	1	0	1.636914	-0.889935	-1.179208
14	35	0	1.862143	1.740905	0.054437
15	1	0	-0.165284	0.809574	0.325546
16	6	0	-2.925847	1.274336	-0.128304
17	6	0	-4.215829	1.375735	-0.419054
18	1	0	-2.270923	2.127326	-0.003119
19	1	0	-4.654439	2.357815	-0.528514
20	1	0	-4.868263	0.523118	-0.555351

```
      21                8                0            2.929962     -2.318778     -0.411532
      22                1                0            3.474632     -1.538419     -0.245769
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.8385849           0.4641032           0.3084044
 Standard basis: 6-311++G(d,p) (5D, 7F)
 There are     358 symmetry adapted cartesian basis functions of A      symmetry.
 There are     345 symmetry adapted basis functions of A      symmetry.
    345 basis functions,      553 primitive gaussians,      358 cartesian basis functions
     55 alpha electrons              55 beta electrons
          nuclear repulsion energy              838.6996491651 Hartrees.
 NAtoms=       22 NActive=       22 NUniq=       22 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      345 RedAO= T EigKep=    4.48D-06    NBF=      345
 NBsUse=      345 1.00D-06 EigRej= -1.00D+00 NBFU=      345
 Initial guess from the checkpoint file:    "."
 B after Tr=          0.000000        0.000000        0.000000
             Rot=        0.999975      -0.001460        0.000570      -0.006855 Ang=    -0.81 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn=                5 AccDes=
0.00D+00
 Harris functional with IExCor=    402 and IRadAn=             5 diagonalized for initial guess.
 HarFok:    IExCor=    402 AccDes= 0.00D+00 IRadAn=                5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=    3500011 ScaDFX=    1.000000    1.000000    1.000000    1.000000
 FoFCou: FMM=F IPFlag=                  0 FMFlag=           100000 FMFlg1=                  0
             NFxFlg=                    0 DoJE=T BraDBF=F KetDBF=T FulRan=T
             wScrn=      0.000000  ICntrl=             500  IOpCl=      0  I1Cent=        200000004  NGrid=
0
             NMat0=         1 NMatS0=            1 NMatT0=         0 NMatD0=         1 NMtDS0=         0
NMtDT0=         0
 Petite list used in FoFCou.
 Keep R1 ints in memory in canonical form, NReq=1804729152.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                       energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3032.34035385          A.U. after      11 cycles
                   NFock= 11    Conv=0.58D-08         -V/T= 2.0017
 Calling FoFJK, ICntrl=              2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 ---------------------------------------------------------------------
```

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000039395	0.000010987	0.000194849
2	6	0.000012061	0.000587518	-0.000309516
3	7	-0.001736454	0.000194874	-0.000458773
4	6	0.002473066	-0.001766334	0.000150186
5	7	0.001400541	-0.000262404	0.000883303
6	6	-0.003636634	-0.000527135	-0.000562594
7	6	-0.000498314	0.000350695	0.001954008
8	1	0.000426914	0.000428205	-0.000191058
9	1	-0.000366991	0.000063717	0.000281743
10	1	0.001028620	-0.000071424	-0.000410760
11	1	0.000483361	-0.000199708	0.000344510
12	1	0.000062272	0.000272819	0.000156021
13	1	-0.000878986	-0.000320038	-0.002052398
14	35	0.000097569	-0.001444570	-0.000363812
15	1	-0.000746750	0.002300878	0.000224021
16	6	0.001948723	-0.000546369	-0.000270633
17	6	-0.000115196	0.000242558	0.000798299
18	1	-0.000749687	0.000237926	-0.000212443
19	1	-0.000021196	0.000098280	-0.000215651
20	1	-0.000047785	-0.000162698	-0.000092756
21	8	0.001101403	0.001269378	0.000532441
22	1	-0.000197142	-0.000757153	-0.000378984

Cartesian Forces: Max 0.003636634 RMS 0.000944582

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.005803041 RMS 0.001027765
Search for a local minimum.
Step number 52 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 49 50 51 52
DE= -3.62D-04 DEPred=-2.36D-04 R= 1.54D+00
TightC=F SS= 1.41D+00 RLast= 1.32D-01 DXNew= 3.7014D-01 3.9727D-01
Trust test= 1.54D+00 RLast= 1.32D-01 DXMaxT set to 3.70D-01
ITU= 1 0 -1 1 1 1 -1 1 0 -1 1 0 -1 0 -1 0 0 1 -1 0
ITU= 1 1 1 1 1 1 0 -1 1 1 1 1 1 0 -1 1 1 1 1 1
ITU= 1 1 1 1 1 1 1 0 0 -1 0 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00097	0.00186	0.00365	0.00615	0.00961
Eigenvalues ---	0.00996	0.01566	0.01758	0.02112	0.02184
Eigenvalues ---	0.02362	0.02761	0.03090	0.03194	0.03838
Eigenvalues ---	0.04185	0.05123	0.05643	0.05750	0.07258
Eigenvalues ---	0.08528	0.09268	0.10750	0.14002	0.14637
Eigenvalues ---	0.15426	0.15723	0.15996	0.16068	0.16513
Eigenvalues ---	0.17150	0.18407	0.21011	0.22506	0.23441
Eigenvalues ---	0.24793	0.25268	0.26538	0.29408	0.33110
Eigenvalues ---	0.33214	0.33864	0.33891	0.34069	0.34229
Eigenvalues ---	0.34332	0.34764	0.35332	0.36306	0.36356
Eigenvalues ---	0.39388	0.43088	0.44332	0.46476	0.49239
Eigenvalues ---	0.53622	0.55245	0.57808	0.60805	0.96869

RFO step: Lambda=-6.26883669D-04 EMin= 9.69562591D-04

Quartic linear search produced a step of 0.81464.

Iteration 1 RMS(Cart)= 0.08276770 RMS(Int)= 0.00438260

Iteration 2 RMS(Cart)= 0.00566038 RMS(Int)= 0.00004064

Iteration 3 RMS(Cart)= 0.00003723 RMS(Int)= 0.00003576

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00003576

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56445	0.00064	0.00031	0.00126	0.00154	2.56600
R2	2.61789	-0.00027	0.00038	-0.00174	-0.00137	2.61652
R3	2.03413	0.00001	0.00020	0.00022	0.00041	2.03454
R4	2.63030	-0.00033	-0.00052	-0.00215	-0.00267	2.62763
R5	2.03054	0.00006	0.00022	0.00026	0.00048	2.03101
R6	2.54377	0.00048	0.00162	0.00328	0.00492	2.54869
R7	2.69161	-0.00092	-0.00195	-0.00331	-0.00526	2.68635
R8	2.52143	-0.00024	0.00009	-0.00051	-0.00040	2.52103
R9	2.09251	0.00170	0.00008	0.01125	0.01133	2.10384
R10	2.80258	-0.00261	-0.00402	-0.00192	-0.00594	2.79664
R11	2.90248	-0.00053	0.00168	0.00115	0.00283	2.90531
R12	2.06141	-0.00044	-0.00006	-0.00074	-0.00080	2.06060
R13	2.05973	0.00034	0.00056	0.00062	0.00118	2.06091
R14	2.06765	-0.00021	-0.00092	-0.00148	-0.00240	2.06525
R15	2.06718	-0.00155	0.00054	-0.00118	-0.00064	2.06654
R16	2.67535	0.00090	0.00042	-0.00022	0.00020	2.67554
R17	5.50748	-0.00090	-0.03978	-0.09867	-0.13845	5.36903
R18	2.50620	-0.00012	0.00022	-0.00006	0.00016	2.50636
R19	2.04596	-0.00005	0.00010	-0.00076	-0.00067	2.04530
R20	2.04304	0.00003	0.00027	0.00029	0.00056	2.04360
R21	2.04510	0.00018	0.00055	0.00063	0.00118	2.04629
R22	1.82542	-0.00079	-0.00011	0.00047	0.00036	1.82579
A1	1.87427	-0.00012	0.00010	0.00116	0.00125	1.87552

A2	2.27431	0.00043	0.00182	0.00246	0.00429	2.27860
A3	2.13436	-0.00031	-0.00191	-0.00372	-0.00563	2.12873
A4	1.86224	-0.00003	0.00026	-0.00111	-0.00087	1.86138
A5	2.27382	0.00041	0.00222	0.00366	0.00588	2.27970
A6	2.14711	-0.00039	-0.00248	-0.00257	-0.00505	2.14206
A7	1.89772	-0.00001	-0.00016	0.00091	0.00078	1.89850
A8	2.24547	0.00025	-0.00001	-0.00046	-0.00050	2.24497
A9	2.14000	-0.00023	0.00019	-0.00045	-0.00028	2.13972
A10	1.88816	-0.00006	-0.00014	-0.00133	-0.00157	1.88659
A11	2.25618	-0.00140	-0.00693	0.00702	-0.00009	2.25609
A12	2.13743	0.00144	0.00632	-0.00348	0.00265	2.14008
A13	1.90238	0.00023	-0.00005	0.00038	0.00034	1.90272
A14	2.21691	0.00129	-0.00020	0.00077	0.00053	2.21745
A15	2.16340	-0.00153	0.00009	-0.00066	-0.00061	2.16279
A16	1.95471	-0.00296	0.00114	0.00190	0.00304	1.95775
A17	1.86310	0.00096	0.00269	0.00624	0.00893	1.87203
A18	1.87436	0.00173	0.00185	0.00082	0.00265	1.87701
A19	1.90860	-0.00039	-0.00362	-0.01446	-0.01809	1.89051
A20	1.94054	0.00121	0.00040	0.00253	0.00290	1.94344
A21	1.92076	-0.00053	-0.00233	0.00352	0.00114	1.92190
A22	1.93182	0.00129	0.00036	0.00548	0.00582	1.93764
A23	1.89216	-0.00358	0.00356	0.00245	0.00601	1.89817
A24	1.89664	0.00117	0.00187	0.00304	0.00493	1.90157
A25	1.92852	0.00036	0.00003	0.00104	0.00098	1.92951
A26	1.88019	-0.00059	-0.00346	-0.00060	-0.00410	1.87609
A27	1.93454	0.00144	-0.00237	-0.01143	-0.01382	1.92072
A28	2.25145	-0.00580	0.00653	-0.10456	-0.09804	2.15341
A29	2.17536	0.00014	0.00003	0.00287	0.00290	2.17826
A30	1.95044	0.00075	0.00375	0.00588	0.00963	1.96007
A31	2.15735	-0.00089	-0.00379	-0.00873	-0.01252	2.14483
A32	2.07860	0.00014	-0.00016	0.00073	0.00056	2.07915
A33	2.15768	-0.00005	-0.00027	-0.00022	-0.00050	2.15718
A34	2.04691	-0.00009	0.00043	-0.00050	-0.00008	2.04683
A35	1.88005	-0.00014	-0.00179	-0.00854	-0.01032	1.86973
D1	0.00235	0.00023	0.00183	0.00346	0.00528	0.00763
D2	-3.13575	0.00005	0.00250	0.00990	0.01244	-3.12331
D3	3.12004	0.00039	0.00258	-0.00131	0.00124	3.12129
D4	-0.01806	0.00020	0.00325	0.00513	0.00841	-0.00965
D5	-0.00053	-0.00022	-0.00331	-0.00815	-0.01145	-0.01198
D6	-3.10927	0.00030	0.00253	-0.02455	-0.02202	-3.13129
D7	-3.12056	-0.00038	-0.00405	-0.00394	-0.00799	-3.12855
D8	0.05388	0.00015	0.00179	-0.02034	-0.01856	0.03532
D9	-0.00338	-0.00016	0.00024	0.00233	0.00258	-0.00080
D10	3.13930	-0.00033	-0.00457	0.00759	0.00304	-3.14085

D11	3.13504	0.00001	-0.00036	-0.00352	-0.00386	3.13118
D12	-0.00547	-0.00016	-0.00517	0.00174	-0.00340	-0.00887
D13	0.00308	0.00003	-0.00230	-0.00742	-0.00972	-0.00664
D14	3.08773	-0.00050	-0.02089	0.03677	0.01596	3.10369
D15	-3.13952	0.00018	0.00215	-0.01229	-0.01014	3.13352
D16	-0.05486	-0.00035	-0.01643	0.03190	0.01553	-0.03933
D17	-0.05657	0.00030	0.01894	-0.10182	-0.08288	-0.13946
D18	3.09370	0.00032	0.02054	-0.10501	-0.08448	3.00922
D19	3.08624	0.00011	0.01353	-0.09591	-0.08237	3.00387
D20	-0.04668	0.00014	0.01514	-0.09910	-0.08396	-0.13064
D21	-0.00159	0.00012	0.00346	0.00961	0.01306	0.01146
D22	3.10838	-0.00032	-0.00216	0.02544	0.02324	3.13163
D23	-3.09095	0.00071	0.02081	-0.03134	-0.01045	-3.10139
D24	0.01903	0.00027	0.01519	-0.01552	-0.00026	0.01877
D25	1.63487	0.00094	0.00132	0.09526	0.09657	1.73145
D26	-2.55988	-0.00063	-0.00074	0.08263	0.08187	-2.47800
D27	-0.50039	0.00012	-0.00113	0.09036	0.08922	-0.41117
D28	-1.46927	0.00150	0.00797	0.07653	0.08452	-1.38476
D29	0.61916	-0.00008	0.00591	0.06391	0.06982	0.68898
D30	2.67865	0.00068	0.00552	0.07163	0.07717	2.75581
D31	-1.08216	-0.00054	-0.02612	-0.02196	-0.04809	-1.13025
D32	1.03568	-0.00160	-0.02357	-0.01571	-0.03928	0.99640
D33	3.13967	-0.00128	-0.02325	-0.02628	-0.04954	3.09013
D34	3.13947	0.00035	-0.02782	-0.02153	-0.04935	3.09012
D35	-1.02588	-0.00072	-0.02528	-0.01528	-0.04054	-1.06641
D36	1.07811	-0.00040	-0.02496	-0.02585	-0.05080	1.02731
D37	1.01492	0.00049	-0.02271	-0.01787	-0.04059	0.97434
D38	3.13276	-0.00058	-0.02016	-0.01161	-0.03177	3.10099
D39	-1.04643	-0.00026	-0.01984	-0.02219	-0.04204	-1.08847
D40	0.64650	-0.00062	0.01020	0.09885	0.10902	0.75552
D41	2.76636	-0.00110	0.01293	0.10782	0.12075	2.88711
D42	-1.43379	-0.00068	0.00710	0.10039	0.10751	-1.32628
D43	-1.55280	0.00176	0.02060	0.06881	0.08941	-1.46338
D44	2.63663	-0.00010	0.02110	0.06089	0.08203	2.71865
D45	0.52479	-0.00104	0.02472	0.06687	0.09154	0.61634
D46	3.13795	0.00020	0.00335	-0.00653	-0.00317	3.13478
D47	-0.00295	0.00006	0.00137	-0.01272	-0.01134	-0.01429
D48	-0.01332	0.00018	0.00160	-0.00289	-0.00129	-0.01462
D49	3.12897	0.00004	-0.00039	-0.00908	-0.00946	3.11951

Item	Value	Threshold	Converged?
Maximum Force	0.005803	0.000450	NO
RMS Force	0.001028	0.000300	NO
Maximum Displacement	0.378412	0.001800	NO
RMS Displacement	0.081927	0.001200	NO

Predicted change in Energy=-5.210996D-04
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.587755	-2.341887	-1.080993
2	6	0	-1.901617	-2.029293	-1.221899
3	7	0	-2.136686	-0.922481	-0.413721
4	6	0	-0.985241	-0.580424	0.199616
5	7	0	-0.038959	-1.437214	-0.187952
6	6	0	1.367974	-1.374904	0.266825
7	6	0	2.174937	-0.305995	-0.488103
8	1	0	-0.006532	-3.136266	-1.517205
9	1	0	-2.672683	-2.495091	-1.808085
10	1	0	1.354647	-1.110666	1.324665
11	1	0	1.800837	-2.366983	0.133448
12	1	0	2.260625	-0.555861	-1.548583
13	1	0	1.682310	0.661929	-0.360319
14	35	0	0.642858	1.571263	2.122603
15	1	0	-0.780076	0.267940	0.890724
16	6	0	-3.352331	-0.214119	-0.210621
17	6	0	-4.469189	-0.414681	-0.897274
18	1	0	-3.269886	0.526689	0.574129
19	1	0	-5.345150	0.173892	-0.661140
20	1	0	-4.558713	-1.138573	-1.697601
21	8	0	3.485691	-0.257657	0.044985
22	1	0	3.455287	0.313504	0.823656

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357868	0.000000			
3	N	2.204348	1.390482	0.000000		
4	C	2.213754	2.227032	1.348707	0.000000	
5	N	1.384605	2.211131	2.171723	1.334073	0.000000
6	C	2.564477	3.651678	3.598676	2.484620	1.479920
7	C	3.482649	4.486258	4.356108	3.245766	2.504213
8	H	1.076633	2.214485	3.264364	3.230739	2.157485
9	H	2.213382	1.074767	2.169019	3.247194	3.268093
10	H	3.328066	4.234634	3.904716	2.649900	2.082494
11	H	2.679714	3.957167	4.229665	3.310348	2.086293

12	H	3.394377	4.427413	4.556167	3.686794	2.813572
13	H	3.833468	4.563938	4.134965	2.995463	2.720088
14	Br	5.204823	5.533901	4.514152	3.313359	3.854151
15	H	3.276561	3.316370	2.226897	1.113304	2.149500
16	C	3.595529	2.534188	1.421556	2.430141	3.531984
17	C	4.337443	3.050373	2.435622	3.656300	4.601701
18	H	4.261689	3.410414	2.088082	2.566235	3.857017
19	H	5.397984	4.126304	3.399631	4.507626	5.565540
20	H	4.194840	2.842504	2.749774	4.084197	4.774558
21	O	4.712197	5.810919	5.680099	4.485234	3.724080
22	H	5.198555	6.194305	5.859088	4.572398	4.037093

		6	7	8	9	10
6	C	0.000000				
7	C	1.537424	0.000000			
8	H	2.859095	3.718642	0.000000		
9	H	4.678352	5.480321	2.757549	0.000000	
10	H	1.090424	2.146276	3.745943	5.286789	0.000000
11	H	1.090587	2.184936	2.565743	4.878354	1.787852
12	H	2.182514	1.092883	3.435037	5.307116	3.063358
13	H	2.154253	1.093567	4.314726	5.570347	2.467514
14	Br	3.556629	3.561903	5.985879	6.555788	2.887230
15	H	2.775302	3.310992	4.240886	4.301148	2.577965
16	C	4.884327	5.534992	4.630386	2.866469	5.031555
17	C	6.029065	6.657601	5.263710	2.895707	6.272039
18	H	5.021976	5.609617	5.332954	3.893938	4.962917
19	H	6.951684	7.537370	6.339624	3.947282	7.104984
20	H	6.248235	6.891888	4.974502	2.325824	6.640986
21	O	2.404617	1.415837	4.787740	6.809225	2.628032
22	H	2.741835	1.934886	5.418924	7.236455	2.586882

		11	12	13	14	15
11	H	0.000000				
12	H	2.514119	0.000000			
13	H	3.071182	1.797062	0.000000		
14	Br	4.561517	4.540863	2.841171	0.000000	
15	H	3.765288	3.984310	2.789925	2.289306	0.000000
16	C	5.595386	5.780329	5.112482	4.959139	2.839338
17	C	6.647338	6.762731	6.268042	6.260724	4.156015
18	H	5.854893	6.021991	5.041402	4.335721	2.523161
19	H	7.625782	7.692067	7.050806	6.749675	4.822554
20	H	6.730944	6.845811	6.631779	6.999537	4.791222
21	O	2.701077	2.032037	2.064484	3.967763	4.380444
22	H	3.224686	2.794733	2.160241	3.343497	4.236138

		16	17	18	19	20
16	C	0.000000				

17	C	1.326306	0.000000			
18	H	1.082325	2.118851	0.000000		
19	H	2.079626	1.081427	2.440712	0.000000	
20	H	2.126284	1.082848	3.097569	1.848053	0.000000
21	O	6.842936	8.012030	6.821512	8.869532	8.277986
22	H	6.905923	8.141816	6.733176	8.925906	8.525811

		21	22
21	O	0.000000	
22	H	0.966166	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.744316	-2.023319	0.345032
2	6	0	-2.798771	-1.193624	0.136383
3	7	0	-2.280047	0.092657	0.037157
4	6	0	-0.940757	0.033208	0.184732
5	7	0	-0.601761	-1.242041	0.381132
6	6	0	0.790277	-1.706381	0.572921
7	6	0	1.552929	-1.818584	-0.757284
8	1	0	-1.710816	-3.089302	0.492334
9	1	0	-3.850091	-1.403688	0.060731
10	1	0	1.294898	-0.967364	1.196006
11	1	0	0.748508	-2.666302	1.088854
12	1	0	1.113518	-2.587727	-1.397386
13	1	0	1.533354	-0.846047	-1.256961
14	35	0	1.969338	1.614833	0.094423
15	1	0	-0.189073	0.852780	0.132611
16	6	0	-2.973112	1.314715	-0.179768
17	6	0	-4.261864	1.411544	-0.477812
18	1	0	-2.326201	2.176853	-0.081528
19	1	0	-4.697583	2.391356	-0.617820
20	1	0	-4.914922	0.556232	-0.598289
21	8	0	2.889929	-2.200149	-0.490015
22	1	0	3.378497	-1.394434	-0.276469

Rotational constants (GHZ): 0.9101431 0.4446239 0.3096270

Standard basis: 6-311++G(d,p) (5D, 7F)
There are 358 symmetry adapted cartesian basis functions of A symmetry.
There are 345 symmetry adapted basis functions of A symmetry.
345 basis functions, 553 primitive gaussians, 358 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 842.4530923705 Hartrees.
NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 345 RedAO= T EigKep= 4.81D-06 NBF= 345
NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345
Initial guess from the checkpoint file: "."
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999936 -0.001918 -0.000995 0.011112 Ang= -1.30 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.34073182 A.U. after 13 cycles
NFock= 13 Conv=0.41D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Atomic Forces (Hartrees/Bohr)
Number Number X Y Z
---
1 6 -0.000135756 -0.000706732 0.000666810

2	6	0.000184211	0.000494831	-0.000452006
3	7	0.000602182	0.001324016	0.000679197
4	6	0.001151596	0.001629440	0.001811064
5	7	0.000468168	0.001195242	0.000430979
6	6	0.000266731	-0.000087358	-0.000811863
7	6	0.001709581	0.000757630	0.001316716
8	1	-0.000093989	0.000247051	-0.000114458
9	1	0.000072700	-0.000171158	0.000211213
10	1	-0.000355445	-0.000349988	0.000157465
11	1	-0.000016297	0.000145446	-0.000144539
12	1	-0.000050058	-0.000185260	-0.000527508
13	1	-0.001921695	-0.000951023	-0.002102354
14	35	-0.000707127	-0.000478394	0.000227285
15	1	-0.000472357	-0.002943758	-0.001349071
16	6	-0.000406696	0.000559836	-0.000394339
17	6	-0.000168798	-0.000216997	-0.000217947
18	1	0.000310444	0.000061598	0.000072967
19	1	0.000131100	-0.000120205	-0.000136094
20	1	-0.000091359	-0.000054414	0.000268957
21	8	-0.000219027	-0.000734862	-0.000339823
22	1	-0.000258111	0.000585058	0.000747348

Cartesian Forces: Max 0.002943758 RMS 0.000807663

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.003339752 RMS 0.001006305
Search for a local minimum.
Step number 53 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 51 52 53
DE= -3.78D-04 DEPred=-5.21D-04 R= 7.25D-01
TightC=F SS= 1.41D+00 RLast= 4.26D-01 DXNew= 6.2250D-01 1.2786D+00
Trust test= 7.25D-01 RLast= 4.26D-01 DXMaxT set to 6.23D-01
ITU= 1 1 0 -1 1 1 1 -1 1 0 -1 1 0 -1 0 -1 0 0 1 -1
ITU= 0 1 1 1 1 1 1 0 -1 1 1 1 1 1 0 -1 1 1 1 1
ITU= 1 1 1 1 1 1 1 1 0 0 -1 0 0
Use linear search instead of GDIIS.
Eigenvalues --- 0.00075 0.00249 0.00341 0.00621 0.00973
Eigenvalues --- 0.01013 0.01563 0.01809 0.02098 0.02182
Eigenvalues --- 0.02392 0.02939 0.03073 0.03203 0.03884

Eigenvalues ---	0.04437	0.05270	0.05718	0.06292	0.07012
Eigenvalues ---	0.08615	0.09301	0.11061	0.14056	0.14335
Eigenvalues ---	0.15347	0.15575	0.15987	0.16075	0.16505
Eigenvalues ---	0.17153	0.18346	0.21005	0.22769	0.23500
Eigenvalues ---	0.25024	0.25325	0.26587	0.29333	0.32943
Eigenvalues ---	0.33219	0.33866	0.33896	0.34067	0.34223
Eigenvalues ---	0.34324	0.34748	0.35302	0.36314	0.36373
Eigenvalues ---	0.40211	0.43034	0.44293	0.46600	0.49259
Eigenvalues ---	0.53500	0.55393	0.57816	0.60805	0.81629

RFO step: Lambda=-8.99484125D-04 EMin= 7.53470107D-04

Quartic linear search produced a step of -0.11915.

Iteration 1 RMS(Cart)= 0.09013447 RMS(Int)= 0.00346994

Iteration 2 RMS(Cart)= 0.00752221 RMS(Int)= 0.00009418

Iteration 3 RMS(Cart)= 0.00004684 RMS(Int)= 0.00008572

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00008572

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56600	0.00025	-0.00018	0.00217	0.00195	2.56795
R2	2.61652	-0.00043	0.00016	-0.00034	-0.00019	2.61633
R3	2.03454	-0.00019	-0.00005	-0.00043	-0.00048	2.03406
R4	2.62763	0.00053	0.00032	-0.00157	-0.00126	2.62637
R5	2.03101	-0.00009	-0.00006	0.00046	0.00040	2.03142
R6	2.54869	-0.00092	-0.00059	0.00061	0.00006	2.54874
R7	2.68635	0.00026	0.00063	0.00125	0.00188	2.68823
R8	2.52103	-0.00093	0.00005	0.00020	0.00027	2.52130
R9	2.10384	-0.00316	-0.00135	-0.00952	-0.01087	2.09297
R10	2.79664	-0.00198	0.00071	-0.00964	-0.00893	2.78772
R11	2.90531	-0.00111	-0.00034	0.00335	0.00301	2.90832
R12	2.06060	0.00008	0.00010	-0.00085	-0.00075	2.05985
R13	2.06091	-0.00012	-0.00014	0.00009	-0.00005	2.06086
R14	2.06525	0.00056	0.00029	-0.00036	-0.00008	2.06517
R15	2.06654	-0.00030	0.00008	0.00004	0.00011	2.06665
R16	2.67554	-0.00029	-0.00002	-0.00155	-0.00158	2.67397
R17	5.36903	0.00029	0.01650	-0.18597	-0.16947	5.19956
R18	2.50636	0.00021	-0.00002	0.00076	0.00074	2.50710
R19	2.04530	0.00012	0.00008	0.00163	0.00171	2.04701
R20	2.04360	-0.00020	-0.00007	0.00030	0.00023	2.04383
R21	2.04629	-0.00016	-0.00014	0.00095	0.00081	2.04709
R22	1.82579	0.00095	-0.00004	0.00227	0.00223	1.82802
A1	1.87552	-0.00069	-0.00015	-0.00034	-0.00047	1.87505
A2	2.27860	0.00030	-0.00051	0.00405	0.00353	2.28213
A3	2.12873	0.00040	0.00067	-0.00384	-0.00318	2.12555
A4	1.86138	0.00024	0.00010	0.00075	0.00089	1.86226
A5	2.27970	-0.00021	-0.00070	0.00769	0.00697	2.28667

A6	2.14206	-0.00003	0.00060	-0.00846	-0.00788	2.13418
A7	1.89850	-0.00050	-0.00009	-0.00100	-0.00114	1.89735
A8	2.24497	-0.00010	0.00006	-0.00457	-0.00469	2.24028
A9	2.13972	0.00060	0.00003	0.00561	0.00544	2.14516
A10	1.88659	0.00043	0.00019	0.00135	0.00158	1.88817
A11	2.25609	0.00009	0.00001	-0.01828	-0.01837	2.23771
A12	2.14008	-0.00053	-0.00032	0.01633	0.01585	2.15593
A13	1.90272	0.00053	-0.00004	-0.00081	-0.00088	1.90184
A14	2.21745	0.00281	-0.00006	0.00742	0.00719	2.22464
A15	2.16279	-0.00334	0.00007	-0.00714	-0.00720	2.15559
A16	1.95775	-0.00320	-0.00036	-0.00971	-0.01010	1.94765
A17	1.87203	-0.00065	-0.00106	0.00407	0.00291	1.87494
A18	1.87701	0.00233	-0.00032	0.01083	0.01052	1.88753
A19	1.89051	0.00111	0.00215	-0.01157	-0.00943	1.88108
A20	1.94344	0.00080	-0.00034	0.01124	0.01093	1.95437
A21	1.92190	-0.00045	-0.00014	-0.00509	-0.00521	1.91669
A22	1.93764	0.00123	-0.00069	0.00402	0.00333	1.94097
A23	1.89817	-0.00299	-0.00072	-0.00149	-0.00220	1.89597
A24	1.90157	-0.00027	-0.00059	0.00391	0.00332	1.90489
A25	1.92951	-0.00020	-0.00012	-0.00038	-0.00049	1.92902
A26	1.87609	-0.00001	0.00049	0.00076	0.00124	1.87733
A27	1.92072	0.00234	0.00165	-0.00685	-0.00520	1.91552
A28	2.15341	-0.00148	0.01168	0.02855	0.04023	2.19364
A29	2.17826	-0.00030	-0.00035	-0.00917	-0.00951	2.16875
A30	1.96007	-0.00015	-0.00115	0.00618	0.00503	1.96510
A31	2.14483	0.00045	0.00149	0.00298	0.00447	2.14931
A32	2.07915	0.00009	-0.00007	0.00321	0.00315	2.08230
A33	2.15718	-0.00001	0.00006	-0.00628	-0.00622	2.15096
A34	2.04683	-0.00008	0.00001	0.00306	0.00307	2.04990
A35	1.86973	-0.00041	0.00123	-0.01098	-0.00975	1.85998
D1	0.00763	-0.00010	-0.00063	0.00222	0.00156	0.00919
D2	-3.12331	-0.00014	-0.00148	0.00551	0.00406	-3.11925
D3	3.12129	0.00029	-0.00015	-0.00303	-0.00316	3.11813
D4	-0.00965	0.00024	-0.00100	0.00026	-0.00066	-0.01031
D5	-0.01198	0.00040	0.00136	-0.00325	-0.00185	-0.01383
D6	-3.13129	0.00058	0.00262	0.02300	0.02583	-3.10546
D7	-3.12855	0.00005	0.00095	0.00131	0.00223	-3.12632
D8	0.03532	0.00023	0.00221	0.02756	0.02991	0.06524
D9	-0.00080	-0.00023	-0.00031	-0.00045	-0.00075	-0.00155
D10	-3.14085	-0.00019	-0.00036	-0.03194	-0.03212	3.11022
D11	3.13118	-0.00019	0.00046	-0.00331	-0.00287	3.12831
D12	-0.00887	-0.00015	0.00040	-0.03479	-0.03424	-0.04311
D13	-0.00664	0.00048	0.00116	-0.00157	-0.00040	-0.00705
D14	3.10369	0.00027	-0.00190	-0.02281	-0.02442	3.07927

D15	3.13352	0.00044	0.00121	0.02761	0.02888	-3.12078
D16	-0.03933	0.00023	-0.00185	0.00637	0.00487	-0.03446
D17	-0.13946	0.00028	0.00988	0.10783	0.11768	-0.02177
D18	3.00922	0.00024	0.01007	0.10868	0.11872	3.12794
D19	3.00387	0.00033	0.00981	0.07246	0.08230	3.08617
D20	-0.13064	0.00029	0.01000	0.07331	0.08334	-0.04731
D21	0.01146	-0.00053	-0.00156	0.00297	0.00139	0.01286
D22	3.13163	-0.00061	-0.00277	-0.02205	-0.02474	3.10689
D23	-3.10139	-0.00036	0.00124	0.02323	0.02475	-3.07664
D24	0.01877	-0.00044	0.00003	-0.00180	-0.00138	0.01739
D25	1.73145	0.00048	-0.01151	0.05495	0.04341	1.77486
D26	-2.47800	-0.00043	-0.00975	0.03774	0.02795	-2.45006
D27	-0.41117	-0.00008	-0.01063	0.03960	0.02895	-0.38222
D28	-1.38476	0.00063	-0.01007	0.08474	0.07470	-1.31006
D29	0.68898	-0.00028	-0.00832	0.06754	0.05923	0.74821
D30	2.75581	0.00007	-0.00919	0.06939	0.06023	2.81605
D31	-1.13025	-0.00145	0.00573	-0.13960	-0.13384	-1.26409
D32	0.99640	-0.00290	0.00468	-0.13849	-0.13378	0.86262
D33	3.09013	-0.00200	0.00590	-0.14536	-0.13943	2.95070
D34	3.09012	0.00055	0.00588	-0.13145	-0.12560	2.96452
D35	-1.06641	-0.00090	0.00483	-0.13034	-0.12554	-1.19196
D36	1.02731	0.00000	0.00605	-0.13720	-0.13119	0.89612
D37	0.97434	-0.00012	0.00484	-0.12453	-0.11968	0.85466
D38	3.10099	-0.00158	0.00379	-0.12342	-0.11963	2.98136
D39	-1.08847	-0.00067	0.00501	-0.13028	-0.12527	-1.21374
D40	0.75552	-0.00121	-0.01299	0.16256	0.14958	0.90510
D41	2.88711	-0.00178	-0.01439	0.16635	0.15196	3.03907
D42	-1.32628	-0.00045	-0.01281	0.16276	0.14995	-1.17634
D43	-1.46338	0.00125	-0.01065	0.04224	0.03159	-1.43179
D44	2.71865	-0.00006	-0.00977	0.03475	0.02497	2.74363
D45	0.61634	-0.00117	-0.01091	0.03873	0.02782	0.64416
D46	3.13478	0.00003	0.00038	0.00912	0.00949	-3.13891
D47	-0.01429	0.00018	0.00135	0.00841	0.00976	-0.00453
D48	-0.01462	0.00007	0.00015	0.00818	0.00834	-0.00628
D49	3.11951	0.00023	0.00113	0.00748	0.00861	3.12811

Item	Value	Threshold	Converged?
Maximum Force	0.003340	0.000450	NO
RMS Force	0.001006	0.000300	NO
Maximum Displacement	0.358432	0.001800	NO
RMS Displacement	0.092821	0.001200	NO

Predicted change in Energy=-6.071255D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.596741	-2.363801	-1.107728
2	6	0	-1.904514	-2.016829	-1.234030
3	7	0	-2.109057	-0.921343	-0.403569
4	6	0	-0.946070	-0.619984	0.209405
5	7	0	-0.022031	-1.491375	-0.199197
6	6	0	1.388294	-1.444387	0.230896
7	6	0	2.156394	-0.309302	-0.469230
8	1	0	-0.035079	-3.163332	-1.559252
9	1	0	-2.695512	-2.448544	-1.820141
10	1	0	1.396408	-1.240667	1.301684
11	1	0	1.835306	-2.419994	0.036737
12	1	0	2.337949	-0.544747	-1.520853
13	1	0	1.576549	0.613397	-0.377449
14	35	0	0.578585	1.655629	1.965310
15	1	0	-0.731077	0.223485	0.894245
16	6	0	-3.301737	-0.170430	-0.210464
17	6	0	-4.443208	-0.405523	-0.844421
18	1	0	-3.178415	0.628313	0.510779
19	1	0	-5.302022	0.218432	-0.637372
20	1	0	-4.564863	-1.196187	-1.574854
21	8	0	3.415578	-0.146914	0.155524
22	1	0	3.265612	0.397226	0.941133

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.358901	0.000000			
3	N	2.205362	1.389817	0.000000		
4	C	2.213089	2.225600	1.348737	0.000000	
5	N	1.384503	2.211499	2.173104	1.334213	0.000000
6	C	2.564683	3.649148	3.592712	2.475754	1.475196
7	C	3.494052	4.471190	4.309638	3.190980	2.493140
8	H	1.076377	2.216986	3.265502	3.229035	2.155311
9	H	2.218006	1.074979	2.164012	3.243953	3.269730
10	H	3.322550	4.234190	3.911284	2.658106	2.080256
11	H	2.688459	3.970346	4.242384	3.317515	2.089904
12	H	3.477361	4.499754	4.600653	3.712713	2.865726
13	H	3.757686	4.446304	3.992467	2.868664	2.649017
14	Br	5.194301	5.467038	4.413138	3.253643	3.866453
15	H	3.274139	3.305376	2.212189	1.107550	2.153857

16	C	3.596242	2.531621	1.422548	2.434657	3.535745
17	C	4.324291	3.032008	2.430778	3.658759	4.598065
18	H	4.270521	3.415253	2.093082	2.575352	3.867804
19	H	5.387841	4.110408	3.398349	4.516004	5.567203
20	H	4.162634	2.804830	2.734672	4.075691	4.755723
21	O	4.754902	5.807824	5.606596	4.387559	3.708174
22	H	5.170965	6.106489	5.695078	4.394134	3.959262

		6	7	8	9	10
6	C	0.000000				
7	C	1.539017	0.000000			
8	H	2.861012	3.759813	0.000000		
9	H	4.678947	5.471956	2.767108	0.000000	
10	H	1.090026	2.140364	3.732393	5.286641	0.000000
11	H	1.090562	2.194111	2.568672	4.896644	1.784247
12	H	2.186280	1.092843	3.534081	5.389782	3.055735
13	H	2.154066	1.093626	4.272901	5.450444	2.507886
14	Br	3.643339	3.503915	6.001792	6.472525	3.081844
15	H	2.777330	3.237347	4.239645	4.285631	2.614563
16	C	4.879974	5.466026	4.631170	2.854535	5.050204
17	C	6.020129	6.610959	5.248628	2.860141	6.277289
18	H	5.022873	5.504519	5.342486	3.890171	5.004761
19	H	6.948322	7.478954	6.326680	3.912237	7.124456
20	H	6.225947	6.869081	4.938506	2.263413	6.619155
21	O	2.408111	1.415002	4.893492	6.822475	2.566519
22	H	2.724023	1.928386	5.461141	7.159472	2.511297

		11	12	13	14	15
11	H	0.000000				
12	H	2.489033	0.000000			
13	H	3.072453	1.796775	0.000000		
14	Br	4.680752	4.482225	2.751490	0.000000	
15	H	3.782806	3.980175	2.663526	2.216626	0.000000
16	C	5.613453	5.802007	4.943676	4.808885	2.825569
17	C	6.652389	6.816234	6.123213	6.112392	4.147111
18	H	5.886790	5.994487	4.837236	4.157654	2.510059
19	H	7.639187	7.728657	6.894802	6.589463	4.820728
20	H	6.712459	6.933694	6.513472	6.864450	4.775964
21	O	2.770967	2.032189	2.060137	3.817462	4.228197
22	H	3.286402	2.794503	2.153677	3.138891	4.000739

		16	17	18	19	20
16	C	0.000000				
17	C	1.326698	0.000000			
18	H	1.083231	2.122518	0.000000		
19	H	2.081972	1.081550	2.448665	0.000000	
20	H	2.123494	1.083274	3.098532	1.850250	0.000000

21	O	6.727319	7.926367	6.648904	8.761205	8.233020
22	H	6.691673	7.953523	6.462515	8.713668	8.377679

		21	22
21	O	0.000000	
22	H	0.967347	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.770197	-2.055344	0.254397
2	6	0	-2.790941	-1.181297	0.052564
3	7	0	-2.231860	0.091095	0.046326
4	6	0	-0.902100	-0.019653	0.242705
5	7	0	-0.607928	-1.313699	0.380665
6	6	0	0.764284	-1.821266	0.569374
7	6	0	1.567476	-1.783780	-0.742895
8	1	0	-1.771040	-3.127886	0.345168
9	1	0	-3.845734	-1.345525	-0.074017
10	1	0	1.260686	-1.162916	1.282336
11	1	0	0.700035	-2.829569	0.979891
12	1	0	1.226421	-2.555593	-1.437368
13	1	0	1.460420	-0.791403	-1.189824
14	35	0	1.914263	1.602268	0.088872
15	1	0	-0.140175	0.784174	0.241967
16	6	0	-2.880795	1.339478	-0.163597
17	6	0	-4.175651	1.474498	-0.419026
18	1	0	-2.198872	2.178758	-0.100522
19	1	0	-4.585459	2.464232	-0.568141
20	1	0	-4.856684	0.635455	-0.494417
21	8	0	2.930710	-2.036236	-0.459891
22	1	0	3.311595	-1.196814	-0.166537

Rotational constants (GHZ): 0.9194700 0.4593147 0.3168295
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 358 symmetry adapted cartesian basis functions of A symmetry.
There are 345 symmetry adapted basis functions of A symmetry.
345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons
nuclear repulsion energy 848.0054350129 Hartrees.
NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 345 RedAO= T EigKep= 4.59D-06 NBF= 345
NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345
Initial guess from the checkpoint file: "."
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999964 -0.008254 0.001843 -0.001200 Ang= -0.98 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.34095985 A.U. after 13 cycles
NFock= 13 Conv=0.24D-08 -V/T= 2.0016
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.001105247	-0.001323073	0.000875437
2	6	0.000209513	-0.000278182	-0.000390704
3	7	0.001999324	0.001222205	-0.000125317
4	6	-0.003097206	-0.001382651	-0.001210545
5	7	-0.002051867	0.000890202	-0.000103660

6	6	0.001584711	0.002074812	0.000108708
7	6	0.003217118	0.001126185	0.000967670
8	1	-0.000278229	0.000093284	-0.000522725
9	1	0.001117777	-0.000613531	-0.000357617
10	1	-0.000675880	-0.001065082	0.000240800
11	1	-0.000533249	0.000136615	0.000044082
12	1	-0.000073799	-0.000404109	-0.000343120
13	1	-0.001370764	-0.001119858	-0.002343607
14	35	0.000811700	0.000966938	0.002217357
15	1	0.001044133	0.000197908	0.001118991
16	6	-0.000267217	-0.000191933	-0.000143440
17	6	0.000089887	0.000082043	-0.000013882
18	1	0.000551158	-0.000611457	-0.000190390
19	1	0.000223439	-0.000311338	-0.000129619
20	1	-0.000691250	0.000510238	0.000426485
21	8	-0.000606454	-0.001748634	-0.000781769
22	1	-0.000097597	0.001749419	0.000656864

Cartesian Forces: Max 0.003217118 RMS 0.001088756

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.003699501 RMS 0.000996253
Search for a local minimum.
Step number 54 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Update second derivatives using D2CorX and points 53 54
DE= -2.28D-04 DEPred=-6.07D-04 R= 3.76D-01
Trust test= 3.76D-01 RLast= 5.62D-01 DXMaxT set to 6.23D-01
ITU= 0 1 1 0 -1 1 1 1 -1 1 0 -1 1 0 -1 0 -1 0 0 1
ITU= -1 0 1 1 1 1 1 1 0 -1 1 1 1 1 1 0 -1 1 1 1
ITU= 1 1 1 1 1 1 1 1 1 0 0 -1 0 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00088	0.00280	0.00383	0.00706	0.00967
Eigenvalues ---	0.01028	0.01602	0.01810	0.02126	0.02191
Eigenvalues ---	0.02389	0.02997	0.03085	0.03206	0.03882
Eigenvalues ---	0.04391	0.05238	0.05697	0.06228	0.07708
Eigenvalues ---	0.08559	0.09266	0.11798	0.14155	0.14291
Eigenvalues ---	0.15516	0.15613	0.16000	0.16083	0.16761
Eigenvalues ---	0.17664	0.18336	0.21684	0.22884	0.23483
Eigenvalues ---	0.24905	0.25438	0.27729	0.29336	0.33095

Eigenvalues --- 0.33530 0.33866 0.33894 0.34053 0.34193
Eigenvalues --- 0.34322 0.34755 0.35496 0.36324 0.36357
Eigenvalues --- 0.40080 0.43077 0.44420 0.46474 0.49499
Eigenvalues --- 0.53600 0.55640 0.57819 0.60802 0.79483
RFO step: Lambda=-4.85170753D-04 EMin= 8.81828577D-04
Quartic linear search produced a step of -0.33492.
Iteration 1 RMS(Cart)= 0.04146556 RMS(Int)= 0.00083093
Iteration 2 RMS(Cart)= 0.00133887 RMS(Int)= 0.00004999
Iteration 3 RMS(Cart)= 0.00000147 RMS(Int)= 0.00004998
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00004998

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56795	-0.00144	-0.00065	-0.00027	-0.00097	2.56699
R2	2.61633	0.00071	0.00006	-0.00014	-0.00007	2.61626
R3	2.03406	0.00000	0.00016	-0.00007	0.00009	2.03415
R4	2.62637	0.00091	0.00042	0.00050	0.00089	2.62727
R5	2.03142	-0.00038	-0.00013	-0.00030	-0.00044	2.03098
R6	2.54874	-0.00117	-0.00002	-0.00020	-0.00020	2.54854
R7	2.68823	-0.00019	-0.00063	0.00019	-0.00043	2.68779
R8	2.52130	-0.00082	-0.00009	-0.00039	-0.00044	2.52086
R9	2.09297	0.00105	0.00364	-0.00191	0.00173	2.09470
R10	2.78772	0.00244	0.00299	0.00010	0.00309	2.79081
R11	2.90832	0.00117	-0.00101	0.00322	0.00221	2.91053
R12	2.05985	0.00003	0.00025	0.00073	0.00098	2.06083
R13	2.06086	-0.00034	0.00002	-0.00065	-0.00064	2.06023
R14	2.06517	0.00041	0.00003	0.00060	0.00062	2.06580
R15	2.06665	0.00015	-0.00004	0.00053	0.00050	2.06715
R16	2.67397	-0.00068	0.00053	-0.00359	-0.00306	2.67090
R17	5.19956	0.00196	0.05676	-0.01319	0.04357	5.24314
R18	2.50710	0.00013	-0.00025	0.00043	0.00018	2.50727
R19	2.04701	-0.00051	-0.00057	-0.00009	-0.00067	2.04634
R20	2.04383	-0.00038	-0.00008	-0.00030	-0.00038	2.04346
R21	2.04709	-0.00059	-0.00027	-0.00050	-0.00077	2.04632
R22	1.82802	0.00153	-0.00075	0.00402	0.00328	1.83130
A1	1.87505	0.00017	0.00016	0.00027	0.00044	1.87549
A2	2.28213	-0.00055	-0.00118	0.00004	-0.00115	2.28098
A3	2.12555	0.00039	0.00107	-0.00045	0.00061	2.12616
A4	1.86226	-0.00040	-0.00030	0.00049	0.00016	1.86242
A5	2.28667	-0.00107	-0.00233	-0.00072	-0.00305	2.28361
A6	2.13418	0.00147	0.00264	0.00013	0.00277	2.13695
A7	1.89735	0.00027	0.00038	-0.00137	-0.00091	1.89644
A8	2.24028	0.00139	0.00157	0.00028	0.00188	2.24216
A9	2.14516	-0.00165	-0.00182	0.00091	-0.00088	2.14429
A10	1.88817	0.00005	-0.00053	0.00146	0.00084	1.88901

A11	2.23771	0.00102	0.00615	0.00484	0.01077	2.24848
A12	2.15593	-0.00107	-0.00531	-0.00482	-0.01037	2.14556
A13	1.90184	-0.00009	0.00029	-0.00089	-0.00058	1.90126
A14	2.22464	-0.00173	-0.00241	0.00466	0.00214	2.22678
A15	2.15559	0.00182	0.00241	-0.00300	-0.00069	2.15490
A16	1.94765	0.00162	0.00338	0.00699	0.01038	1.95803
A17	1.87494	-0.00026	-0.00097	0.00010	-0.00087	1.87406
A18	1.88753	-0.00156	-0.00352	-0.00511	-0.00863	1.87890
A19	1.88108	0.00092	0.00316	-0.00200	0.00114	1.88223
A20	1.95437	-0.00061	-0.00366	0.00183	-0.00182	1.95255
A21	1.91669	-0.00010	0.00174	-0.00191	-0.00018	1.91651
A22	1.94097	-0.00178	-0.00111	0.00214	0.00103	1.94200
A23	1.89597	0.00065	0.00074	-0.00343	-0.00271	1.89325
A24	1.90489	0.00140	-0.00111	-0.00137	-0.00249	1.90240
A25	1.92902	0.00093	0.00016	0.00688	0.00704	1.93606
A26	1.87733	0.00020	-0.00041	0.00301	0.00261	1.87994
A27	1.91552	-0.00142	0.00174	-0.00742	-0.00569	1.90983
A28	2.19364	-0.00370	-0.01347	-0.03373	-0.04720	2.14644
A29	2.16875	0.00221	0.00319	0.00190	0.00509	2.17384
A30	1.96510	-0.00179	-0.00168	-0.00172	-0.00340	1.96170
A31	2.14931	-0.00042	-0.00150	-0.00017	-0.00167	2.14763
A32	2.08230	-0.00035	-0.00105	-0.00168	-0.00274	2.07956
A33	2.15096	0.00094	0.00208	0.00078	0.00286	2.15383
A34	2.04990	-0.00059	-0.00103	0.00091	-0.00012	2.04978
A35	1.85998	-0.00006	0.00326	-0.00695	-0.00369	1.85629
D1	0.00919	-0.00032	-0.00052	-0.00235	-0.00292	0.00628
D2	-3.11925	-0.00030	-0.00136	0.00698	0.00558	-3.11367
D3	3.11813	0.00023	0.00106	-0.00763	-0.00658	3.11155
D4	-0.01031	0.00025	0.00022	0.00170	0.00192	-0.00839
D5	-0.01383	0.00050	0.00062	-0.00159	-0.00094	-0.01477
D6	-3.10546	0.00033	-0.00865	-0.01847	-0.02713	-3.13259
D7	-3.12632	0.00003	-0.00075	0.00310	0.00236	-3.12396
D8	0.06524	-0.00015	-0.01002	-0.01378	-0.02382	0.04141
D9	-0.00155	0.00003	0.00025	0.00547	0.00576	0.00421
D10	3.11022	0.00026	0.01076	-0.00127	0.00951	3.11973
D11	3.12831	-0.00001	0.00096	-0.00286	-0.00191	3.12640
D12	-0.04311	0.00022	0.01147	-0.00960	0.00184	-0.04127
D13	-0.00705	0.00028	0.00014	-0.00652	-0.00641	-0.01345
D14	3.07927	0.00016	0.00818	0.02330	0.03163	3.11090
D15	-3.12078	0.00001	-0.00967	-0.00022	-0.00996	-3.13074
D16	-0.03446	-0.00011	-0.00163	0.02960	0.02807	-0.00639
D17	-0.02177	0.00002	-0.03941	0.01032	-0.02911	-0.05088
D18	3.12794	-0.00010	-0.03976	0.00828	-0.03150	3.09644
D19	3.08617	0.00031	-0.02756	0.00268	-0.02486	3.06130

D20	-0.04731	0.00019	-0.02791	0.00064	-0.02725	-0.07456
D21	0.01286	-0.00049	-0.00047	0.00504	0.00457	0.01742
D22	3.10689	-0.00044	0.00828	0.02136	0.02954	3.13643
D23	-3.07664	-0.00045	-0.00829	-0.02343	-0.03153	-3.10817
D24	0.01739	-0.00040	0.00046	-0.00710	-0.00656	0.01084
D25	1.77486	-0.00095	-0.01454	0.07934	0.06478	1.83964
D26	-2.45006	0.00092	-0.00936	0.08091	0.07155	-2.37851
D27	-0.38222	-0.00017	-0.00970	0.07598	0.06630	-0.31592
D28	-1.31006	-0.00108	-0.02502	0.06009	0.03507	-1.27499
D29	0.74821	0.00079	-0.01984	0.06167	0.04184	0.79005
D30	2.81605	-0.00030	-0.02017	0.05674	0.03658	2.85263
D31	-1.26409	0.00127	0.04482	-0.08618	-0.04136	-1.30544
D32	0.86262	0.00174	0.04481	-0.07852	-0.03372	0.82890
D33	2.95070	0.00122	0.04670	-0.09032	-0.04362	2.90708
D34	2.96452	0.00010	0.04207	-0.08905	-0.04698	2.91754
D35	-1.19196	0.00057	0.04205	-0.08139	-0.03934	-1.23130
D36	0.89612	0.00005	0.04394	-0.09319	-0.04924	0.84688
D37	0.85466	-0.00001	0.04008	-0.08648	-0.04640	0.80826
D38	2.98136	0.00045	0.04007	-0.07882	-0.03876	2.94260
D39	-1.21374	-0.00007	0.04196	-0.09062	-0.04866	-1.26240
D40	0.90510	0.00289	-0.05010	0.12453	0.07444	0.97954
D41	3.03907	0.00170	-0.05089	0.12931	0.07842	3.11749
D42	-1.17634	0.00164	-0.05022	0.13261	0.08238	-1.09396
D43	-1.43179	-0.00129	-0.01058	-0.01345	-0.02404	-1.45584
D44	2.74363	-0.00007	-0.00836	-0.01703	-0.02539	2.71823
D45	0.64416	-0.00051	-0.00932	-0.02287	-0.03218	0.61198
D46	-3.13891	-0.00009	-0.00318	-0.00146	-0.00464	3.13963
D47	-0.00453	0.00009	-0.00327	-0.00026	-0.00353	-0.00805
D48	-0.00628	0.00003	-0.00279	0.00078	-0.00201	-0.00828
D49	3.12811	0.00021	-0.00288	0.00199	-0.00089	3.12722

Item	Value	Threshold	Converged?
Maximum Force	0.003700	0.000450	NO
RMS Force	0.000996	0.000300	NO
Maximum Displacement	0.184431	0.001800	NO
RMS Displacement	0.041473	0.001200	NO

Predicted change in Energy=-3.467413D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.610779	-2.384541	-1.102603

2	6	0	-1.919556	-2.040633	-1.221154
3	7	0	-2.112977	-0.921469	-0.419303
4	6	0	-0.939802	-0.599962	0.163021
5	7	0	-0.022355	-1.484989	-0.230072
6	6	0	1.388427	-1.443128	0.204638
7	6	0	2.169513	-0.296817	-0.464723
8	1	0	-0.057594	-3.200429	-1.535044
9	1	0	-2.717735	-2.494553	-1.779682
10	1	0	1.392520	-1.266516	1.280778
11	1	0	1.830066	-2.416125	-0.011745
12	1	0	2.395914	-0.528025	-1.508903
13	1	0	1.575941	0.618735	-0.387080
14	35	0	0.676181	1.634763	2.032887
15	1	0	-0.709616	0.245292	0.842177
16	6	0	-3.304071	-0.169556	-0.222044
17	6	0	-4.452690	-0.402494	-0.843970
18	1	0	-3.173035	0.630019	0.496382
19	1	0	-5.306433	0.224228	-0.625649
20	1	0	-4.586600	-1.192134	-1.572764
21	8	0	3.397394	-0.119803	0.212494
22	1	0	3.207633	0.441259	0.979511

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.358390	0.000000			
3	N	2.205465	1.390289	0.000000		
4	C	2.212415	2.225172	1.348631	0.000000	
5	N	1.384466	2.211415	2.173490	1.333980	0.000000
6	C	2.567482	3.651390	3.594616	2.476553	1.476832
7	C	3.534899	4.509276	4.328045	3.186503	2.504216
8	H	1.076425	2.215977	3.265445	3.228644	2.155674
9	H	2.215807	1.074749	2.165861	3.244165	3.268881
10	H	3.308125	4.222413	3.911245	2.670843	2.081411
11	H	2.673704	3.957693	4.236471	3.316800	2.084741
12	H	3.556956	4.581928	4.655333	3.731958	2.898140
13	H	3.783304	4.470617	3.997672	2.849000	2.646669
14	Br	5.257601	5.552943	4.508543	3.331937	3.916859
15	H	3.272302	3.308587	2.218577	1.108465	2.148469
16	C	3.596577	2.532989	1.422319	2.433781	3.535546
17	C	4.330783	3.040154	2.433914	3.659700	4.601797
18	H	4.267257	3.413726	2.090292	2.571247	3.863648
19	H	5.392803	4.117664	3.399024	4.513175	5.567708
20	H	4.177324	2.820763	2.742726	4.082003	4.766646

21	O	4.787899	5.832229	5.604108	4.363975	3.708677
22	H	5.186581	6.106618	5.667680	4.353392	3.950487

		6	7	8	9	10
6	C	0.000000				
7	C	1.540185	0.000000			
8	H	2.864538	3.812684	0.000000		
9	H	4.680127	5.517640	2.763052	0.000000	
10	H	1.090544	2.142617	3.711025	5.269600	0.000000
11	H	1.090224	2.193600	2.549282	4.879984	1.784282
12	H	2.188303	1.093173	3.627965	5.485431	3.055240
13	H	2.153270	1.093888	4.309556	5.483389	2.523800
14	Br	3.650096	3.492720	6.053730	6.565485	3.081595
15	H	2.767491	3.207999	4.236663	4.291088	2.626197
16	C	4.880941	5.480439	4.631390	2.859307	5.051709
17	C	6.025044	6.633896	5.255748	2.874428	6.279137
18	H	5.018964	5.506866	5.339007	3.892392	5.005638
19	H	6.949144	7.495809	6.332896	3.927457	7.122692
20	H	6.238839	6.904666	4.954449	2.287305	6.625565
21	O	2.405660	1.413382	4.947837	6.855874	2.544741
22	H	2.731457	1.925685	5.499690	7.165342	2.510358

		11	12	13	14	15
11	H	0.000000				
12	H	2.475194	0.000000			
13	H	3.068523	1.801639	0.000000		
14	Br	4.682057	4.492150	2.774548	0.000000	
15	H	3.776547	3.971136	2.621889	2.295398	0.000000
16	C	5.608089	5.854429	4.946024	4.917590	2.834759
17	C	6.649837	6.881953	6.131562	6.223508	4.156119
18	H	5.879474	6.031205	4.830467	4.264602	2.517146
19	H	7.634000	7.789234	6.897798	6.696947	4.825524
20	H	6.716289	7.014316	6.531616	6.977746	4.788438
21	O	2.789246	2.032933	2.054901	3.714476	4.171011
22	H	3.323391	2.791166	2.135764	2.990368	3.924552

		16	17	18	19	20
16	C	0.000000				
17	C	1.326793	0.000000			
18	H	1.082879	2.121354	0.000000		
19	H	2.080244	1.081351	2.444382	0.000000	
20	H	2.124851	1.082869	3.098350	1.849667	0.000000
21	O	6.715723	7.925898	6.619167	8.750854	8.251134
22	H	6.649746	7.919442	6.401717	8.666773	8.362545

		21	22
21	O	0.000000	
22	H	0.969080	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.847055	-2.019817	0.287623
2	6	0	-2.854298	-1.129132	0.094323
3	7	0	-2.268372	0.130278	0.035313
4	6	0	-0.935118	-0.006693	0.185232
5	7	0	-0.664875	-1.302219	0.352818
6	6	0	0.700835	-1.831428	0.542044
7	6	0	1.521745	-1.801867	-0.760800
8	1	0	-1.869826	-3.088666	0.413062
9	1	0	-3.915937	-1.275421	0.013030
10	1	0	1.201523	-1.188911	1.267143
11	1	0	0.611473	-2.841309	0.942974
12	1	0	1.205151	-2.591776	-1.446978
13	1	0	1.407115	-0.815881	-1.220456
14	35	0	2.011319	1.546848	0.102634
15	1	0	-0.149538	0.775073	0.165185
16	6	0	-2.895740	1.388882	-0.177567
17	6	0	-4.190568	1.553564	-0.415640
18	1	0	-2.194549	2.212712	-0.130022
19	1	0	-4.576038	2.553035	-0.563261
20	1	0	-4.894508	0.733025	-0.477186
21	8	0	2.883409	-2.020986	-0.451757
22	1	0	3.245621	-1.161151	-0.189837

Rotational constants (GHZ): 0.9397834 0.4445382 0.3119072
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 358 symmetry adapted cartesian basis functions of A symmetry.
There are 345 symmetry adapted basis functions of A symmetry.
345 basis functions, 553 primitive gaussians, 358 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 845.2192268598 Hartrees.
NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.

Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 345 RedAO= T EigKep= 4.74D-06 NBF= 345
NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345
Initial guess from the checkpoint file: "."
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999931 -0.001266 -0.000196 0.011677 Ang= -1.35 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.34135247 A.U. after 12 cycles
NFock= 12 Conv=0.48D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000364693	-0.001141415	0.001188584
2	6	-0.000086880	-0.000132878	0.000223723
3	7	0.001786855	0.001765590	-0.000622569
4	6	-0.000456958	-0.000038502	0.001517538
5	7	-0.001687606	0.001281456	-0.000625497
6	6	0.001493546	0.000724764	0.000151232
7	6	0.002313317	0.001583960	0.002247933
8	1	-0.000194160	0.000214606	-0.000535795
9	1	0.000666103	-0.000324939	-0.000366197
10	1	-0.000501344	-0.000723097	-0.000216495

11	1	-0.000127597	-0.000083997	0.000358181
12	1	-0.000506435	-0.000007595	-0.000191843
13	1	-0.001347682	-0.001108977	-0.003272385
14	35	-0.000312324	-0.001281882	0.000313682
15	1	-0.000108388	-0.000439648	-0.000075841
16	6	-0.000393930	0.000136049	-0.000078156
17	6	0.000512301	0.000046448	0.000194238
18	1	0.000323447	-0.000323557	-0.000070476
19	1	0.000048045	-0.000232264	-0.000188967
20	1	-0.000483692	0.000235994	0.000253146
21	8	-0.000099416	-0.001423387	-0.001003863
22	1	-0.000472509	0.001273270	0.000799826

Cartesian Forces: Max 0.003272385 RMS 0.000933414

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.005200241 RMS 0.001034929
Search for a local minimum.
Step number 55 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 54 55
DE= -3.93D-04 DEPred=-3.47D-04 R= 1.13D+00
TightC=F SS= 1.41D+00 RLast= 2.63D-01 DXNew= 1.0469D+00 7.8877D-01
Trust test= 1.13D+00 RLast= 2.63D-01 DXMaxT set to 7.89D-01
ITU= 1 0 1 1 0 -1 1 1 1 -1 1 0 -1 1 0 -1 0 -1 0 0
ITU= 1 -1 0 1 1 1 1 1 1 0 -1 1 1 1 1 1 0 -1 1 1
ITU= 1 1 1 1 1 1 1 1 1 1 0 0 -1 0 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00091	0.00273	0.00384	0.00699	0.00973
Eigenvalues ---	0.00997	0.01548	0.01759	0.02114	0.02224
Eigenvalues ---	0.02357	0.03024	0.03067	0.03207	0.03886
Eigenvalues ---	0.04387	0.05164	0.05612	0.06236	0.07707
Eigenvalues ---	0.08589	0.09311	0.10603	0.13947	0.14382
Eigenvalues ---	0.15081	0.15574	0.15920	0.16068	0.16191
Eigenvalues ---	0.17075	0.18333	0.21045	0.22858	0.23619
Eigenvalues ---	0.25013	0.25370	0.26052	0.29377	0.32863
Eigenvalues ---	0.33191	0.33865	0.33893	0.34054	0.34215
Eigenvalues ---	0.34368	0.34804	0.35299	0.36314	0.36356
Eigenvalues ---	0.40005	0.43119	0.44233	0.46459	0.49248
Eigenvalues ---	0.53528	0.54727	0.57867	0.60801	1.10705

RFO step: Lambda=-3.95935301D-04 EMin= 9.05949105D-04
Quartic linear search produced a step of 0.18162.
Iteration 1 RMS(Cart)= 0.03035425 RMS(Int)= 0.00063957
Iteration 2 RMS(Cart)= 0.00073573 RMS(Int)= 0.00002818
Iteration 3 RMS(Cart)= 0.00000031 RMS(Int)= 0.00002818

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56699	-0.00045	-0.00018	-0.00026	-0.00044	2.56654
R2	2.61626	-0.00019	-0.00001	-0.00086	-0.00087	2.61539
R3	2.03415	-0.00005	0.00002	-0.00026	-0.00024	2.03391
R4	2.62727	0.00089	0.00016	-0.00023	-0.00008	2.62719
R5	2.03098	-0.00017	-0.00008	-0.00047	-0.00055	2.03043
R6	2.54854	-0.00140	-0.00004	-0.00242	-0.00245	2.54609
R7	2.68779	-0.00005	-0.00008	-0.00122	-0.00130	2.68650
R8	2.52086	-0.00048	-0.00008	-0.00079	-0.00086	2.52000
R9	2.09470	-0.00040	0.00031	0.00317	0.00348	2.09818
R10	2.79081	0.00015	0.00056	0.00279	0.00336	2.79416
R11	2.91053	-0.00046	0.00040	0.00221	0.00261	2.91314
R12	2.06083	-0.00033	0.00018	-0.00175	-0.00158	2.05925
R13	2.06023	-0.00005	-0.00012	-0.00001	-0.00013	2.06010
R14	2.06580	0.00008	0.00011	0.00080	0.00092	2.06671
R15	2.06715	-0.00132	0.00009	-0.00302	-0.00293	2.06422
R16	2.67090	-0.00061	-0.00056	-0.00143	-0.00199	2.66892
R17	5.24314	-0.00010	0.00791	0.00821	0.01613	5.25927
R18	2.50727	-0.00020	0.00003	-0.00060	-0.00057	2.50670
R19	2.04634	-0.00024	-0.00012	-0.00130	-0.00142	2.04492
R20	2.04346	-0.00021	-0.00007	-0.00072	-0.00079	2.04267
R21	2.04632	-0.00029	-0.00014	-0.00091	-0.00105	2.04527
R22	1.83130	0.00146	0.00059	0.00263	0.00323	1.83452
A1	1.87549	-0.00061	0.00008	-0.00022	-0.00017	1.87532
A2	2.28098	-0.00003	-0.00021	-0.00152	-0.00181	2.27917
A3	2.12616	0.00067	0.00011	0.00241	0.00244	2.12860
A4	1.86242	-0.00003	0.00003	-0.00058	-0.00053	1.86189
A5	2.28361	-0.00077	-0.00055	-0.00453	-0.00511	2.27851
A6	2.13695	0.00080	0.00050	0.00527	0.00575	2.14270
A7	1.89644	0.00013	-0.00017	0.00064	0.00047	1.89691
A8	2.24216	0.00082	0.00034	0.00404	0.00432	2.24647
A9	2.14429	-0.00094	-0.00016	-0.00428	-0.00451	2.13978
A10	1.88901	-0.00022	0.00015	0.00000	0.00013	1.88914
A11	2.24848	0.00013	0.00196	-0.00235	-0.00049	2.24798
A12	2.14556	0.00008	-0.00188	0.00247	0.00049	2.14605
A13	1.90126	0.00074	-0.00010	0.00028	0.00019	1.90145
A14	2.22678	0.00161	0.00039	0.00309	0.00342	2.23020
A15	2.15490	-0.00236	-0.00013	-0.00328	-0.00346	2.15144

A16	1.95803	-0.00326	0.00188	-0.00624	-0.00435	1.95368
A17	1.87406	-0.00041	-0.00016	0.00147	0.00131	1.87538
A18	1.87890	0.00188	-0.00157	0.00023	-0.00133	1.87757
A19	1.88223	0.00137	0.00021	0.00479	0.00499	1.88722
A20	1.95255	0.00106	-0.00033	0.00364	0.00330	1.95585
A21	1.91651	-0.00070	-0.00003	-0.00408	-0.00412	1.91239
A22	1.94200	0.00118	0.00019	0.00066	0.00082	1.94282
A23	1.89325	-0.00379	-0.00049	-0.00561	-0.00612	1.88713
A24	1.90240	0.00049	-0.00045	0.00152	0.00103	1.90342
A25	1.93606	0.00032	0.00128	-0.00168	-0.00039	1.93567
A26	1.87994	-0.00021	0.00047	0.01004	0.01051	1.89045
A27	1.90983	0.00211	-0.00103	-0.00491	-0.00596	1.90387
A28	2.14644	-0.00520	-0.00857	-0.02579	-0.03437	2.11207
A29	2.17384	0.00090	0.00092	0.00501	0.00593	2.17977
A30	1.96170	-0.00085	-0.00062	-0.00404	-0.00467	1.95703
A31	2.14763	-0.00005	-0.00030	-0.00094	-0.00125	2.14639
A32	2.07956	-0.00005	-0.00050	0.00075	0.00025	2.07981
A33	2.15383	0.00054	0.00052	0.00292	0.00343	2.15726
A34	2.04978	-0.00048	-0.00002	-0.00365	-0.00367	2.04611
A35	1.85629	-0.00053	-0.00067	-0.00669	-0.00736	1.84894
D1	0.00628	-0.00017	-0.00053	-0.00307	-0.00361	0.00267
D2	-3.11367	-0.00043	0.00101	-0.01207	-0.01101	-3.12468
D3	3.11155	0.00050	-0.00119	0.01883	0.01759	3.12914
D4	-0.00839	0.00024	0.00035	0.00983	0.01018	0.00179
D5	-0.01477	0.00052	-0.00017	0.00645	0.00629	-0.00848
D6	-3.13259	0.00064	-0.00493	0.00215	-0.00279	-3.13537
D7	-3.12396	-0.00006	0.00043	-0.01300	-0.01259	-3.13654
D8	0.04141	0.00005	-0.00433	-0.01730	-0.02166	0.01975
D9	0.00421	-0.00024	0.00105	-0.00129	-0.00025	0.00397
D10	3.11973	0.00002	0.00173	0.01621	0.01799	3.13773
D11	3.12640	-0.00003	-0.00035	0.00664	0.00629	3.13269
D12	-0.04127	0.00023	0.00033	0.02413	0.02453	-0.01674
D13	-0.01345	0.00057	-0.00116	0.00532	0.00416	-0.00929
D14	3.11090	0.00009	0.00574	0.01309	0.01885	3.12975
D15	-3.13074	0.00030	-0.00181	-0.01113	-0.01288	3.13956
D16	-0.00639	-0.00019	0.00510	-0.00337	0.00180	-0.00458
D17	-0.05088	0.00000	-0.00529	0.02344	0.01815	-0.03274
D18	3.09644	-0.00008	-0.00572	0.01837	0.01265	3.10908
D19	3.06130	0.00032	-0.00452	0.04326	0.03875	3.10005
D20	-0.07456	0.00023	-0.00495	0.03819	0.03324	-0.04132
D21	0.01742	-0.00067	0.00083	-0.00726	-0.00644	0.01098
D22	3.13643	-0.00072	0.00536	-0.00307	0.00225	3.13868
D23	-3.10817	-0.00022	-0.00573	-0.01441	-0.02007	-3.12824
D24	0.01084	-0.00027	-0.00119	-0.01022	-0.01138	-0.00055

D25	1.83964	0.00030	0.01177	0.01233	0.02409	1.86373
D26	-2.37851	-0.00016	0.01299	0.01553	0.02852	-2.34999
D27	-0.31592	-0.00022	0.01204	0.01164	0.02368	-0.29225
D28	-1.27499	0.00039	0.00637	0.00739	0.01376	-1.26123
D29	0.79005	-0.00008	0.00760	0.01059	0.01819	0.80823
D30	2.85263	-0.00013	0.00664	0.00670	0.01335	2.86598
D31	-1.30544	-0.00075	-0.00751	-0.00690	-0.01441	-1.31985
D32	0.82890	-0.00214	-0.00612	-0.01234	-0.01846	0.81044
D33	2.90708	-0.00151	-0.00792	-0.02063	-0.02855	2.87853
D34	2.91754	0.00079	-0.00853	-0.00811	-0.01664	2.90091
D35	-1.23130	-0.00060	-0.00714	-0.01355	-0.02069	-1.25199
D36	0.84688	0.00003	-0.00894	-0.02184	-0.03078	0.81610
D37	0.80826	0.00011	-0.00843	-0.00844	-0.01687	0.79139
D38	2.94260	-0.00128	-0.00704	-0.01388	-0.02093	2.92168
D39	-1.26240	-0.00065	-0.00884	-0.02217	-0.03101	-1.29341
D40	0.97954	-0.00120	0.01352	0.01803	0.03156	1.01110
D41	3.11749	-0.00205	0.01424	0.01404	0.02828	-3.13741
D42	-1.09396	-0.00079	0.01496	0.02231	0.03725	-1.05671
D43	-1.45584	0.00125	-0.00437	-0.05867	-0.06302	-1.51886
D44	2.71823	-0.00033	-0.00461	-0.06629	-0.07092	2.64732
D45	0.61198	-0.00181	-0.00584	-0.06743	-0.07326	0.53872
D46	3.13963	-0.00004	-0.00084	0.00087	0.00003	3.13965
D47	-0.00805	0.00010	-0.00064	0.00324	0.00260	-0.00545
D48	-0.00828	0.00005	-0.00036	0.00646	0.00609	-0.00219
D49	3.12722	0.00019	-0.00016	0.00883	0.00867	3.13589

Item	Value	Threshold	Converged?
Maximum Force	0.005200	0.000450	NO
RMS Force	0.001035	0.000300	NO
Maximum Displacement	0.143540	0.001800	NO
RMS Displacement	0.030199	0.001200	NO

Predicted change in Energy=-2.154404D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.614001	-2.398094	-1.101021
2	6	0	-1.918915	-2.044309	-1.229968
3	7	0	-2.105412	-0.913578	-0.442912
4	6	0	-0.933289	-0.595630	0.140482
5	7	0	-0.020945	-1.490265	-0.241022
6	6	0	1.388489	-1.451846	0.204288

7	6	0	2.170466	-0.300061	-0.457784
8	1	0	-0.064416	-3.216555	-1.532871
9	1	0	-2.713433	-2.498522	-1.792896
10	1	0	1.386538	-1.285323	1.281197
11	1	0	1.829350	-2.424692	-0.014014
12	1	0	2.415113	-0.532104	-1.498164
13	1	0	1.562253	0.604967	-0.392918
14	35	0	0.708264	1.585387	2.067779
15	1	0	-0.702764	0.248334	0.824125
16	6	0	-3.291686	-0.156595	-0.240988
17	6	0	-4.456737	-0.401260	-0.826113
18	1	0	-3.141753	0.658245	0.455108
19	1	0	-5.301948	0.234645	-0.603270
20	1	0	-4.616648	-1.209932	-1.527454
21	8	0	3.377271	-0.096909	0.247219
22	1	0	3.164553	0.517217	0.968348

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.358157	0.000000			
3	N	2.204813	1.390249	0.000000		
4	C	2.211820	2.224469	1.347335	0.000000	
5	N	1.384005	2.210717	2.172172	1.333525	0.000000
6	C	2.570833	3.653358	3.593876	2.475445	1.478607
7	C	3.545244	4.512395	4.319694	3.174678	2.503168
8	H	1.076298	2.214740	3.264564	3.228668	2.156581
9	H	2.212779	1.074457	2.168916	3.244667	3.267169
10	H	3.303843	4.219956	3.912092	2.675538	2.083305
11	H	2.674371	3.958879	4.236717	3.316852	2.085252
12	H	3.579829	4.598096	4.657706	3.728403	2.903938
13	H	3.775694	4.453970	3.969917	2.820227	2.630510
14	Br	5.259068	5.563443	4.523845	3.341558	3.914325
15	H	3.273782	3.309764	2.218749	1.110309	2.149917
16	C	3.596382	2.534965	1.421633	2.429055	3.532198
17	C	4.339302	3.050123	2.436810	3.658794	4.604837
18	H	4.260548	3.411541	2.085922	2.559005	3.852289
19	H	5.399622	4.126900	3.400290	4.508626	5.567364
20	H	4.196994	2.839445	2.751430	4.089806	4.780585
21	O	4.800360	5.833012	5.585968	4.340627	3.705089
22	H	5.201807	6.102103	5.640156	4.326211	3.954738

		6	7	8	9	10
6	C	0.000000				
7	C	1.541569	0.000000			

8	H	2.871037	3.828374	0.000000		
9	H	4.680817	5.519804	2.756896	0.000000	
10	H	1.089710	2.146937	3.708625	5.266086	0.000000
11	H	1.090158	2.197123	2.553493	4.879217	1.780959
12	H	2.190484	1.093657	3.654524	5.500514	3.057802
13	H	2.148796	1.092340	4.306921	5.465627	2.531153
14	Br	3.627684	3.474395	6.051476	6.579600	3.052826
15	H	2.765529	3.193663	4.238912	4.293811	2.631769
16	C	4.876472	5.468335	4.631154	2.868348	5.047460
17	C	6.027614	6.638203	5.264777	2.893490	6.274248
18	H	5.003847	5.474614	5.332554	3.898995	4.996529
19	H	6.946824	7.492934	6.340874	3.947889	7.113183
20	H	6.254529	6.930872	4.974875	2.313688	6.628156
21	O	2.406855	1.412330	4.974547	6.857586	2.538593
22	H	2.759602	1.920939	5.533841	7.160299	2.551150

		11	12	13	14	15
11	H	0.000000				
12	H	2.475421	0.000000			
13	H	3.064921	1.800519	0.000000		
14	Br	4.655258	4.484758	2.783083	0.000000	
15	H	3.776129	3.965258	2.595898	2.307680	0.000000
16	C	5.605425	5.855685	4.915667	4.936041	2.828595
17	C	6.653471	6.905874	6.117875	6.244887	4.151816
18	H	5.868257	6.009239	4.780131	4.275854	2.500573
19	H	7.633788	7.806521	6.877401	6.714287	4.815614
20	H	6.731793	7.064416	6.539102	7.006725	4.793220
21	O	2.807646	2.039976	2.048583	3.642548	4.135057
22	H	3.376778	2.783239	2.104308	2.895357	3.879335

		16	17	18	19	20
16	C	0.000000				
17	C	1.326491	0.000000			
18	H	1.082125	2.119732	0.000000		
19	H	2.079777	1.080933	2.442549	0.000000	
20	H	2.126039	1.082313	3.097734	1.846769	0.000000
21	O	6.687069	7.913049	6.565907	8.727090	8.263838
22	H	6.602995	7.883385	6.328728	8.615769	8.352196

		21	22
21	O	0.000000	
22	H	0.970787	0.000000

Stoichiometry C7H11BrN2O

Framework group C1[X(C7H11BrN2O)]

Deg. of freedom 60

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.861572	-2.011367	0.312636
2	6	0	-2.866338	-1.121257	0.105900
3	7	0	-2.274972	0.133511	0.012975
4	6	0	-0.942532	-0.005602	0.156374
5	7	0	-0.675981	-1.298180	0.347374
6	6	0	0.692332	-1.824324	0.540173
7	6	0	1.508503	-1.799398	-0.767373
8	1	0	-1.888603	-3.078645	0.449034
9	1	0	-3.927663	-1.270942	0.030797
10	1	0	1.191268	-1.180046	1.263662
11	1	0	0.603378	-2.831316	0.948215
12	1	0	1.201644	-2.602855	-1.442933
13	1	0	1.370244	-0.822268	-1.235677
14	35	0	2.029744	1.520754	0.113714
15	1	0	-0.154390	0.775947	0.128099
16	6	0	-2.894394	1.394446	-0.204743
17	6	0	-4.194003	1.578410	-0.396451
18	1	0	-2.179241	2.206544	-0.197837
19	1	0	-4.566802	2.581046	-0.551879
20	1	0	-4.917263	0.773363	-0.410406
21	8	0	2.875917	-1.975240	-0.460890
22	1	0	3.223745	-1.088074	-0.275474

Rotational constants (GHZ): 0.9553223 0.4417275 0.3123565

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 846.2945609738 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 4.74D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Initial guess from the checkpoint file: "."
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999997 -0.001024 -0.000161 0.002227 Ang= -0.28 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.34157097 A.U. after 11 cycles
NFock= 11 Conv=0.99D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000050592	-0.000324370	0.000224099
2	6	0.000021149	-0.000260768	0.000052439
3	7	0.000207125	0.000979778	-0.000537538
4	6	0.000680959	0.001302373	0.002560699
5	7	-0.000497111	0.000842660	0.000537923
6	6	0.001214556	-0.000127292	-0.000978198
7	6	0.001689649	0.000930171	0.003445306
8	1	-0.000061594	-0.000007512	-0.000140812
9	1	0.000038831	-0.000039115	-0.000208737
10	1	-0.000403338	0.000114633	0.000077766
11	1	-0.000052151	-0.000142725	-0.000010220
12	1	-0.000199326	-0.000127860	0.000110762
13	1	-0.001884365	-0.000347294	-0.003893629
14	35	-0.000449843	-0.000946302	0.000036662
15	1	-0.000118590	-0.001493640	-0.001131215

16	6	-0.000515438	0.000196032	0.000068829
17	6	0.000418169	-0.000191799	-0.000085886
18	1	0.000117131	0.000288940	0.000142294
19	1	-0.000083086	0.000071891	0.000039454
20	1	-0.000105290	-0.000168365	-0.000061713
21	8	0.000161246	-0.000160627	-0.001445226
22	1	-0.000229275	-0.000388809	0.001196944

Cartesian Forces: Max 0.003893629 RMS 0.000935832

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.002845722 RMS 0.000863549

Search for a local minimum.

Step number 56 out of a maximum of 116

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 54 55 56

DE= -2.18D-04 DEPred=-2.15D-04 R= 1.01D+00

TightC=F SS= 1.41D+00 RLast= 1.83D-01 DXNew= 1.3266D+00 5.4884D-01

Trust test= 1.01D+00 RLast= 1.83D-01 DXMaxT set to 7.89D-01

ITU= 1 1 0 1 1 0 -1 1 1 1 -1 1 0 -1 1 0 -1 0 -1 0

ITU= 0 1 -1 0 1 1 1 1 1 1 0 -1 1 1 1 1 1 0 -1 1

ITU= 1 1 1 1 1 1 1 1 1 1 1 0 0 -1 0 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00076	0.00311	0.00431	0.00869	0.00936
Eigenvalues ---	0.01064	0.01563	0.01707	0.02119	0.02225
Eigenvalues ---	0.02335	0.03009	0.03034	0.03206	0.03888
Eigenvalues ---	0.04390	0.04991	0.05529	0.06407	0.07873
Eigenvalues ---	0.08629	0.09137	0.09634	0.13486	0.14307
Eigenvalues ---	0.14725	0.15584	0.15901	0.16069	0.16164
Eigenvalues ---	0.17083	0.18344	0.21511	0.22917	0.23722
Eigenvalues ---	0.24808	0.25307	0.25782	0.29377	0.32707
Eigenvalues ---	0.33376	0.33874	0.33900	0.34057	0.34263
Eigenvalues ---	0.34502	0.34805	0.35325	0.36315	0.36356
Eigenvalues ---	0.40561	0.43112	0.44272	0.46522	0.49096
Eigenvalues ---	0.53592	0.54432	0.57908	0.60803	1.15265

RFO step: Lambda=-4.24897840D-04 EMin= 7.55869676D-04

Quartic linear search produced a step of 0.01852.

Iteration 1 RMS(Cart)= 0.05206744 RMS(Int)= 0.00182202

Iteration 2 RMS(Cart)= 0.00311365 RMS(Int)= 0.00005064

Iteration 3 RMS(Cart)= 0.00000750 RMS(Int)= 0.00005023

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00005023

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56654	0.00019	-0.00001	-0.00087	-0.00091	2.56563
R2	2.61539	-0.00010	-0.00002	-0.00054	-0.00056	2.61483
R3	2.03391	0.00003	0.00000	-0.00009	-0.00009	2.03382
R4	2.62719	0.00072	0.00000	0.00099	0.00097	2.62816
R5	2.03043	0.00010	-0.00001	-0.00046	-0.00047	2.02996
R6	2.54609	0.00001	-0.00005	-0.00116	-0.00119	2.54491
R7	2.68650	0.00026	-0.00002	0.00189	0.00187	2.68836
R8	2.52000	-0.00010	-0.00002	-0.00127	-0.00125	2.51875
R9	2.09818	-0.00186	0.00006	0.00010	0.00016	2.09834
R10	2.79416	-0.00062	0.00006	0.00419	0.00425	2.79841
R11	2.91314	-0.00101	0.00005	0.00456	0.00461	2.91775
R12	2.05925	0.00009	-0.00003	0.00002	-0.00001	2.05924
R13	2.06010	0.00011	0.00000	-0.00044	-0.00044	2.05966
R14	2.06671	-0.00012	0.00002	-0.00037	-0.00035	2.06636
R15	2.06422	0.00000	-0.00005	0.00065	0.00059	2.06482
R16	2.66892	-0.00026	-0.00004	-0.00679	-0.00683	2.66209
R17	5.25927	-0.00016	0.00030	0.04019	0.04049	5.29976
R18	2.50670	-0.00010	-0.00001	0.00002	0.00001	2.50672
R19	2.04492	0.00033	-0.00003	-0.00032	-0.00035	2.04457
R20	2.04267	0.00012	-0.00001	-0.00002	-0.00004	2.04263
R21	2.04527	0.00018	-0.00002	-0.00060	-0.00062	2.04465
R22	1.83452	0.00069	0.00006	0.00760	0.00766	1.84218
A1	1.87532	-0.00042	0.00000	0.00005	0.00004	1.87536
A2	2.27917	0.00009	-0.00003	-0.00241	-0.00249	2.27668
A3	2.12860	0.00033	0.00005	0.00254	0.00254	2.13114
A4	1.86189	0.00017	-0.00001	-0.00011	-0.00012	1.86178
A5	2.27851	-0.00020	-0.00009	-0.00573	-0.00582	2.27268
A6	2.14270	0.00004	0.00011	0.00584	0.00595	2.14865
A7	1.89691	-0.00020	0.00001	-0.00064	-0.00060	1.89630
A8	2.24647	-0.00007	0.00008	0.00230	0.00233	2.24880
A9	2.13978	0.00027	-0.00008	-0.00157	-0.00171	2.13807
A10	1.88914	-0.00012	0.00000	0.00072	0.00066	1.88981
A11	2.24798	0.00035	-0.00001	0.00735	0.00711	2.25509
A12	2.14605	-0.00024	0.00001	-0.00799	-0.00820	2.13785
A13	1.90145	0.00058	0.00000	0.00002	0.00005	1.90149
A14	2.23020	0.00169	0.00006	0.00511	0.00506	2.23526
A15	2.15144	-0.00227	-0.00006	-0.00485	-0.00503	2.14641
A16	1.95368	-0.00242	-0.00008	-0.00002	-0.00009	1.95359
A17	1.87538	-0.00061	0.00002	-0.00503	-0.00501	1.87037
A18	1.87757	0.00178	-0.00002	-0.00471	-0.00473	1.87284
A19	1.88722	0.00067	0.00009	0.00623	0.00631	1.89353

A20	1.95585	0.00078	0.00006	0.00555	0.00560	1.96145
A21	1.91239	-0.00025	-0.00008	-0.00259	-0.00271	1.90968
A22	1.94282	0.00136	0.00002	-0.00131	-0.00130	1.94152
A23	1.88713	-0.00280	-0.00011	-0.00724	-0.00735	1.87978
A24	1.90342	-0.00053	0.00002	0.00607	0.00609	1.90952
A25	1.93567	-0.00049	-0.00001	0.00329	0.00327	1.93894
A26	1.89045	-0.00032	0.00019	-0.00146	-0.00127	1.88918
A27	1.90387	0.00285	-0.00011	0.00084	0.00074	1.90461
A28	2.11207	-0.00276	-0.00064	-0.07261	-0.07325	2.03882
A29	2.17977	-0.00046	0.00011	0.00504	0.00515	2.18491
A30	1.95703	0.00018	-0.00009	-0.00448	-0.00458	1.95246
A31	2.14639	0.00028	-0.00002	-0.00056	-0.00059	2.14579
A32	2.07981	-0.00007	0.00000	-0.00081	-0.00082	2.07900
A33	2.15726	0.00010	0.00006	0.00357	0.00363	2.16089
A34	2.04611	-0.00003	-0.00007	-0.00274	-0.00281	2.04330
A35	1.84894	0.00030	-0.00014	-0.01137	-0.01150	1.83743
D1	0.00267	-0.00005	-0.00007	-0.00468	-0.00478	-0.00211
D2	-3.12468	-0.00024	-0.00020	-0.00558	-0.00577	-3.13045
D3	3.12914	0.00025	0.00033	0.00988	0.01016	3.13930
D4	0.00179	0.00005	0.00019	0.00898	0.00917	0.01097
D5	-0.00848	0.00028	0.00012	0.00533	0.00548	-0.00300
D6	-3.13537	0.00043	-0.00005	-0.01600	-0.01606	3.13175
D7	-3.13654	0.00002	-0.00023	-0.00766	-0.00789	3.13875
D8	0.01975	0.00017	-0.00040	-0.02898	-0.02944	-0.00968
D9	0.00397	-0.00020	0.00000	0.00247	0.00250	0.00646
D10	3.13773	-0.00009	0.00033	0.01488	0.01528	-3.13018
D11	3.13269	-0.00003	0.00012	0.00317	0.00328	3.13597
D12	-0.01674	0.00008	0.00045	0.01558	0.01606	-0.00068
D13	-0.00929	0.00038	0.00008	0.00082	0.00089	-0.00840
D14	3.12975	-0.00003	0.00035	0.03458	0.03506	-3.11837
D15	3.13956	0.00028	-0.00024	-0.01069	-0.01094	3.12862
D16	-0.00458	-0.00013	0.00003	0.02306	0.02323	0.01865
D17	-0.03274	0.00003	0.00034	0.01639	0.01671	-0.01603
D18	3.10908	0.00005	0.00023	0.00927	0.00949	3.11858
D19	3.10005	0.00015	0.00072	0.03034	0.03107	3.13112
D20	-0.04132	0.00017	0.00062	0.02323	0.02386	-0.01746
D21	0.01098	-0.00041	-0.00012	-0.00377	-0.00391	0.00708
D22	3.13868	-0.00051	0.00004	0.01649	0.01641	-3.12810
D23	-3.12824	-0.00003	-0.00037	-0.03515	-0.03532	3.11962
D24	-0.00055	-0.00013	-0.00021	-0.01489	-0.01500	-0.01555
D25	1.86373	0.00042	0.00045	0.06370	0.06413	1.92786
D26	-2.34999	-0.00054	0.00053	0.06813	0.06863	-2.28136
D27	-0.29225	-0.00023	0.00044	0.06000	0.06043	-0.23181
D28	-1.26123	0.00056	0.00025	0.03952	0.03978	-1.22145

D29	0.80823	-0.00040	0.00034	0.04395	0.04429	0.85253
D30	2.86598	-0.00008	0.00025	0.03582	0.03609	2.90207
D31	-1.31985	-0.00117	-0.00027	-0.05884	-0.05911	-1.37896
D32	0.81044	-0.00279	-0.00034	-0.06039	-0.06072	0.74972
D33	2.87853	-0.00128	-0.00053	-0.06012	-0.06065	2.81788
D34	2.90091	0.00057	-0.00031	-0.05659	-0.05690	2.84401
D35	-1.25199	-0.00104	-0.00038	-0.05814	-0.05851	-1.31050
D36	0.81610	0.00047	-0.00057	-0.05787	-0.05844	0.75766
D37	0.79139	-0.00004	-0.00031	-0.06099	-0.06131	0.73008
D38	2.92168	-0.00166	-0.00039	-0.06253	-0.06292	2.85876
D39	-1.29341	-0.00015	-0.00057	-0.06227	-0.06285	-1.35627
D40	1.01110	-0.00140	0.00058	0.09744	0.09803	1.10913
D41	-3.13741	-0.00186	0.00052	0.09311	0.09363	-3.04379
D42	-1.05671	-0.00076	0.00069	0.09384	0.09453	-0.96218
D43	-1.51886	0.00169	-0.00117	0.09020	0.08903	-1.42983
D44	2.64732	0.00054	-0.00131	0.08906	0.08774	2.73506
D45	0.53872	-0.00035	-0.00136	0.08545	0.08410	0.62282
D46	3.13965	0.00000	0.00000	-0.00455	-0.00455	3.13510
D47	-0.00545	0.00008	0.00005	0.00219	0.00223	-0.00322
D48	-0.00219	-0.00002	0.00011	0.00331	0.00342	0.00123
D49	3.13589	0.00006	0.00016	0.01004	0.01021	-3.13709

Item	Value	Threshold	Converged?
Maximum Force	0.002846	0.000450	NO
RMS Force	0.000864	0.000300	NO
Maximum Displacement	0.230773	0.001800	NO
RMS Displacement	0.051970	0.001200	NO

Predicted change in Energy=-2.374967D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.623166	-2.419863	-1.097822
2	6	0	-1.925416	-2.058727	-1.228215
3	7	0	-2.097344	-0.905154	-0.470634
4	6	0	-0.918309	-0.580678	0.093468
5	7	0	-0.015671	-1.490888	-0.271621
6	6	0	1.393763	-1.455274	0.181325
7	6	0	2.174183	-0.284115	-0.453730
8	1	0	-0.083517	-3.250561	-1.518572
9	1	0	-2.722991	-2.525154	-1.776159
10	1	0	1.380824	-1.316271	1.262049

11	1	0	1.834564	-2.423868	-0.054159
12	1	0	2.475489	-0.518272	-1.478458
13	1	0	1.530554	0.598389	-0.425026
14	35	0	0.812416	1.558627	2.110225
15	1	0	-0.674750	0.260362	0.776337
16	6	0	-3.278906	-0.139641	-0.266307
17	6	0	-4.462898	-0.403316	-0.803179
18	1	0	-3.106642	0.698361	0.396015
19	1	0	-5.299154	0.242714	-0.575807
20	1	0	-4.651763	-1.239248	-1.463662
21	8	0	3.336650	-0.032335	0.301094
22	1	0	3.042433	0.518034	1.049991

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357673	0.000000			
3	N	2.204746	1.390762	0.000000		
4	C	2.211081	2.223902	1.346707	0.000000	
5	N	1.383710	2.210122	2.171648	1.332865	0.000000
6	C	2.575782	3.656215	3.593816	2.473523	1.480856
7	C	3.577909	4.533849	4.316470	3.154501	2.506975
8	H	1.076249	2.213000	3.264139	3.228595	2.157762
9	H	2.209184	1.074208	2.172609	3.245516	3.265414
10	H	3.286774	4.205221	3.907539	2.681920	2.081546
11	H	2.670147	3.955905	4.235545	3.316241	2.083533
12	H	3.655488	4.669431	4.698530	3.740682	2.933993
13	H	3.768422	4.432731	3.927386	2.766941	2.603732
14	Br	5.308563	5.632598	4.604102	3.411649	3.957078
15	H	3.270893	3.310675	2.221967	1.110396	2.144640
16	C	3.597747	2.537734	1.422621	2.428244	3.531940
17	C	4.347047	3.059388	2.440958	3.660539	4.609035
18	H	4.257055	3.411004	2.083512	2.552699	3.846121
19	H	5.406170	4.135743	3.402977	4.507516	5.568940
20	H	4.213939	2.856562	2.760938	4.098420	4.793499
21	O	4.830880	5.842464	5.557487	4.295167	3.700464
22	H	5.165361	6.042304	5.545726	4.220140	3.890299

		6	7	8	9	10
6	C	0.000000				
7	C	1.544008	0.000000			
8	H	2.880115	3.876970	0.000000		
9	H	4.682313	5.545574	2.749435	0.000000	
10	H	1.089703	2.153755	3.690207	5.247229	0.000000
11	H	1.089923	2.203076	2.550874	4.873074	1.779060

12	H	2.191570	1.093472	3.743731	5.580358	3.057036
13	H	2.145670	1.092654	4.314566	5.447452	2.556279
14	Br	3.625220	3.438601	6.090908	6.654349	3.050825
15	H	2.752489	3.150546	4.235888	4.297631	2.635731
16	C	4.874946	5.458221	4.632117	2.877389	5.043155
17	C	6.031281	6.647343	5.272340	2.911385	6.264802
18	H	4.993784	5.438238	5.329063	3.905967	4.994608
19	H	6.946333	7.492877	6.347806	3.967185	7.101426
20	H	6.269054	6.966044	4.991720	2.339096	6.620237
21	O	2.411204	1.408717	5.036438	6.873746	2.529265
22	H	2.714154	1.912715	5.529140	7.105508	2.484067

		11	12	13	14	15
11	H	0.000000				
12	H	2.463881	0.000000			
13	H	3.060065	1.802651	0.000000		
14	Br	4.646463	4.467434	2.804510	0.000000	
15	H	3.767157	3.951503	2.533950	2.382523	0.000000
16	C	5.604487	5.892854	4.868345	5.027021	2.833502
17	C	6.655951	6.972118	6.088340	6.337672	4.157572
18	H	5.862293	6.012821	4.710380	4.363208	2.500117
19	H	7.633656	7.863774	6.840625	6.804240	4.818061
20	H	6.742585	7.163640	6.532741	7.103381	4.804483
21	O	2.846383	2.035814	2.046227	3.489394	4.050044
22	H	3.366435	2.790772	2.113743	2.679535	3.736139

		16	17	18	19	20
16	C	0.000000				
17	C	1.326497	0.000000			
18	H	1.081939	2.119243	0.000000		
19	H	2.079275	1.080914	2.441139	0.000000	
20	H	2.127799	1.081984	3.098407	1.844888	0.000000
21	O	6.640711	7.886063	6.485286	8.684567	8.269567
22	H	6.490339	7.785443	6.186382	8.503005	8.282943

		21	22
21	O	0.000000	
22	H	0.974841	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-1.926649	-1.981206	0.341544
2	6	0	-2.917553	-1.077380	0.130632
3	7	0	-2.303435	0.162561	-0.009455
4	6	0	-0.971786	-0.000721	0.107458
5	7	0	-0.726607	-1.292508	0.325869
6	6	0	0.638561	-1.832176	0.520823
7	6	0	1.464873	-1.795367	-0.782947
8	1	0	-1.973796	-3.044701	0.499871
9	1	0	-3.981929	-1.213876	0.081696
10	1	0	1.131233	-1.201238	1.260177
11	1	0	0.534417	-2.841866	0.917827
12	1	0	1.197128	-2.623291	-1.445168
13	1	0	1.282657	-0.831735	-1.264719
14	35	0	2.113007	1.456317	0.128341
15	1	0	-0.165294	0.761679	0.071460
16	6	0	-2.900953	1.434095	-0.233111
17	6	0	-4.202139	1.654206	-0.367499
18	1	0	-2.163003	2.224127	-0.276374
19	1	0	-4.550766	2.664541	-0.528928
20	1	0	-4.952228	0.875719	-0.322633
21	8	0	2.834570	-1.904410	-0.472269
22	1	0	3.113934	-1.004254	-0.223292

Rotational constants (GHZ): 0.9864826 0.4297936 0.3095833
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 358 symmetry adapted cartesian basis functions of A symmetry.
There are 345 symmetry adapted basis functions of A symmetry.
345 basis functions, 553 primitive gaussians, 358 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 845.8919040543 Hartrees.
NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 345 RedAO= T EigKep= 4.91D-06 NBF= 345
NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345
Initial guess from the checkpoint file: "."
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999948 -0.002830 -0.000361 0.009765 Ang= -1.17 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes=

0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid=
0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0
NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.34166922 A.U. after 12 cycles
NFock= 12 Conv=0.48D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000871415	0.000426043	-0.000432457
2	6	-0.000013649	-0.000090793	0.000469294
3	7	-0.001590639	0.001135090	-0.000593873
4	6	0.002769745	0.002298641	0.004480809
5	7	0.000385590	0.000231564	0.001083417
6	6	0.000354728	-0.001423305	-0.001576194
7	6	0.001323873	0.000397147	0.004038978
8	1	0.000127336	-0.000058341	0.000147816
9	1	-0.000591276	0.000437058	-0.000127261
10	1	0.000101720	0.000679649	0.000009622
11	1	0.000302810	-0.000174705	-0.000135968
12	1	-0.000587332	0.000224120	0.000064902
13	1	-0.001181693	0.000174416	-0.004481178
14	35	-0.001636280	-0.002233345	-0.000856685
15	1	-0.001142992	-0.001758393	-0.002298712
16	6	-0.000074415	0.000003246	0.000328490
17	6	0.000511459	-0.000359051	0.000071689
18	1	-0.000164130	0.000603360	0.000062492
19	1	-0.000007164	0.000257893	0.000054720

20	1	0.000269700	-0.000385572	-0.000325076
21	8	-0.000373775	-0.000981754	-0.000574355
22	1	0.000344970	0.000597032	0.000589529

Cartesian Forces: Max 0.004481178 RMS 0.001276559

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.005026979 RMS 0.001604534

Search for a local minimum.

Step number 57 out of a maximum of 116

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 55 56 57

DE= -9.82D-05 DEPred=-2.37D-04 R= 4.14D-01

Trust test= 4.14D-01 RLast= 3.40D-01 DXMaxT set to 7.89D-01

ITU= 0 1 1 0 1 1 0 -1 1 1 1 -1 1 0 -1 1 0 -1 0 -1

ITU= 0 0 1 -1 0 1 1 1 1 1 1 0 -1 1 1 1 1 1 0 -1

ITU= 1 1 1 1 1 1 1 1 1 1 1 1 0 0 -1 0 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00141	0.00219	0.00576	0.00865	0.01018
Eigenvalues ---	0.01065	0.01569	0.01684	0.02140	0.02219
Eigenvalues ---	0.02384	0.03021	0.03151	0.03235	0.03896
Eigenvalues ---	0.04335	0.04780	0.05420	0.06202	0.08182
Eigenvalues ---	0.08460	0.08846	0.09435	0.13122	0.14261
Eigenvalues ---	0.14711	0.15604	0.15905	0.16090	0.16155
Eigenvalues ---	0.17210	0.18334	0.21751	0.23001	0.23796
Eigenvalues ---	0.24407	0.25289	0.25614	0.29419	0.32609
Eigenvalues ---	0.33348	0.33874	0.33900	0.34058	0.34272
Eigenvalues ---	0.34688	0.34809	0.35374	0.36315	0.36356
Eigenvalues ---	0.40786	0.43141	0.44255	0.46537	0.48985
Eigenvalues ---	0.53521	0.54120	0.58085	0.60803	1.20809

RFO step: Lambda=-4.28133299D-04 EMin= 1.40704394D-03

Quartic linear search produced a step of -0.34374.

Iteration 1 RMS(Cart)= 0.04578906 RMS(Int)= 0.00107714

Iteration 2 RMS(Cart)= 0.00154611 RMS(Int)= 0.00002681

Iteration 3 RMS(Cart)= 0.00000116 RMS(Int)= 0.00002679

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00002679

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56563	0.00121	0.00031	-0.00079	-0.00045	2.56518
R2	2.61483	-0.00071	0.00019	0.00023	0.00043	2.61526

R3	2.03382	0.00005	0.00003	-0.00009	-0.00006	2.03376
R4	2.62816	0.00036	-0.00033	0.00109	0.00076	2.62892
R5	2.02996	0.00031	0.00016	-0.00042	-0.00026	2.02970
R6	2.54491	0.00045	0.00041	-0.00174	-0.00135	2.54355
R7	2.68836	-0.00036	-0.00064	-0.00011	-0.00075	2.68761
R8	2.51875	0.00073	0.00043	-0.00058	-0.00017	2.51857
R9	2.09834	-0.00300	-0.00006	0.00440	0.00435	2.10269
R10	2.79841	-0.00225	-0.00146	0.00378	0.00232	2.80073
R11	2.91775	-0.00194	-0.00158	0.00376	0.00217	2.91993
R12	2.05924	0.00009	0.00000	-0.00114	-0.00114	2.05810
R13	2.05966	0.00031	0.00015	0.00013	0.00028	2.05993
R14	2.06636	-0.00027	0.00012	0.00046	0.00058	2.06695
R15	2.06482	-0.00014	-0.00020	0.00005	-0.00016	2.06466
R16	2.66209	-0.00008	0.00235	-0.00476	-0.00241	2.65968
R17	5.29976	-0.00112	-0.01392	0.13687	0.12295	5.42271
R18	2.50672	-0.00051	0.00000	-0.00078	-0.00079	2.50593
R19	2.04457	0.00048	0.00012	-0.00047	-0.00035	2.04422
R20	2.04263	0.00017	0.00001	-0.00042	-0.00041	2.04223
R21	2.04465	0.00045	0.00021	-0.00060	-0.00039	2.04427
R22	1.84218	0.00069	-0.00263	0.00693	0.00430	1.84648
A1	1.87536	-0.00075	-0.00001	0.00006	0.00000	1.87536
A2	2.27668	0.00054	0.00085	-0.00351	-0.00278	2.27391
A3	2.13114	0.00022	-0.00087	0.00346	0.00246	2.13360
A4	1.86178	0.00058	0.00004	-0.00030	-0.00024	1.86153
A5	2.27268	0.00037	0.00200	-0.00772	-0.00577	2.26692
A6	2.14865	-0.00094	-0.00205	0.00818	0.00608	2.15473
A7	1.89630	-0.00044	0.00021	-0.00009	0.00010	1.89641
A8	2.24880	-0.00066	-0.00080	0.00460	0.00379	2.25259
A9	2.13807	0.00110	0.00059	-0.00458	-0.00400	2.13407
A10	1.88981	-0.00019	-0.00023	0.00059	0.00038	1.89018
A11	2.25509	-0.00057	-0.00244	-0.00082	-0.00320	2.25189
A12	2.13785	0.00078	0.00282	0.00017	0.00305	2.14090
A13	1.90149	0.00081	-0.00002	-0.00023	-0.00023	1.90127
A14	2.23526	0.00340	-0.00174	0.00292	0.00121	2.23647
A15	2.14641	-0.00420	0.00173	-0.00273	-0.00098	2.14543
A16	1.95359	-0.00424	0.00003	-0.00545	-0.00542	1.94817
A17	1.87037	-0.00072	0.00172	-0.00105	0.00068	1.87105
A18	1.87284	0.00362	0.00163	-0.00189	-0.00027	1.87257
A19	1.89353	0.00045	-0.00217	0.01226	0.01010	1.90363
A20	1.96145	0.00115	-0.00193	0.00230	0.00037	1.96182
A21	1.90968	-0.00030	0.00093	-0.00666	-0.00572	1.90396
A22	1.94152	0.00291	0.00045	-0.00701	-0.00659	1.93493
A23	1.87978	-0.00449	0.00253	-0.00502	-0.00254	1.87724
A24	1.90952	-0.00128	-0.00209	0.00697	0.00487	1.91439

A25	1.93894	-0.00108	-0.00112	-0.00641	-0.00757	1.93137
A26	1.88918	-0.00050	0.00044	0.00318	0.00364	1.89281
A27	1.90461	0.00451	-0.00025	0.00879	0.00853	1.91314
A28	2.03882	-0.00212	0.02518	-0.04246	-0.01728	2.02154
A29	2.18491	-0.00177	-0.00177	0.00534	0.00357	2.18849
A30	1.95246	0.00120	0.00157	-0.00612	-0.00455	1.94791
A31	2.14579	0.00056	0.00020	0.00075	0.00095	2.14675
A32	2.07900	0.00000	0.00028	-0.00042	-0.00014	2.07886
A33	2.16089	-0.00035	-0.00125	0.00505	0.00381	2.16469
A34	2.04330	0.00035	0.00097	-0.00465	-0.00369	2.03961
A35	1.83743	0.00100	0.00395	-0.00297	0.00098	1.83842
D1	-0.00211	0.00010	0.00164	-0.00630	-0.00464	-0.00676
D2	-3.13045	-0.00019	0.00198	-0.01964	-0.01759	3.13515
D3	3.13930	0.00018	-0.00349	0.02632	0.02279	-3.12110
D4	0.01097	-0.00012	-0.00315	0.01298	0.00984	0.02081
D5	-0.00300	0.00009	-0.00188	0.00841	0.00652	0.00351
D6	3.13175	0.00031	0.00552	0.00166	0.00720	3.13895
D7	3.13875	0.00002	0.00271	-0.02090	-0.01822	3.12053
D8	-0.00968	0.00024	0.01012	-0.02765	-0.01754	-0.02722
D9	0.00646	-0.00026	-0.00086	0.00212	0.00125	0.00771
D10	-3.13018	-0.00028	-0.00525	0.01815	0.01290	-3.11729
D11	3.13597	0.00002	-0.00113	0.01414	0.01305	-3.13417
D12	-0.00068	0.00000	-0.00552	0.03017	0.02470	0.02402
D13	-0.00840	0.00032	-0.00030	0.00309	0.00280	-0.00560
D14	-3.11837	-0.00029	-0.01205	0.00515	-0.00694	-3.12531
D15	3.12862	0.00034	0.00376	-0.01168	-0.00787	3.12075
D16	0.01865	-0.00028	-0.00799	-0.00962	-0.01761	0.00104
D17	-0.01603	-0.00002	-0.00574	0.09203	0.08629	0.07026
D18	3.11858	0.00015	-0.00326	0.08664	0.08338	-3.08123
D19	3.13112	-0.00004	-0.01068	0.11002	0.09933	-3.05274
D20	-0.01746	0.00013	-0.00820	0.10463	0.09642	0.07896
D21	0.00708	-0.00025	0.00134	-0.00707	-0.00574	0.00134
D22	-3.12810	-0.00049	-0.00564	-0.00077	-0.00639	-3.13448
D23	3.11962	0.00028	0.01214	-0.00899	0.00312	3.12274
D24	-0.01555	0.00004	0.00516	-0.00268	0.00247	-0.01308
D25	1.92786	0.00094	-0.02204	-0.00520	-0.02724	1.90062
D26	-2.28136	-0.00140	-0.02359	0.00599	-0.01760	-2.29895
D27	-0.23181	-0.00028	-0.02077	-0.00327	-0.02405	-0.25586
D28	-1.22145	0.00121	-0.01368	-0.01279	-0.02647	-1.24791
D29	0.85253	-0.00113	-0.01522	-0.00160	-0.01683	0.83570
D30	2.90207	-0.00001	-0.01241	-0.01087	-0.02328	2.87879
D31	-1.37896	-0.00254	0.02032	-0.01527	0.00503	-1.37393
D32	0.74972	-0.00503	0.02087	-0.03084	-0.00996	0.73975
D33	2.81788	-0.00291	0.02085	-0.01934	0.00151	2.81939

D34	2.84401	0.00058	0.01956	-0.01852	0.00102	2.84503
D35	-1.31050	-0.00191	0.02011	-0.03410	-0.01397	-1.32447
D36	0.75766	0.00021	0.02009	-0.02260	-0.00250	0.75516
D37	0.73008	-0.00007	0.02107	-0.02000	0.00106	0.73114
D38	2.85876	-0.00257	0.02163	-0.03557	-0.01393	2.84482
D39	-1.35627	-0.00045	0.02160	-0.02407	-0.00246	-1.35873
D40	1.10913	-0.00470	-0.03370	0.00287	-0.03085	1.07828
D41	-3.04379	-0.00471	-0.03218	-0.01305	-0.04521	-3.08899
D42	-0.96218	-0.00311	-0.03249	-0.00747	-0.03997	-1.00216
D43	-1.42983	0.00187	-0.03060	-0.01214	-0.04276	-1.47259
D44	2.73506	-0.00061	-0.03016	-0.00974	-0.03990	2.69516
D45	0.62282	-0.00168	-0.02891	-0.00909	-0.03799	0.58483
D46	3.13510	0.00018	0.00157	0.00520	0.00676	-3.14132
D47	-0.00322	0.00001	-0.00077	0.01103	0.01026	0.00704
D48	0.00123	-0.00001	-0.00118	0.01118	0.01000	0.01124
D49	-3.13709	-0.00018	-0.00351	0.01701	0.01351	-3.12358

Item	Value	Threshold	Converged?
Maximum Force	0.005027	0.000450	NO
RMS Force	0.001605	0.000300	NO
Maximum Displacement	0.216374	0.001800	NO
RMS Displacement	0.046126	0.001200	NO

Predicted change in Energy=-2.820337D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.615137	-2.407153	-1.113496
2	6	0	-1.912006	-2.035113	-1.263002
3	7	0	-2.088987	-0.888511	-0.495327
4	6	0	-0.918122	-0.578414	0.091704
5	7	0	-0.014303	-1.488331	-0.270850
6	6	0	1.390594	-1.460514	0.200375
7	6	0	2.185823	-0.305188	-0.447965
8	1	0	-0.071705	-3.227202	-1.549895
9	1	0	-2.696243	-2.487942	-1.840535
10	1	0	1.365632	-1.313785	1.279258
11	1	0	1.824510	-2.436655	-0.016696
12	1	0	2.488048	-0.563987	-1.466807
13	1	0	1.542341	0.577785	-0.449310
14	35	0	0.726502	1.533971	2.130334
15	1	0	-0.682027	0.259693	0.784473

16	6	0	-3.268658	-0.121395	-0.288854
17	6	0	-4.472373	-0.422703	-0.756587
18	1	0	-3.073795	0.753960	0.316107
19	1	0	-5.301355	0.235097	-0.537496
20	1	0	-4.689055	-1.301425	-1.349162
21	8	0	3.344262	-0.044432	0.307624
22	1	0	3.056403	0.555366	1.023260

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357437	0.000000			
3	N	2.204686	1.391166	0.000000		
4	C	2.211016	2.223737	1.345990	0.000000	
5	N	1.383938	2.210116	2.171287	1.332772	0.000000
6	C	2.577855	3.657705	3.594256	2.473880	1.482081
7	C	3.564627	4.522072	4.314685	3.162336	2.504347
8	H	1.076217	2.211355	3.263589	3.229140	2.159380
9	H	2.205928	1.074070	2.176355	3.246776	3.264343
10	H	3.293049	4.210263	3.906968	2.677048	2.082672
11	H	2.675017	3.959301	4.235717	3.314640	2.084502
12	H	3.626547	4.643945	4.690238	3.745818	2.923437
13	H	3.742420	4.407022	3.916463	2.771889	2.593034
14	Br	5.277772	5.587022	4.548570	3.364962	3.930495
15	H	3.273961	3.312270	2.221665	1.112696	2.148290
16	C	3.598041	2.540037	1.422225	2.424605	3.529825
17	C	4.352436	3.067866	2.442492	3.657396	4.609327
18	H	4.252223	3.409145	2.079900	2.544112	3.838343
19	H	5.410536	4.143416	3.403466	4.502269	5.567245
20	H	4.227882	2.873625	2.767650	4.101070	4.801145
21	O	4.824818	5.835926	5.556743	4.301124	3.701275
22	H	5.179039	6.051666	5.555711	4.236756	3.909048

		6	7	8	9	10
6	C	0.000000				
7	C	1.545158	0.000000			
8	H	2.884952	3.853420	0.000000		
9	H	4.682218	5.526141	2.742112	0.000000	
10	H	1.089101	2.161778	3.705565	5.254577	0.000000
11	H	1.090070	2.204471	2.563454	4.875062	1.775079
12	H	2.188073	1.093780	3.694855	5.542396	3.059884
13	H	2.144710	1.092571	4.277190	5.412927	2.568503
14	Br	3.623907	3.487083	6.070419	6.607478	3.040153
15	H	2.756092	3.172153	4.240307	4.300840	2.629363
16	C	4.872496	5.459896	4.632146	2.887199	5.035614

17	C	6.030524	6.666381	5.278299	2.931688	6.246679
18	H	4.984783	5.419334	5.323924	3.911979	4.991166
19	H	6.942747	7.507180	6.353086	3.987412	7.081549
20	H	6.276027	7.004898	5.006879	2.370774	6.600605
21	O	2.415286	1.407440	5.024861	6.860978	2.543680
22	H	2.741502	1.913888	5.542022	7.110273	2.533371

		11	12	13	14	15
11	H	0.000000				
12	H	2.459674	0.000000			
13	H	3.058370	1.798139	0.000000		
14	Br	4.645560	4.521493	2.869573	0.000000	
15	H	3.767610	3.974429	2.563438	2.327892	0.000000
16	C	5.601327	5.892633	4.864186	4.955200	2.826291
17	C	6.652382	6.997988	6.105095	6.260287	4.148163
18	H	5.855269	5.987475	4.682479	4.282767	2.486810
19	H	7.628069	7.885236	6.852838	6.718590	4.804831
20	H	6.744682	7.215848	6.570499	7.033820	4.800600
21	O	2.852641	2.037559	2.051103	3.558974	4.065818
22	H	3.398715	2.788622	2.112190	2.758935	3.757699

		16	17	18	19	20
16	C	0.000000				
17	C	1.326081	0.000000			
18	H	1.081756	2.119252	0.000000		
19	H	2.078645	1.080700	2.441287	0.000000	
20	H	2.129379	1.081781	3.099483	1.842447	0.000000
21	O	6.640212	7.897811	6.467531	8.691320	8.298141
22	H	6.495079	7.797881	6.174045	8.508269	8.310727

		21	22
21	O	0.000000	
22	H	0.977116	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.891261	-2.000421	0.343431
2	6	0	-2.886579	-1.108247	0.106782
3	7	0	-2.280945	0.135788	-0.037881

4	6	0	-0.950490	-0.014392	0.100056
5	7	0	-0.696576	-1.301926	0.332578
6	6	0	0.672928	-1.827463	0.544319
7	6	0	1.491892	-1.826896	-0.765953
8	1	0	-1.932549	-3.065185	0.494483
9	1	0	-3.946946	-1.262739	0.033428
10	1	0	1.159687	-1.175674	1.268459
11	1	0	0.574511	-2.825151	0.972321
12	1	0	1.217497	-2.676953	-1.397195
13	1	0	1.290526	-0.884118	-1.280086
14	35	0	2.056296	1.496047	0.128052
15	1	0	-0.150467	0.757958	0.060936
16	6	0	-2.881924	1.403499	-0.271235
17	6	0	-4.186221	1.637523	-0.321569
18	1	0	-2.138834	2.179479	-0.397208
19	1	0	-4.532982	2.644262	-0.506350
20	1	0	-4.943419	0.877628	-0.182068
21	8	0	2.864239	-1.918483	-0.467352
22	1	0	3.151287	-1.001942	-0.287598

Rotational constants (GHZ): 0.9653302 0.4387101 0.3119283

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 846.3602460850 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 5.23D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Initial guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999981 0.002132 0.000396 -0.005778 Ang= 0.71 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.34190843 A.U. after 12 cycles
NFock= 12 Conv=0.26D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.001270927	0.001156900	-0.001531670
2	6	0.000043564	-0.000434312	0.000561843
3	7	-0.002112018	-0.000095183	-0.000780473
4	6	0.002577026	0.002953644	0.003843008
5	7	0.000915559	-0.000378326	0.002113976
6	6	-0.000120485	-0.001904286	-0.002226234
7	6	-0.000689796	-0.000767202	0.003445939
8	1	0.000215496	-0.000339261	0.000658766
9	1	-0.001185226	0.000734916	0.000093737
10	1	0.000203657	0.001628779	0.000213063
11	1	0.000335088	-0.000107997	-0.000508217
12	1	-0.000113706	0.000342049	0.000141342
13	1	-0.000680963	0.000439607	-0.003794437
14	35	-0.000503125	-0.001482566	-0.001047622
15	1	-0.000839684	-0.002280152	-0.002270572
16	6	0.000345092	0.000260670	0.000415034
17	6	0.000010219	-0.000446906	-0.000238491
18	1	-0.000510223	0.000846933	0.000158466
19	1	-0.000065725	0.000456479	0.000265345
20	1	0.000709382	-0.000646661	-0.000531546
21	8	-0.001170255	0.002610093	0.001894587
22	1	0.001365198	-0.002547219	-0.000875845

Cartesian Forces: Max 0.003843008 RMS 0.001389818

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.003423479 RMS 0.001196343
Search for a local minimum.
Step number 58 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 55 56 57 58
DE= -2.39D-04 DEPred=-2.82D-04 R= 8.48D-01
TightC=F SS= 1.41D+00 RLast= 2.58D-01 DXNew= 1.3266D+00 7.7270D-01
Trust test= 8.48D-01 RLast= 2.58D-01 DXMaxT set to 7.89D-01
ITU= 1 0 1 1 0 1 1 0 -1 1 1 1 -1 1 0 -1 1 0 -1 0
ITU= -1 0 0 1 -1 0 1 1 1 1 1 1 0 -1 1 1 1 1 1 0
ITU= -1 1 1 1 1 1 1 1 1 1 1 1 1 0 0 -1 0 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00102	0.00294	0.00565	0.00855	0.01064
Eigenvalues ---	0.01298	0.01529	0.01674	0.02144	0.02269
Eigenvalues ---	0.02389	0.03033	0.03158	0.03251	0.03902
Eigenvalues ---	0.04449	0.04803	0.05497	0.06081	0.07758
Eigenvalues ---	0.08445	0.09313	0.09462	0.13272	0.14306
Eigenvalues ---	0.14715	0.15741	0.15899	0.16102	0.16144
Eigenvalues ---	0.17567	0.18335	0.22537	0.23354	0.23862
Eigenvalues ---	0.24949	0.25300	0.27484	0.29444	0.32612
Eigenvalues ---	0.33365	0.33874	0.33902	0.34058	0.34273
Eigenvalues ---	0.34647	0.34870	0.35372	0.36321	0.36375
Eigenvalues ---	0.41661	0.43195	0.45095	0.46896	0.49019
Eigenvalues ---	0.53606	0.56062	0.58832	0.60843	1.05190

RFO step: Lambda=-2.98233031D-04 EMin= 1.01595243D-03
Quartic linear search produced a step of -0.09364.
Iteration 1 RMS(Cart)= 0.03213284 RMS(Int)= 0.00058203
Iteration 2 RMS(Cart)= 0.00108019 RMS(Int)= 0.00000425
Iteration 3 RMS(Cart)= 0.00000076 RMS(Int)= 0.00000420

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56518	0.00137	0.00004	0.00053	0.00057	2.56576
R2	2.61526	-0.00042	-0.00004	-0.00001	-0.00006	2.61521
R3	2.03376	0.00010	0.00001	0.00006	0.00007	2.03383
R4	2.62892	-0.00018	-0.00007	-0.00040	-0.00047	2.62845
R5	2.02970	0.00051	0.00002	0.00024	0.00027	2.02997
R6	2.54355	0.00126	0.00013	0.00078	0.00090	2.54446
R7	2.68761	-0.00014	0.00007	-0.00188	-0.00181	2.68581

R8	2.51857	0.00081	0.00002	0.00043	0.00045	2.51903
R9	2.10269	-0.00331	-0.00041	-0.00067	-0.00108	2.10162
R10	2.80073	-0.00222	-0.00022	0.00086	0.00064	2.80137
R11	2.91993	-0.00187	-0.00020	0.00166	0.00146	2.92138
R12	2.05810	0.00042	0.00011	-0.00028	-0.00018	2.05793
R13	2.05993	0.00033	-0.00003	0.00036	0.00033	2.06027
R14	2.06695	-0.00024	-0.00005	-0.00014	-0.00020	2.06675
R15	2.06466	-0.00014	0.00001	0.00032	0.00033	2.06499
R16	2.65968	0.00072	0.00023	-0.00331	-0.00309	2.65659
R17	5.42271	-0.00129	-0.01151	0.01370	0.00219	5.42490
R18	2.50593	-0.00027	0.00007	-0.00055	-0.00047	2.50546
R19	2.04422	0.00068	0.00003	-0.00016	-0.00013	2.04409
R20	2.04223	0.00038	0.00004	-0.00002	0.00002	2.04225
R21	2.04427	0.00067	0.00004	0.00026	0.00030	2.04456
R22	1.84648	-0.00261	-0.00040	0.00253	0.00213	1.84861
A1	1.87536	-0.00046	0.00000	0.00026	0.00026	1.87562
A2	2.27391	0.00063	0.00026	-0.00055	-0.00029	2.27362
A3	2.13360	-0.00016	-0.00023	0.00008	-0.00015	2.13345
A4	1.86153	0.00049	0.00002	0.00014	0.00016	1.86169
A5	2.26692	0.00108	0.00054	-0.00060	-0.00006	2.26686
A6	2.15473	-0.00157	-0.00057	0.00046	-0.00011	2.15462
A7	1.89641	-0.00030	-0.00001	-0.00026	-0.00026	1.89614
A8	2.25259	-0.00148	-0.00035	0.00020	-0.00015	2.25244
A9	2.13407	0.00178	0.00037	-0.00003	0.00034	2.13441
A10	1.89018	-0.00026	-0.00004	0.00028	0.00024	1.89042
A11	2.25189	-0.00009	0.00030	-0.00246	-0.00217	2.24972
A12	2.14090	0.00036	-0.00029	0.00204	0.00174	2.14264
A13	1.90127	0.00053	0.00002	-0.00042	-0.00039	1.90087
A14	2.23647	0.00191	-0.00011	0.00155	0.00143	2.23790
A15	2.14543	-0.00243	0.00009	-0.00111	-0.00102	2.14441
A16	1.94817	-0.00167	0.00051	-0.00404	-0.00354	1.94463
A17	1.87105	-0.00059	-0.00006	-0.00027	-0.00035	1.87071
A18	1.87257	0.00216	0.00003	0.00192	0.00195	1.87452
A19	1.90363	-0.00068	-0.00095	-0.00205	-0.00300	1.90063
A20	1.96182	0.00037	-0.00003	0.00478	0.00475	1.96658
A21	1.90396	0.00043	0.00054	-0.00047	0.00007	1.90403
A22	1.93493	0.00208	0.00062	-0.00137	-0.00076	1.93417
A23	1.87724	-0.00158	0.00024	-0.00005	0.00019	1.87743
A24	1.91439	-0.00186	-0.00046	0.00293	0.00247	1.91686
A25	1.93137	-0.00142	0.00071	-0.00510	-0.00439	1.92698
A26	1.89281	0.00000	-0.00034	0.00257	0.00222	1.89504
A27	1.91314	0.00278	-0.00080	0.00108	0.00028	1.91342
A28	2.02154	-0.00205	0.00162	-0.04285	-0.04123	1.98030
A29	2.18849	-0.00275	-0.00033	-0.00086	-0.00120	2.18729

A30	1.94791	0.00209	0.00043	0.00140	0.00183	1.94974
A31	2.14675	0.00066	-0.00009	-0.00053	-0.00062	2.14612
A32	2.07886	0.00006	0.00001	-0.00012	-0.00011	2.07875
A33	2.16469	-0.00088	-0.00036	0.00077	0.00041	2.16511
A34	2.03961	0.00082	0.00035	-0.00064	-0.00030	2.03931
A35	1.83842	0.00167	-0.00009	-0.00037	-0.00046	1.83795
D1	-0.00676	0.00024	0.00043	-0.00005	0.00039	-0.00637
D2	3.13515	0.00005	0.00165	-0.00715	-0.00551	3.12964
D3	-3.12110	-0.00011	-0.00213	0.00939	0.00727	-3.11383
D4	0.02081	-0.00031	-0.00092	0.00229	0.00137	0.02217
D5	0.00351	-0.00014	-0.00061	-0.00064	-0.00126	0.00226
D6	3.13895	0.00012	-0.00067	0.00314	0.00246	3.14141
D7	3.12053	0.00019	0.00171	-0.00917	-0.00746	3.11307
D8	-0.02722	0.00045	0.00164	-0.00539	-0.00374	-0.03097
D9	0.00771	-0.00026	-0.00012	0.00071	0.00059	0.00830
D10	-3.11729	-0.00031	-0.00121	0.00613	0.00491	-3.11237
D11	-3.13417	-0.00008	-0.00122	0.00724	0.00602	-3.12815
D12	0.02402	-0.00013	-0.00231	0.01266	0.01034	0.03436
D13	-0.00560	0.00018	-0.00026	-0.00112	-0.00138	-0.00699
D14	-3.12531	-0.00011	0.00065	0.00652	0.00716	-3.11815
D15	3.12075	0.00019	0.00074	-0.00609	-0.00536	3.11539
D16	0.00104	-0.00010	0.00165	0.00155	0.00319	0.00423
D17	0.07026	-0.00019	-0.00808	0.03709	0.02901	0.09927
D18	-3.08123	-0.00001	-0.00781	0.03802	0.03022	-3.05101
D19	-3.05274	-0.00022	-0.00930	0.04316	0.03386	-3.01888
D20	0.07896	-0.00005	-0.00903	0.04410	0.03507	0.11403
D21	0.00134	-0.00003	0.00054	0.00109	0.00163	0.00297
D22	-3.13448	-0.00029	0.00060	-0.00246	-0.00186	-3.13634
D23	3.12274	0.00024	-0.00029	-0.00603	-0.00634	3.11640
D24	-0.01308	-0.00002	-0.00023	-0.00958	-0.00982	-0.02291
D25	1.90062	0.00069	0.00255	0.01594	0.01849	1.91911
D26	-2.29895	-0.00148	0.00165	0.01093	0.01258	-2.28637
D27	-0.25586	-0.00019	0.00225	0.01122	0.01348	-0.24239
D28	-1.24791	0.00099	0.00248	0.02021	0.02268	-1.22523
D29	0.83570	-0.00118	0.00158	0.01520	0.01677	0.85247
D30	2.87879	0.00012	0.00218	0.01549	0.01767	2.89646
D31	-1.37393	-0.00193	-0.00047	-0.05189	-0.05236	-1.42629
D32	0.73975	-0.00342	0.00093	-0.05901	-0.05807	0.68168
D33	2.81939	-0.00205	-0.00014	-0.05610	-0.05624	2.76315
D34	2.84503	0.00025	-0.00010	-0.04781	-0.04791	2.79712
D35	-1.32447	-0.00125	0.00131	-0.05493	-0.05363	-1.37810
D36	0.75516	0.00013	0.00023	-0.05202	-0.05179	0.70337
D37	0.73114	-0.00007	-0.00010	-0.04893	-0.04902	0.68212
D38	2.84482	-0.00156	0.00130	-0.05604	-0.05474	2.79008

D39	-1.35873	-0.00019	0.00023	-0.05313	-0.05290	-1.41163
D40	1.07828	-0.00291	0.00289	0.05520	0.05809	1.13637
D41	-3.08899	-0.00221	0.00423	0.05044	0.05467	-3.03432
D42	-1.00216	-0.00132	0.00374	0.05111	0.05486	-0.94730
D43	-1.47259	0.00166	0.00400	0.00983	0.01384	-1.45875
D44	2.69516	0.00024	0.00374	0.00814	0.01187	2.70703
D45	0.58483	0.00029	0.00356	0.01214	0.01570	0.60053
D46	-3.14132	0.00009	-0.00063	0.00450	0.00386	-3.13746
D47	0.00704	-0.00011	-0.00096	0.00410	0.00314	0.01019
D48	0.01124	-0.00010	-0.00094	0.00345	0.00252	0.01375
D49	-3.12358	-0.00030	-0.00126	0.00306	0.00179	-3.12179

Item	Value	Threshold	Converged?
Maximum Force	0.003423	0.000450	NO
RMS Force	0.001196	0.000300	NO
Maximum Displacement	0.162562	0.001800	NO
RMS Displacement	0.032267	0.001200	NO

Predicted change in Energy=-1.583473D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.618294	-2.412994	-1.120253
2	6	0	-1.912600	-2.031359	-1.270533
3	7	0	-2.081176	-0.882377	-0.504982
4	6	0	-0.907390	-0.579715	0.081192
5	7	0	-0.010460	-1.497810	-0.278719
6	6	0	1.395252	-1.476863	0.191505
7	6	0	2.184775	-0.307897	-0.441004
8	1	0	-0.079704	-3.234492	-1.560008
9	1	0	-2.698993	-2.476592	-1.851296
10	1	0	1.371131	-1.342431	1.271914
11	1	0	1.830098	-2.450140	-0.037142
12	1	0	2.529766	-0.570154	-1.445160
13	1	0	1.518091	0.556992	-0.480931
14	35	0	0.755077	1.532527	2.108904
15	1	0	-0.668769	0.254595	0.776759
16	6	0	-3.255741	-0.109896	-0.295992
17	6	0	-4.467567	-0.423970	-0.732639
18	1	0	-3.050742	0.782049	0.280600
19	1	0	-5.292152	0.240973	-0.518522
20	1	0	-4.695564	-1.319618	-1.295150

21	8	0	3.304933	-0.004534	0.352411
22	1	0	2.970379	0.586828	1.056201

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357740	0.000000			
3	N	2.204852	1.390915	0.000000		
4	C	2.210873	2.223708	1.346469	0.000000	
5	N	1.383909	2.210544	2.172054	1.333011	0.000000
6	C	2.579034	3.658812	3.595005	2.473703	1.482422
7	C	3.570716	4.521827	4.304935	3.147707	2.502256
8	H	1.076254	2.211523	3.263651	3.229001	2.159296
9	H	2.206303	1.074212	2.176185	3.246920	3.264846
10	H	3.290347	4.209697	3.909916	2.681644	2.082643
11	H	2.677524	3.962880	4.239673	3.317580	2.086372
12	H	3.662227	4.679768	4.716164	3.760835	2.945145
13	H	3.713986	4.369516	3.876479	2.736977	2.568963
14	Br	5.280222	5.589130	4.550658	3.367043	3.933158
15	H	3.273719	3.311209	2.220464	1.112127	2.149030
16	C	3.597192	2.538853	1.421269	2.424407	3.529653
17	C	4.350100	3.066087	2.440661	3.655330	4.607058
18	H	4.252940	3.408320	2.080267	2.547180	3.841082
19	H	5.408379	4.141302	3.401832	4.501035	5.565711
20	H	4.224949	2.872642	2.765966	4.097809	4.797404
21	O	4.833336	5.827917	5.524121	4.260054	3.690533
22	H	5.158920	6.009332	5.487629	4.165160	3.874678

		6	7	8	9	10
6	C	0.000000				
7	C	1.545929	0.000000			
8	H	2.886615	3.865875	0.000000		
9	H	4.683517	5.526604	2.742251	0.000000	
10	H	1.089008	2.160178	3.701972	5.254206	0.000000
11	H	1.090247	2.208644	2.565476	4.878987	1.775190
12	H	2.188130	1.093675	3.731115	5.580266	3.053087
13	H	2.145653	1.092746	4.253552	5.372553	2.588798
14	Br	3.625283	3.454451	6.073075	6.609600	3.057035
15	H	2.756928	3.153103	4.240425	4.299752	2.637587
16	C	4.872164	5.446049	4.631204	2.886207	5.038395
17	C	6.027875	6.659744	5.276071	2.931298	6.241170
18	H	4.987734	5.396234	5.324238	3.909917	5.004907
19	H	6.940927	7.497446	6.350840	3.985714	7.078995
20	H	6.271595	7.006584	5.004304	2.373644	6.587498
21	O	2.416718	1.405806	5.054280	6.856714	2.524885

22	H	2.736338	1.912937	5.545272	7.069643	2.515187
		11	12	13	14	15
11	H	0.000000				
12	H	2.450795	0.000000			
13	H	3.055674	1.795461	0.000000		
14	Br	4.650035	4.494681	2.870732	0.000000	
15	H	3.771255	3.980924	2.540784	2.331321	0.000000
16	C	5.604418	5.916461	4.823735	4.956585	2.824194
17	C	6.652043	7.035035	6.070729	6.259254	4.143622
18	H	5.862646	5.995729	4.637329	4.288376	2.489615
19	H	7.628910	7.918268	6.817675	6.718664	4.801417
20	H	6.741286	7.265644	6.541722	7.030775	4.794376
21	O	2.882340	2.037664	2.050018	3.456818	4.004688
22	H	3.423276	2.790977	2.114900	2.628706	3.664951
		16	17	18	19	20
16	C	0.000000				
17	C	1.325830	0.000000			
18	H	1.081688	2.118615	0.000000		
19	H	2.078364	1.080710	2.440343	0.000000	
20	H	2.129515	1.081937	3.099263	1.842420	0.000000
21	O	6.593479	7.859073	6.404567	8.644574	8.273564
22	H	6.409245	7.716521	6.074008	8.418360	8.241970
		21	22			
21	O	0.000000				
22	H	0.978241	0.000000			

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.911226	-1.995720	0.330766
2	6	0	-2.897777	-1.094020	0.091784
3	7	0	-2.280852	0.144837	-0.047075
4	6	0	-0.951893	-0.017731	0.095819
5	7	0	-0.710289	-1.308011	0.327605
6	6	0	0.654771	-1.845092	0.541450
7	6	0	1.482993	-1.817940	-0.763620
8	1	0	-1.962233	-3.061302	0.473094

9	1	0	-3.958786	-1.239804	0.008486
10	1	0	1.139167	-1.207938	1.279918
11	1	0	0.549343	-2.849758	0.951535
12	1	0	1.246973	-2.681515	-1.391839
13	1	0	1.243417	-0.889117	-1.287056
14	35	0	2.069903	1.467057	0.129443
15	1	0	-0.147436	0.749659	0.067759
16	6	0	-2.869952	1.418118	-0.274499
17	6	0	-4.171859	1.668184	-0.292701
18	1	0	-2.121362	2.183890	-0.426993
19	1	0	-4.510743	2.677196	-0.479750
20	1	0	-4.934916	0.919720	-0.124975
21	8	0	2.854948	-1.847715	-0.458421
22	1	0	3.098036	-0.918873	-0.271030

Rotational constants (GHZ): 0.9830915 0.4382173 0.3132686

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 848.4235687983 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 5.47D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Initial guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999994 -0.002424 0.000163 0.002543 Ang= -0.40 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.34212652 A.U. after 11 cycles
NFock= 11 Conv=0.57D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.001220465	0.001300518	-0.001647506
2	6	0.000180001	-0.000578200	0.000414686
3	7	-0.001133207	-0.000370162	-0.000454088
4	6	0.002136262	0.002296349	0.004107169
5	7	0.000541603	-0.000579008	0.001940797
6	6	-0.000666241	-0.001340073	-0.001964474
7	6	0.000033732	-0.000421868	0.003412953
8	1	0.000161850	-0.000409098	0.000783227
9	1	-0.001126535	0.000768450	0.000166682
10	1	0.000139800	0.001386979	0.000227068
11	1	0.000115666	0.000035992	-0.000555229
12	1	0.000078031	0.000292513	0.000138560
13	1	-0.000477267	0.000360896	-0.003663287
14	35	-0.000927808	-0.001120566	-0.000498524
15	1	-0.000659005	-0.002093695	-0.002535860
16	6	0.000061722	0.000585363	0.000271645
17	6	-0.000440951	-0.000430493	-0.000451729
18	1	-0.000415500	0.000812268	0.000249853
19	1	-0.000089894	0.000421085	0.000312119
20	1	0.000775678	-0.000592591	-0.000462970
21	8	-0.000386314	0.001524367	0.000515103
22	1	0.000877912	-0.001849025	-0.000306197

Cartesian Forces: Max 0.004107169 RMS 0.001230749

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.003298576 RMS 0.001080330
Search for a local minimum.
Step number 59 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 56 57 58 59
DE= -2.18D-04 DEPred=-1.58D-04 R= 1.38D+00
TightC=F SS= 1.41D+00 RLast= 2.09D-01 DXNew= 1.3266D+00 6.2659D-01
Trust test= 1.38D+00 RLast= 2.09D-01 DXMaxT set to 7.89D-01
ITU= 1 1 0 1 1 0 1 1 0 -1 1 1 1 -1 1 0 -1 1 0 -1
ITU= 0 -1 0 0 1 -1 0 1 1 1 1 1 1 0 -1 1 1 1 1 1
ITU= 0 -1 1 1 1 1 1 1 1 1 1 1 1 1 0 0 -1 0 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00165	0.00245	0.00522	0.00804	0.01106
Eigenvalues ---	0.01217	0.01571	0.01887	0.02143	0.02285
Eigenvalues ---	0.02451	0.03040	0.03168	0.03379	0.03898
Eigenvalues ---	0.04436	0.04615	0.05390	0.05792	0.07618
Eigenvalues ---	0.08485	0.09345	0.09997	0.13289	0.14317
Eigenvalues ---	0.14719	0.15806	0.15878	0.16059	0.16166
Eigenvalues ---	0.17222	0.18532	0.22324	0.23084	0.23520
Eigenvalues ---	0.24964	0.25565	0.28102	0.29968	0.32615
Eigenvalues ---	0.33788	0.33885	0.33980	0.34220	0.34381
Eigenvalues ---	0.34509	0.34847	0.35393	0.36327	0.36367
Eigenvalues ---	0.41692	0.43105	0.45210	0.46355	0.49223
Eigenvalues ---	0.53640	0.56149	0.58952	0.60884	0.69517

RFO step: Lambda=-5.92936373D-04 EMin= 1.65228483D-03
Quartic linear search produced a step of 0.43593.
Iteration 1 RMS(Cart)= 0.03996131 RMS(Int)= 0.00091260
Iteration 2 RMS(Cart)= 0.00132798 RMS(Int)= 0.00002917
Iteration 3 RMS(Cart)= 0.00000112 RMS(Int)= 0.00002916
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00002916

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56576	0.00108	0.00025	0.00012	0.00038	2.56613
R2	2.61521	-0.00048	-0.00002	0.00047	0.00044	2.61565
R3	2.03383	0.00007	0.00003	0.00012	0.00015	2.03397
R4	2.62845	-0.00014	-0.00021	0.00012	-0.00008	2.62837
R5	2.02997	0.00042	0.00012	0.00040	0.00051	2.03048
R6	2.54446	0.00095	0.00039	0.00082	0.00121	2.54567
R7	2.68581	0.00051	-0.00079	0.00173	0.00094	2.68675
R8	2.51903	0.00052	0.00020	0.00015	0.00034	2.51936
R9	2.10162	-0.00330	-0.00047	-0.00095	-0.00142	2.10020
R10	2.80137	-0.00203	0.00028	0.00227	0.00255	2.80392
R11	2.92138	-0.00115	0.00064	0.00202	0.00266	2.92404

R12	2.05793	0.00039	-0.00008	0.00027	0.00019	2.05812
R13	2.06027	0.00013	0.00015	0.00022	0.00037	2.06064
R14	2.06675	-0.00017	-0.00009	-0.00022	-0.00031	2.06644
R15	2.06499	0.00041	0.00014	0.00240	0.00255	2.06754
R16	2.65659	0.00044	-0.00135	-0.00606	-0.00741	2.64918
R17	5.42490	-0.00058	0.00096	0.16605	0.16701	5.59191
R18	2.50546	0.00012	-0.00021	-0.00040	-0.00060	2.50485
R19	2.04409	0.00072	-0.00006	0.00056	0.00050	2.04460
R20	2.04225	0.00039	0.00001	0.00064	0.00064	2.04289
R21	2.04456	0.00057	0.00013	0.00063	0.00076	2.04532
R22	1.84861	-0.00164	0.00093	0.00335	0.00428	1.85289
A1	1.87562	-0.00047	0.00011	-0.00011	0.00000	1.87562
A2	2.27362	0.00063	-0.00013	-0.00171	-0.00188	2.27174
A3	2.13345	-0.00015	-0.00007	0.00148	0.00137	2.13482
A4	1.86169	0.00041	0.00007	0.00008	0.00015	1.86183
A5	2.26686	0.00112	-0.00003	-0.00156	-0.00164	2.26522
A6	2.15462	-0.00153	-0.00005	0.00142	0.00132	2.15595
A7	1.89614	-0.00024	-0.00011	0.00015	0.00003	1.89618
A8	2.25244	-0.00157	-0.00007	-0.00191	-0.00200	2.25044
A9	2.13441	0.00181	0.00015	0.00161	0.00174	2.13615
A10	1.89042	-0.00028	0.00010	-0.00038	-0.00028	1.89014
A11	2.24972	0.00003	-0.00095	0.00133	0.00037	2.25009
A12	2.14264	0.00026	0.00076	-0.00078	-0.00003	2.14261
A13	1.90087	0.00058	-0.00017	0.00029	0.00011	1.90099
A14	2.23790	0.00157	0.00062	-0.00169	-0.00108	2.23682
A15	2.14441	-0.00215	-0.00045	0.00142	0.00095	2.14535
A16	1.94463	-0.00047	-0.00154	-0.00327	-0.00482	1.93981
A17	1.87071	-0.00085	-0.00015	-0.00592	-0.00607	1.86464
A18	1.87452	0.00148	0.00085	0.00056	0.00142	1.87594
A19	1.90063	-0.00075	-0.00131	0.00473	0.00339	1.90402
A20	1.96658	0.00005	0.00207	0.00224	0.00430	1.97088
A21	1.90403	0.00053	0.00003	0.00124	0.00126	1.90529
A22	1.93417	0.00208	-0.00033	-0.00593	-0.00628	1.92789
A23	1.87743	-0.00168	0.00008	0.00048	0.00039	1.87782
A24	1.91686	-0.00158	0.00108	0.00957	0.01056	1.92742
A25	1.92698	-0.00132	-0.00191	-0.01244	-0.01436	1.91262
A26	1.89504	-0.00040	0.00097	-0.00729	-0.00625	1.88879
A27	1.91342	0.00293	0.00012	0.01612	0.01616	1.92958
A28	1.98030	-0.00044	-0.01797	-0.06502	-0.08299	1.89732
A29	2.18729	-0.00255	-0.00052	-0.00316	-0.00368	2.18361
A30	1.94974	0.00188	0.00080	0.00181	0.00260	1.95234
A31	2.14612	0.00067	-0.00027	0.00133	0.00106	2.14718
A32	2.07875	0.00012	-0.00005	0.00089	0.00084	2.07959
A33	2.16511	-0.00097	0.00018	0.00040	0.00058	2.16568

A34	2.03931	0.00085	-0.00013	-0.00131	-0.00144	2.03787
A35	1.83795	0.00107	-0.00020	0.00306	0.00286	1.84081
D1	-0.00637	0.00022	0.00017	0.00070	0.00087	-0.00550
D2	3.12964	0.00004	-0.00240	-0.01138	-0.01377	3.11587
D3	-3.11383	-0.00018	0.00317	0.01200	0.01515	-3.09868
D4	0.02217	-0.00036	0.00060	-0.00008	0.00051	0.02269
D5	0.00226	-0.00010	-0.00055	0.00282	0.00227	0.00453
D6	3.14141	0.00010	0.00107	0.01092	0.01199	-3.12978
D7	3.11307	0.00028	-0.00325	-0.00745	-0.01071	3.10235
D8	-0.03097	0.00048	-0.00163	0.00065	-0.00100	-0.03196
D9	0.00830	-0.00027	0.00026	-0.00394	-0.00368	0.00462
D10	-3.11237	-0.00035	0.00214	0.00417	0.00630	-3.10607
D11	-3.12815	-0.00012	0.00262	0.00718	0.00982	-3.11834
D12	0.03436	-0.00021	0.00451	0.01530	0.01980	0.05416
D13	-0.00699	0.00021	-0.00060	0.00574	0.00514	-0.00185
D14	-3.11815	-0.00026	0.00312	-0.00063	0.00248	-3.11567
D15	3.11539	0.00025	-0.00234	-0.00176	-0.00411	3.11128
D16	0.00423	-0.00022	0.00139	-0.00814	-0.00676	-0.00254
D17	0.09927	-0.00020	0.01265	0.05335	0.06599	0.16526
D18	-3.05101	-0.00009	0.01317	0.05140	0.06457	-2.98644
D19	-3.01888	-0.00027	0.01476	0.06246	0.07722	-2.94165
D20	0.11403	-0.00016	0.01529	0.06052	0.07580	0.18983
D21	0.00297	-0.00007	0.00071	-0.00530	-0.00460	-0.00162
D22	-3.13634	-0.00026	-0.00081	-0.01288	-0.01369	3.13315
D23	3.11640	0.00036	-0.00276	0.00064	-0.00213	3.11427
D24	-0.02291	0.00017	-0.00428	-0.00693	-0.01123	-0.03414
D25	1.91911	0.00054	0.00806	-0.03598	-0.02793	1.89118
D26	-2.28637	-0.00117	0.00548	-0.03577	-0.03027	-2.31664
D27	-0.24239	-0.00023	0.00587	-0.03706	-0.03118	-0.27357
D28	-1.22523	0.00076	0.00989	-0.02685	-0.01698	-1.24221
D29	0.85247	-0.00095	0.00731	-0.02665	-0.01932	0.83315
D30	2.89646	-0.00001	0.00770	-0.02794	-0.02024	2.87622
D31	-1.42629	-0.00173	-0.02283	-0.01189	-0.03473	-1.46102
D32	0.68168	-0.00317	-0.02532	-0.03034	-0.05566	0.62602
D33	2.76315	-0.00153	-0.02452	-0.00525	-0.02975	2.73340
D34	2.79712	0.00007	-0.02089	-0.00563	-0.02652	2.77059
D35	-1.37810	-0.00137	-0.02338	-0.02408	-0.04745	-1.42556
D36	0.70337	0.00027	-0.02258	0.00101	-0.02154	0.68183
D37	0.68212	-0.00012	-0.02137	-0.01195	-0.03334	0.64878
D38	2.79008	-0.00156	-0.02386	-0.03040	-0.05427	2.73581
D39	-1.41163	0.00008	-0.02306	-0.00530	-0.02836	-1.43998
D40	1.13637	-0.00301	0.02532	-0.02553	-0.00020	1.13617
D41	-3.03432	-0.00230	0.02383	-0.03985	-0.01596	-3.05028
D42	-0.94730	-0.00177	0.02391	-0.04642	-0.02256	-0.96986

D43	-1.45875	0.00152	0.00603	0.08582	0.09177	-1.36698
D44	2.70703	0.00019	0.00518	0.09180	0.09697	2.80400
D45	0.60053	0.00028	0.00684	0.10175	0.10869	0.70922
D46	-3.13746	-0.00001	0.00168	0.00177	0.00345	-3.13401
D47	0.01019	-0.00013	0.00137	0.00598	0.00735	0.01754
D48	0.01375	-0.00014	0.00110	0.00392	0.00502	0.01877
D49	-3.12179	-0.00027	0.00078	0.00814	0.00892	-3.11287

Item	Value	Threshold	Converged?
Maximum Force	0.003299	0.000450	NO
RMS Force	0.001080	0.000300	NO
Maximum Displacement	0.171786	0.001800	NO
RMS Displacement	0.040109	0.001200	NO

Predicted change in Energy=-3.643960D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.612694	-2.399022	-1.125629
2	6	0	-1.903346	-2.009271	-1.287833
3	7	0	-2.073780	-0.863029	-0.518674
4	6	0	-0.905396	-0.572155	0.085455
5	7	0	-0.008914	-1.491808	-0.272245
6	6	0	1.396936	-1.474796	0.201964
7	6	0	2.192100	-0.318852	-0.450534
8	1	0	-0.072300	-3.214710	-1.574091
9	1	0	-2.681825	-2.441695	-1.889078
10	1	0	1.364475	-1.320982	1.279670
11	1	0	1.825020	-2.455703	-0.006912
12	1	0	2.562781	-0.617823	-1.434902
13	1	0	1.511823	0.531337	-0.557515
14	35	0	0.731894	1.467990	2.138912
15	1	0	-0.670445	0.254791	0.789811
16	6	0	-3.249756	-0.090434	-0.314705
17	6	0	-4.468510	-0.440600	-0.700709
18	1	0	-3.039822	0.831772	0.210739
19	1	0	-5.295884	0.226054	-0.501468
20	1	0	-4.701732	-1.369854	-1.204245
21	8	0	3.292673	0.028448	0.345335
22	1	0	2.927050	0.573463	1.073808

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357939	0.000000			
3	N	2.205095	1.390872	0.000000		
4	C	2.211300	2.224214	1.347108	0.000000	
5	N	1.384143	2.210895	2.172502	1.333189	0.000000
6	C	2.579789	3.660193	3.597144	2.475695	1.483771
7	C	3.556646	4.509020	4.300989	3.153717	2.500415
8	H	1.076332	2.210827	3.263469	3.229743	2.160373
9	H	2.205896	1.074484	2.177134	3.248024	3.265101
10	H	3.294971	4.212417	3.907090	2.671929	2.079379
11	H	2.682759	3.967464	4.242541	3.318352	2.088734
12	H	3.654034	4.680176	4.732578	3.787060	2.954528
13	H	3.663787	4.318730	3.847378	2.733872	2.546986
14	Br	5.236309	5.547830	4.513116	3.325597	3.888815
15	H	3.273373	3.310985	2.220586	1.111377	2.148533
16	C	3.597398	2.538058	1.421769	2.426563	3.531106
17	C	4.345491	3.063579	2.438507	3.651184	4.601806
18	H	4.256156	3.407172	2.082698	2.557827	3.849507
19	H	5.404893	4.138159	3.401228	4.500889	5.563780
20	H	4.217298	2.871726	2.762790	4.088009	4.786026
21	O	4.827861	5.815337	5.508181	4.248770	3.686877
22	H	5.118885	5.964946	5.441306	4.120306	3.833678

		6	7	8	9	10
6	C	0.000000				
7	C	1.547335	0.000000			
8	H	2.887962	3.843941	0.000000		
9	H	4.684404	5.507360	2.739780	0.000000	
10	H	1.089111	2.163986	3.714092	5.260181	0.000000
11	H	1.090442	2.213071	2.575261	4.884097	1.776228
12	H	2.184703	1.093512	3.702276	5.571237	3.049470
13	H	2.148157	1.094095	4.192343	5.310241	2.613053
14	Br	3.585253	3.468463	6.029992	6.569917	2.986105
15	H	2.758822	3.172016	4.240666	4.300364	2.619908
16	C	4.875977	5.448341	4.630700	2.886109	5.034620
17	C	6.023939	6.666419	5.271162	2.934083	6.222595
18	H	5.000515	5.397612	5.325957	3.905506	5.017449
19	H	6.941293	7.507957	6.346275	3.984425	7.065844
20	H	6.259568	7.014100	4.997191	2.387019	6.555234
21	O	2.423658	1.401887	5.052258	6.840236	2.532171
22	H	2.701245	1.913112	5.509784	7.023485	2.464334

		11	12	13	14	15
11	H	0.000000				
12	H	2.441567	0.000000			

13	H	3.053468	1.787425	0.000000		
14	Br	4.603786	4.524921	2.959109	0.000000	
15	H	3.769468	4.020517	2.579547	2.293138	0.000000
16	C	5.607369	5.942942	4.808138	4.929752	2.827009
17	C	6.644586	7.071740	6.060491	6.224979	4.138903
18	H	5.875504	6.016528	4.625791	4.283511	2.506427
19	H	7.625201	7.958771	6.814779	6.696874	4.802386
20	H	6.723925	7.306976	6.530012	6.982432	4.781946
21	O	2.906732	2.029693	2.058995	3.441916	3.994383
22	H	3.399745	2.800978	2.160059	2.598718	3.622731

		16	17	18	19	20
16	C	0.000000				
17	C	1.325511	0.000000			
18	H	1.081955	2.119155	0.000000		
19	H	2.078866	1.081051	2.442120	0.000000	
20	H	2.129890	1.082337	3.100207	1.842236	0.000000
21	O	6.576713	7.845392	6.384664	8.632464	8.262382
22	H	6.365662	7.672779	6.034498	8.379668	8.195384

		21	22
21	O	0.000000	
22	H	0.980506	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.877244	-1.999550	0.352190
2	6	0	-2.872244	-1.113126	0.090990
3	7	0	-2.267863	0.129132	-0.070390
4	6	0	-0.937689	-0.015584	0.085804
5	7	0	-0.683436	-1.299154	0.341138
6	6	0	0.688130	-1.821778	0.558500
7	6	0	1.496689	-1.833033	-0.760724
8	1	0	-1.918230	-3.064426	0.503349
9	1	0	-3.930031	-1.275453	-0.005197
10	1	0	1.172383	-1.151628	1.267415
11	1	0	0.594419	-2.810987	1.007664
12	1	0	1.278817	-2.737824	-1.334877

13	1	0	1.200088	-0.952136	-1.337865
14	35	0	2.035306	1.473823	0.136401
15	1	0	-0.141956	0.759411	0.049069
16	6	0	-2.872667	1.391580	-0.319114
17	6	0	-4.174359	1.636560	-0.268506
18	1	0	-2.138143	2.151670	-0.550119
19	1	0	-4.531138	2.634332	-0.482586
20	1	0	-4.921533	0.895884	-0.014372
21	8	0	2.872277	-1.805125	-0.491901
22	1	0	3.076796	-0.871885	-0.271382

Rotational constants (GHZ): 0.9868375 0.4427769 0.3165643

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 850.7626030257 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 6.01D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Initial guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999988 0.001532 -0.000205 -0.004587 Ang= 0.55 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Keep R1 ints in memory in canonical form, NReq=1804729152.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.34253278 A.U. after 12 cycles
NFock= 12 Conv=0.22D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.001141244	0.001717554	-0.002082084
2	6	0.000434501	-0.000631279	0.000017073
3	7	-0.000937503	-0.000956293	0.000289373
4	6	0.001238758	0.001709757	0.002455774
5	7	0.000845319	-0.001397164	0.002008629
6	6	-0.002042552	-0.000920477	-0.001522231
7	6	-0.001050831	-0.001227584	0.000827509
8	1	0.000184948	-0.000514359	0.001090030
9	1	-0.001193837	0.000885249	0.000429557
10	1	0.000619215	0.001374680	0.000178065
11	1	0.000040116	0.000243203	-0.000739358
12	1	0.000395846	0.000324209	-0.000024273
13	1	0.000295690	0.000526859	-0.002098700
14	35	-0.000156827	-0.000227582	0.000273469
15	1	-0.000444461	-0.001694658	-0.002132931
16	6	0.000578262	0.000426717	0.000224276
17	6	-0.001328833	-0.000401170	-0.000557638
18	1	-0.000363554	0.000543016	0.000203820
19	1	0.000106210	0.000381669	0.000281298
20	1	0.001028964	-0.000385354	-0.000416902
21	8	-0.000848409	0.001787558	0.003227243
22	1	0.001457734	-0.001564552	-0.001931999

Cartesian Forces: Max 0.003227243 RMS 0.001141470

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.002849760 RMS 0.000770244
Search for a local minimum.
Step number 60 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS
Update second derivatives using D2CorX and points 58 59 60
DE= -4.06D-04 DEPred=-3.64D-04 R= 1.11D+00
TightC=F SS= 1.41D+00 RLast= 3.25D-01 DXNew= 1.3266D+00 9.7377D-01
Trust test= 1.11D+00 RLast= 3.25D-01 DXMaxT set to 9.74D-01
ITU= 1 1 1 0 1 1 0 1 1 0 -1 1 1 1 -1 1 0 -1 1 0
ITU= -1 0 -1 0 0 1 -1 0 1 1 1 1 1 1 0 -1 1 1 1 1
ITU= 1 0 -1 1 1 1 1 1 1 1 1 1 1 1 1 0 0 -1 0 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00158	0.00304	0.00498	0.00774	0.01068
Eigenvalues ---	0.01323	0.01559	0.01928	0.02141	0.02269
Eigenvalues ---	0.02449	0.03045	0.03168	0.03385	0.03903
Eigenvalues ---	0.04320	0.04702	0.05249	0.05706	0.07116
Eigenvalues ---	0.08635	0.09312	0.10052	0.13476	0.14330
Eigenvalues ---	0.14695	0.15596	0.15981	0.16011	0.16205
Eigenvalues ---	0.16793	0.18566	0.21536	0.22965	0.23593
Eigenvalues ---	0.24938	0.25639	0.27859	0.29816	0.32639
Eigenvalues ---	0.33778	0.33886	0.33952	0.34214	0.34235
Eigenvalues ---	0.34700	0.34855	0.35389	0.36326	0.36352
Eigenvalues ---	0.39947	0.43057	0.44323	0.45954	0.49408
Eigenvalues ---	0.53631	0.55224	0.57898	0.60897	0.70108

RFO step: Lambda=-5.29480443D-04 EMin= 1.58045188D-03
Quartic linear search produced a step of 0.25688.
Iteration 1 RMS(Cart)= 0.03636036 RMS(Int)= 0.00101863
Iteration 2 RMS(Cart)= 0.00180526 RMS(Int)= 0.00002725
Iteration 3 RMS(Cart)= 0.00000212 RMS(Int)= 0.00002722
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00002722

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56613	0.00071	0.00010	0.00142	0.00153	2.56766
R2	2.61565	-0.00038	0.00011	0.00011	0.00023	2.61588
R3	2.03397	0.00003	0.00004	0.00022	0.00026	2.03423
R4	2.62837	-0.00050	-0.00002	-0.00147	-0.00149	2.62688
R5	2.03048	0.00027	0.00013	0.00078	0.00091	2.03139
R6	2.54567	0.00059	0.00031	0.00356	0.00386	2.54952
R7	2.68675	0.00025	0.00024	-0.00113	-0.00088	2.68587
R8	2.51936	0.00024	0.00009	0.00167	0.00175	2.52111
R9	2.10020	-0.00271	-0.00036	-0.00499	-0.00535	2.09484
R10	2.80392	-0.00180	0.00065	-0.00393	-0.00327	2.80065
R11	2.92404	-0.00033	0.00068	0.00045	0.00113	2.92517
R12	2.05812	0.00035	0.00005	0.00083	0.00088	2.05900
R13	2.06064	-0.00006	0.00009	0.00020	0.00029	2.06093
R14	2.06644	0.00007	-0.00008	-0.00019	-0.00027	2.06617
R15	2.06754	0.00033	0.00065	0.00269	0.00334	2.07088

R16	2.64918	0.00127	-0.00190	-0.00200	-0.00390	2.64528
R17	5.59191	0.00022	0.04290	0.05418	0.09708	5.68898
R18	2.50485	0.00049	-0.00016	0.00051	0.00035	2.50520
R19	2.04460	0.00049	0.00013	0.00094	0.00107	2.04567
R20	2.04289	0.00020	0.00017	0.00067	0.00084	2.04373
R21	2.04532	0.00030	0.00019	0.00117	0.00136	2.04668
R22	1.85289	-0.00285	0.00110	-0.00117	-0.00007	1.85282
A1	1.87562	-0.00020	0.00000	0.00045	0.00041	1.87603
A2	2.27174	0.00067	-0.00048	0.00382	0.00325	2.27499
A3	2.13482	-0.00043	0.00035	-0.00324	-0.00297	2.13185
A4	1.86183	0.00018	0.00004	0.00052	0.00057	1.86241
A5	2.26522	0.00144	-0.00042	0.00844	0.00800	2.27322
A6	2.15595	-0.00162	0.00034	-0.00886	-0.00854	2.14741
A7	1.89618	-0.00003	0.00001	-0.00011	-0.00013	1.89604
A8	2.25044	-0.00153	-0.00051	-0.00653	-0.00709	2.24336
A9	2.13615	0.00157	0.00045	0.00713	0.00754	2.14369
A10	1.89014	-0.00019	-0.00007	-0.00057	-0.00064	1.88950
A11	2.25009	0.00008	0.00010	-0.00149	-0.00140	2.24869
A12	2.14261	0.00012	-0.00001	0.00207	0.00206	2.14467
A13	1.90099	0.00025	0.00003	-0.00025	-0.00024	1.90075
A14	2.23682	0.00005	-0.00028	-0.00224	-0.00256	2.23426
A15	2.14535	-0.00030	0.00024	0.00242	0.00262	2.14797
A16	1.93981	0.00211	-0.00124	0.00562	0.00437	1.94418
A17	1.86464	-0.00042	-0.00156	0.00185	0.00029	1.86493
A18	1.87594	-0.00029	0.00036	0.00164	0.00199	1.87793
A19	1.90402	-0.00143	0.00087	-0.01478	-0.01391	1.89010
A20	1.97088	-0.00084	0.00111	0.00149	0.00258	1.97345
A21	1.90529	0.00091	0.00032	0.00453	0.00485	1.91014
A22	1.92789	0.00067	-0.00161	0.00169	0.00008	1.92797
A23	1.87782	0.00078	0.00010	0.00511	0.00514	1.88296
A24	1.92742	-0.00130	0.00271	-0.00148	0.00118	1.92860
A25	1.91262	-0.00074	-0.00369	-0.00645	-0.01012	1.90249
A26	1.88879	0.00016	-0.00161	-0.00200	-0.00358	1.88521
A27	1.92958	0.00043	0.00415	0.00311	0.00721	1.93679
A28	1.89732	-0.00103	-0.02132	-0.05993	-0.08125	1.81607
A29	2.18361	-0.00211	-0.00094	-0.00867	-0.00963	2.17398
A30	1.95234	0.00154	0.00067	0.00866	0.00932	1.96166
A31	2.14718	0.00057	0.00027	0.00010	0.00036	2.14754
A32	2.07959	0.00014	0.00021	0.00059	0.00080	2.08039
A33	2.16568	-0.00117	0.00015	-0.00517	-0.00503	2.16065
A34	2.03787	0.00103	-0.00037	0.00464	0.00426	2.04214
A35	1.84081	0.00081	0.00073	0.00250	0.00323	1.84404
D1	-0.00550	0.00017	0.00022	0.00539	0.00561	0.00011
D2	3.11587	0.00021	-0.00354	0.01068	0.00720	3.12307

D3	-3.09868	-0.00045	0.00389	-0.01917	-0.01535	-3.11403
D4	0.02269	-0.00041	0.00013	-0.01388	-0.01377	0.00892
D5	0.00453	-0.00022	0.00058	-0.01060	-0.01002	-0.00549
D6	-3.12978	-0.00005	0.00308	0.00132	0.00438	-3.12540
D7	3.10235	0.00038	-0.00275	0.01184	0.00905	3.11140
D8	-0.03196	0.00055	-0.00026	0.02376	0.02345	-0.00851
D9	0.00462	-0.00008	-0.00095	0.00155	0.00061	0.00523
D10	-3.10607	-0.00027	0.00162	-0.01695	-0.01526	-3.12134
D11	-3.11834	-0.00015	0.00252	-0.00356	-0.00106	-3.11940
D12	0.05416	-0.00035	0.00509	-0.02207	-0.01693	0.03723
D13	-0.00185	-0.00006	0.00132	-0.00818	-0.00685	-0.00870
D14	-3.11567	-0.00025	0.00064	-0.00834	-0.00774	-3.12340
D15	3.11128	0.00006	-0.00105	0.00859	0.00762	3.11890
D16	-0.00254	-0.00013	-0.00174	0.00842	0.00674	0.00420
D17	0.16526	-0.00033	0.01695	-0.01580	0.00115	0.16641
D18	-2.98644	-0.00018	0.01659	-0.00699	0.00960	-2.97683
D19	-2.94165	-0.00052	0.01984	-0.03641	-0.01658	-2.95823
D20	0.18983	-0.00037	0.01947	-0.02761	-0.00813	0.18170
D21	-0.00162	0.00017	-0.00118	0.01159	0.01040	0.00878
D22	3.13315	0.00001	-0.00352	0.00040	-0.00316	3.12999
D23	3.11427	0.00035	-0.00055	0.01168	0.01116	3.12543
D24	-0.03414	0.00019	-0.00288	0.00049	-0.00241	-0.03654
D25	1.89118	-0.00001	-0.00717	0.01028	0.00310	1.89428
D26	-2.31664	-0.00081	-0.00778	-0.00332	-0.01111	-2.32775
D27	-0.27357	-0.00012	-0.00801	0.00370	-0.00432	-0.27789
D28	-1.24221	0.00018	-0.00436	0.02373	0.01937	-1.22283
D29	0.83315	-0.00063	-0.00496	0.01012	0.00517	0.83831
D30	2.87622	0.00006	-0.00520	0.01715	0.01195	2.88818
D31	-1.46102	-0.00068	-0.00892	-0.07660	-0.08553	-1.54655
D32	0.62602	-0.00071	-0.01430	-0.08033	-0.09464	0.53138
D33	2.73340	-0.00047	-0.00764	-0.07424	-0.08188	2.65152
D34	2.77059	-0.00053	-0.00681	-0.07308	-0.07989	2.69070
D35	-1.42556	-0.00056	-0.01219	-0.07681	-0.08900	-1.51456
D36	0.68183	-0.00033	-0.00553	-0.07072	-0.07624	0.60559
D37	0.64878	-0.00012	-0.00856	-0.06936	-0.07793	0.57085
D38	2.73581	-0.00014	-0.01394	-0.07310	-0.08704	2.64877
D39	-1.43998	0.00009	-0.00728	-0.06701	-0.07428	-1.51426
D40	1.13617	-0.00103	-0.00005	0.05744	0.05741	1.19358
D41	-3.05028	-0.00018	-0.00410	0.05882	0.05474	-2.99554
D42	-0.96986	-0.00018	-0.00580	0.05422	0.04839	-0.92148
D43	-1.36698	-0.00008	0.02357	-0.00383	0.01972	-1.34727
D44	2.80400	-0.00021	0.02491	-0.00374	0.02117	2.82516
D45	0.70922	0.00034	0.02792	0.00354	0.03150	0.74072
D46	-3.13401	0.00002	0.00089	0.00497	0.00585	-3.12816

D47	0.01754	-0.00021	0.00189	-0.00225	-0.00037	0.01716
D48	0.01877	-0.00015	0.00129	-0.00481	-0.00352	0.01526
D49	-3.11287	-0.00038	0.00229	-0.01204	-0.00974	-3.12261

Item	Value	Threshold	Converged?
Maximum Force	0.002850	0.000450	NO
RMS Force	0.000770	0.000300	NO
Maximum Displacement	0.195375	0.001800	NO
RMS Displacement	0.036514	0.001200	NO

Predicted change in Energy=-3.090190D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.618461	-2.396033	-1.128930
2	6	0	-1.910588	-2.002684	-1.276836
3	7	0	-2.072138	-0.860965	-0.500491
4	6	0	-0.895778	-0.574316	0.094669
5	7	0	-0.006233	-1.499090	-0.270527
6	6	0	1.403758	-1.489674	0.185842
7	6	0	2.196668	-0.324514	-0.454311
8	1	0	-0.084368	-3.216956	-1.575715
9	1	0	-2.701662	-2.425144	-1.869528
10	1	0	1.385552	-1.338888	1.264780
11	1	0	1.828894	-2.469027	-0.036716
12	1	0	2.629908	-0.635832	-1.408693
13	1	0	1.497758	0.500651	-0.631910
14	35	0	0.771538	1.450977	2.130784
15	1	0	-0.653349	0.250907	0.794029
16	6	0	-3.245820	-0.084563	-0.301073
17	6	0	-4.458857	-0.438688	-0.701833
18	1	0	-3.043900	0.841227	0.222375
19	1	0	-5.291216	0.226070	-0.515012
20	1	0	-4.677333	-1.369214	-1.211149
21	8	0	3.242314	0.076585	0.385476
22	1	0	2.823662	0.612293	1.091923

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.358746	0.000000			
3	N	2.205572	1.390083	0.000000		

4	C	2.211957	2.225107	1.349150	0.000000	
5	N	1.384264	2.211974	2.174408	1.334116	0.000000
6	C	2.576719	3.658893	3.598358	2.476703	1.482038
7	C	3.559670	4.512466	4.302629	3.150714	2.503233
8	H	1.076469	2.213338	3.264664	3.229879	2.158862
9	H	2.211122	1.074967	2.171916	3.247284	3.267983
10	H	3.295978	4.214851	3.911548	2.675480	2.078437
11	H	2.681008	3.967253	4.244879	3.321299	2.088812
12	H	3.705196	4.743604	4.794242	3.833320	2.998312
13	H	3.621629	4.277784	3.823013	2.722588	2.528152
14	Br	5.230423	5.543776	4.511671	3.320771	3.882540
15	H	3.271893	3.308746	2.219235	1.108543	2.148145
16	C	3.596005	2.532616	1.421301	2.432934	3.535073
17	C	4.331542	3.044731	2.432136	3.653539	4.597427
18	H	4.264814	3.408792	2.089095	2.575753	3.866194
19	H	5.393234	4.120239	3.397694	4.509125	5.564800
20	H	4.187549	2.839098	2.747799	4.078871	4.766636
21	O	4.828338	5.799917	5.468760	4.199053	3.669625
22	H	5.082364	5.904425	5.354916	4.029489	3.784509

		6	7	8	9	10
6	C	0.000000				
7	C	1.547933	0.000000			
8	H	2.881164	3.850570	0.000000		
9	H	4.685523	5.514446	2.750185	0.000000	
10	H	1.089576	2.154562	3.708937	5.263948	0.000000
11	H	1.090598	2.215531	2.566805	4.887439	1.779791
12	H	2.185185	1.093371	3.749319	5.642663	3.031529
13	H	2.153822	1.095863	4.149036	5.265653	2.644604
14	Br	3.581889	3.444718	6.021654	6.564292	2.985017
15	H	2.762464	3.164184	4.238573	4.295506	2.627960
16	C	4.881598	5.449929	4.629403	2.869578	5.047259
17	C	6.021860	6.661104	5.255340	2.897802	6.231777
18	H	5.021564	5.411138	5.334867	3.893888	5.045747
19	H	6.946774	7.508345	6.331729	3.945813	7.084913
20	H	6.240655	6.994004	4.964110	2.334893	6.549025
21	O	2.423491	1.399821	5.075480	6.831877	2.494856
22	H	2.693580	1.913522	5.498734	6.966018	2.430051

		11	12	13	14	15
11	H	0.000000				
12	H	2.425809	0.000000			
13	H	3.046784	1.782344	0.000000		
14	Br	4.602444	4.509569	3.010481	0.000000	
15	H	3.774878	4.051922	2.592863	2.292899	0.000000
16	C	5.613222	6.004573	4.790977	4.940746	2.834200

17	C	6.640818	7.126648	6.030631	6.241121	4.146690
18	H	5.896527	6.085572	4.633838	4.309454	2.527845
19	H	7.628125	8.017840	6.795531	6.727379	4.819131
20	H	6.702229	7.346608	6.477937	6.986573	4.778910
21	O	2.942132	2.025245	2.063585	3.322618	3.920905
22	H	3.428982	2.801506	2.177633	2.448231	3.508411

		16	17	18	19	20
16	C	0.000000				
17	C	1.325697	0.000000			
18	H	1.082523	2.120010	0.000000		
19	H	2.079883	1.081493	2.443888	0.000000	
20	H	2.127863	1.083058	3.099862	1.845642	0.000000
21	O	6.526346	7.794600	6.334648	8.582212	8.207336
22	H	6.266151	7.573454	5.936060	8.281465	8.092925

		21	22
21	O	0.000000	
22	H	0.980469	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.892308	-1.988442	0.341875
2	6	0	-2.880345	-1.090107	0.090937
3	7	0	-2.266102	0.147707	-0.060230
4	6	0	-0.934810	-0.010295	0.091107
5	7	0	-0.692534	-1.297987	0.342137
6	6	0	0.671642	-1.838685	0.549760
7	6	0	1.487062	-1.834284	-0.765979
8	1	0	-1.940705	-3.052713	0.496056
9	1	0	-3.941422	-1.233391	-0.004662
10	1	0	1.167639	-1.179709	1.261739
11	1	0	0.569348	-2.833062	0.985825
12	1	0	1.328374	-2.765124	-1.317175
13	1	0	1.136847	-0.994082	-1.376163
14	35	0	2.051601	1.441104	0.139120
15	1	0	-0.134926	0.756246	0.052782
16	6	0	-2.868366	1.410144	-0.312479

17	6	0	-4.172793	1.642902	-0.270480
18	1	0	-2.139298	2.175835	-0.544930
19	1	0	-4.538727	2.636622	-0.490117
20	1	0	-4.911353	0.890434	-0.022820
21	8	0	2.855494	-1.719965	-0.494273
22	1	0	3.004174	-0.775420	-0.277364

Rotational constants (GHZ): 1.0093730 0.4415091 0.3181703

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 853.2868399775 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 5.80D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Initial guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999995 -0.002056 -0.000115 0.002234 Ang= -0.35 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Keep R1 ints in memory in canonical form, NReq=1804729152.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3032.34279973 A.U. after 11 cycles

NFock= 11 Conv=0.69D-08 -V/T= 2.0016

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000226377	0.000938751	-0.000891315
2	6	0.000637099	-0.000725256	-0.000205297
3	7	0.001679083	0.000071741	0.000646371
4	6	-0.000489197	-0.000217346	0.001465661
5	7	-0.000549948	-0.000735726	0.000570193
6	6	-0.001973989	0.000367065	0.000084902
7	6	0.000280348	-0.000301814	-0.000664416
8	1	-0.000028472	-0.000271582	0.000694329
9	1	-0.000182109	0.000413281	0.000306885
10	1	0.000281275	0.000163873	-0.000032516
11	1	-0.000293353	0.000349512	-0.000436429
12	1	0.000282297	0.000126110	-0.000193653
13	1	0.000646305	0.000082079	-0.001073467
14	35	-0.001078042	0.000513340	0.001084774
15	1	-0.000227404	-0.000994576	-0.001316613
16	6	0.000139355	0.000364466	-0.000170065
17	6	-0.001580095	0.000021191	-0.000591446
18	1	0.000114516	-0.000182850	0.000263077
19	1	0.000203769	-0.000066955	0.000198041
20	1	0.000543252	0.000198969	0.000078734
21	8	0.000988786	-0.000048895	0.000237001
22	1	0.000380148	-0.000065377	-0.000054748

Cartesian Forces: Max 0.001973989 RMS 0.000644343

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.003277143 RMS 0.000637115

Search for a local minimum.

Step number 61 out of a maximum of 116

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 59 60 61

DE= -2.67D-04 DEPred=-3.09D-04 R= 8.64D-01

TightC=F SS= 1.41D+00 RLast= 3.05D-01 DXNew= 1.6377D+00 9.1643D-01

Trust test= 8.64D-01 RLast= 3.05D-01 DXMaxT set to 9.74D-01

ITU= 1 1 1 1 0 1 1 0 1 1 0 -1 1 1 1 -1 1 0 -1 1

ITU= 0 -1 0 -1 0 0 1 -1 0 1 1 1 1 1 1 0 -1 1 1 1

ITU= 1 1 0 -1 1 1 1 1 1 1 1 1 1 1 1 1 0 0 -1 0

ITU= 0

Eigenvalues ---	0.00195	0.00313	0.00437	0.00712	0.01030
Eigenvalues ---	0.01371	0.01520	0.01907	0.02139	0.02258
Eigenvalues ---	0.02479	0.03040	0.03163	0.03434	0.03905
Eigenvalues ---	0.04483	0.04924	0.05207	0.05717	0.07552
Eigenvalues ---	0.08703	0.09232	0.11635	0.13519	0.14358
Eigenvalues ---	0.14517	0.15160	0.15950	0.16001	0.16189
Eigenvalues ---	0.16549	0.18733	0.21490	0.23018	0.23698
Eigenvalues ---	0.25040	0.25769	0.26707	0.29649	0.32686
Eigenvalues ---	0.33639	0.33869	0.33893	0.34093	0.34247
Eigenvalues ---	0.34814	0.34954	0.35422	0.36314	0.36411
Eigenvalues ---	0.38518	0.43118	0.43855	0.45916	0.49250
Eigenvalues ---	0.53660	0.56033	0.57543	0.60913	0.71197

En-DIIS/RFO-DIIS IScMMF= 0 using points: 61 60

RFO step: Lambda=-1.11687135D-04.

DidBck=F Rises=F RFO-DIIS coefs: 0.86329 0.13671

Iteration 1 RMS(Cart)= 0.03356198 RMS(Int)= 0.00045867

Iteration 2 RMS(Cart)= 0.00124826 RMS(Int)= 0.00001821

Iteration 3 RMS(Cart)= 0.00000100 RMS(Int)= 0.00001820

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001820

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56766	-0.00046	-0.00021	-0.00004	-0.00025	2.56741
R2	2.61588	-0.00052	-0.00003	0.00043	0.00041	2.61629
R3	2.03423	-0.00009	-0.00004	-0.00001	-0.00004	2.03419
R4	2.62688	0.00011	0.00020	-0.00013	0.00006	2.62694
R5	2.03139	-0.00020	-0.00012	0.00016	0.00004	2.03143
R6	2.54952	-0.00124	-0.00053	0.00118	0.00065	2.55017
R7	2.68587	0.00063	0.00012	-0.00087	-0.00075	2.68512
R8	2.52111	-0.00078	-0.00024	0.00021	-0.00002	2.52109
R9	2.09484	-0.00162	0.00073	-0.00489	-0.00416	2.09069
R10	2.80065	-0.00078	0.00045	-0.00251	-0.00206	2.79859
R11	2.92517	0.00129	-0.00015	0.00129	0.00114	2.92631
R12	2.05900	-0.00001	-0.00012	0.00087	0.00075	2.05975
R13	2.06093	-0.00034	-0.00004	-0.00018	-0.00022	2.06071
R14	2.06617	0.00025	0.00004	0.00020	0.00023	2.06640
R15	2.07088	0.00073	-0.00046	0.00240	0.00194	2.07282
R16	2.64528	0.00110	0.00053	-0.00088	-0.00035	2.64493
R17	5.68898	0.00142	-0.01327	0.19327	0.18000	5.86898

R18	2.50520	0.00082	-0.00005	0.00082	0.00077	2.50597
R19	2.04567	-0.00001	-0.00015	0.00004	-0.00011	2.04557
R20	2.04373	-0.00017	-0.00011	0.00004	-0.00008	2.04365
R21	2.04668	-0.00032	-0.00019	0.00004	-0.00014	2.04654
R22	1.85282	-0.00024	0.00001	-0.00223	-0.00222	1.85060
A1	1.87603	-0.00030	-0.00006	-0.00008	-0.00014	1.87589
A2	2.27499	0.00039	-0.00044	0.00190	0.00143	2.27641
A3	2.13185	-0.00009	0.00041	-0.00144	-0.00106	2.13079
A4	1.86241	-0.00014	-0.00008	0.00027	0.00019	1.86259
A5	2.27322	0.00058	-0.00109	0.00459	0.00350	2.27672
A6	2.14741	-0.00044	0.00117	-0.00485	-0.00368	2.14373
A7	1.89604	0.00010	0.00002	-0.00001	0.00002	1.89606
A8	2.24336	-0.00009	0.00097	-0.00339	-0.00242	2.24094
A9	2.14369	-0.00001	-0.00103	0.00346	0.00243	2.14612
A10	1.88950	-0.00002	0.00009	-0.00041	-0.00032	1.88918
A11	2.24869	0.00004	0.00019	0.00034	0.00050	2.24919
A12	2.14467	-0.00001	-0.00028	0.00035	0.00004	2.14471
A13	1.90075	0.00036	0.00003	0.00021	0.00024	1.90099
A14	2.23426	-0.00024	0.00035	-0.00536	-0.00506	2.22920
A15	2.14797	-0.00012	-0.00036	0.00479	0.00438	2.15235
A16	1.94418	0.00262	-0.00060	0.00696	0.00637	1.95055
A17	1.86493	-0.00063	-0.00004	-0.00115	-0.00118	1.86375
A18	1.87793	-0.00093	-0.00027	-0.00072	-0.00099	1.87694
A19	1.89010	-0.00056	0.00190	-0.00559	-0.00369	1.88641
A20	1.97345	-0.00102	-0.00035	-0.00366	-0.00401	1.96944
A21	1.91014	0.00052	-0.00066	0.00439	0.00372	1.91386
A22	1.92797	0.00047	-0.00001	-0.00163	-0.00164	1.92633
A23	1.88296	0.00022	-0.00070	0.00349	0.00272	1.88568
A24	1.92860	-0.00044	-0.00016	0.00265	0.00243	1.93103
A25	1.90249	-0.00057	0.00138	-0.01123	-0.00982	1.89268
A26	1.88521	-0.00045	0.00049	-0.00826	-0.00775	1.87746
A27	1.93679	0.00078	-0.00099	0.01486	0.01384	1.95063
A28	1.81607	0.00328	0.01111	-0.04871	-0.03761	1.77846
A29	2.17398	0.00021	0.00132	-0.00375	-0.00243	2.17155
A30	1.96166	-0.00028	-0.00127	0.00355	0.00227	1.96393
A31	2.14754	0.00006	-0.00005	0.00021	0.00016	2.14770
A32	2.08039	0.00010	-0.00011	0.00007	-0.00004	2.08035
A33	2.16065	-0.00054	0.00069	-0.00330	-0.00262	2.15804
A34	2.04214	0.00044	-0.00058	0.00324	0.00266	2.04480
A35	1.84404	0.00057	-0.00044	0.01231	0.01187	1.85591
D1	0.00011	-0.00006	-0.00077	0.00355	0.00278	0.00289
D2	3.12307	0.00001	-0.00098	0.00426	0.00328	3.12634
D3	-3.11403	-0.00026	0.00210	-0.01232	-0.01024	-3.12428
D4	0.00892	-0.00020	0.00188	-0.01161	-0.00974	-0.00082

D5	-0.00549	0.00017	0.00137	-0.00411	-0.00274	-0.00823
D6	-3.12540	0.00015	-0.00060	0.01419	0.01355	-3.11185
D7	3.11140	0.00036	-0.00124	0.01024	0.00901	3.12041
D8	-0.00851	0.00034	-0.00321	0.02854	0.02529	0.01678
D9	0.00523	-0.00007	-0.00008	-0.00181	-0.00188	0.00334
D10	-3.12134	-0.00009	0.00209	-0.00695	-0.00487	-3.12620
D11	-3.11940	-0.00014	0.00014	-0.00257	-0.00243	-3.12182
D12	0.03723	-0.00016	0.00231	-0.00771	-0.00541	0.03182
D13	-0.00870	0.00017	0.00094	-0.00073	0.00020	-0.00850
D14	-3.12340	-0.00019	0.00106	-0.01285	-0.01181	-3.13521
D15	3.11890	0.00019	-0.00104	0.00399	0.00294	3.12184
D16	0.00420	-0.00018	-0.00092	-0.00813	-0.00907	-0.00487
D17	0.16641	-0.00024	-0.00016	-0.00595	-0.00610	0.16031
D18	-2.97683	-0.00034	-0.00131	-0.00196	-0.00327	-2.98011
D19	-2.95823	-0.00026	0.00227	-0.01171	-0.00945	-2.96768
D20	0.18170	-0.00036	0.00111	-0.00772	-0.00661	0.17509
D21	0.00878	-0.00021	-0.00142	0.00297	0.00155	0.01033
D22	3.12999	-0.00019	0.00043	-0.01438	-0.01400	3.11599
D23	3.12543	0.00013	-0.00153	0.01421	0.01269	3.13812
D24	-0.03654	0.00015	0.00033	-0.00315	-0.00286	-0.03941
D25	1.89428	-0.00042	-0.00042	-0.05644	-0.05686	1.83742
D26	-2.32775	-0.00003	0.00152	-0.06004	-0.05852	-2.38628
D27	-0.27789	-0.00022	0.00059	-0.05589	-0.05530	-0.33319
D28	-1.22283	-0.00045	-0.00265	-0.03571	-0.03836	-1.26119
D29	0.83831	-0.00006	-0.00071	-0.03931	-0.04002	0.79830
D30	2.88818	-0.00025	-0.00163	-0.03515	-0.03679	2.85139
D31	-1.54655	-0.00011	0.01169	-0.01836	-0.00667	-1.55321
D32	0.53138	-0.00040	0.01294	-0.03080	-0.01787	0.51351
D33	2.65152	0.00044	0.01119	-0.00873	0.00247	2.65400
D34	2.69070	-0.00050	0.01092	-0.01754	-0.00661	2.68409
D35	-1.51456	-0.00080	0.01217	-0.02998	-0.01781	-1.53237
D36	0.60559	0.00004	0.01042	-0.00791	0.00252	0.60811
D37	0.57085	-0.00011	0.01065	-0.01680	-0.00615	0.56470
D38	2.64877	-0.00040	0.01190	-0.02925	-0.01735	2.63142
D39	-1.51426	0.00044	0.01015	-0.00717	0.00298	-1.51128
D40	1.19358	-0.00104	-0.00785	-0.04158	-0.04940	1.14418
D41	-2.99554	-0.00068	-0.00748	-0.04791	-0.05538	-3.05092
D42	-0.92148	-0.00112	-0.00661	-0.05614	-0.06280	-0.98427
D43	-1.34727	-0.00018	-0.00270	0.05134	0.04862	-1.29865
D44	2.82516	-0.00020	-0.00289	0.05695	0.05405	2.87921
D45	0.74072	0.00032	-0.00431	0.06707	0.06281	0.80352
D46	-3.12816	-0.00021	-0.00080	0.00125	0.00045	-3.12771
D47	0.01716	-0.00014	0.00005	-0.00007	-0.00002	0.01715
D48	0.01526	-0.00010	0.00048	-0.00316	-0.00268	0.01258

D49	-3.12261	-0.00003	0.00133	-0.00447	-0.00314	-3.12574

Item	Value	Threshold	Converged?
Maximum Force	0.003277	0.000450	NO
RMS Force	0.000637	0.000300	NO
Maximum Displacement	0.147569	0.001800	NO
RMS Displacement	0.034152	0.001200	NO

Predicted change in Energy=-2.494878D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.610998	-2.375006	-1.126832
2	6	0	-1.904309	-1.986397	-1.275691
3	7	0	-2.075847	-0.856201	-0.484709
4	6	0	-0.904343	-0.572736	0.122214
5	7	0	-0.008670	-1.488615	-0.250306
6	6	0	1.402854	-1.475417	0.197619
7	6	0	2.208778	-0.338559	-0.477664
8	1	0	-0.071441	-3.191558	-1.575003
9	1	0	-2.692763	-2.402406	-1.876421
10	1	0	1.390560	-1.289627	1.271568
11	1	0	1.819272	-2.463919	0.001114
12	1	0	2.641459	-0.686408	-1.419746
13	1	0	1.517372	0.484432	-0.696319
14	35	0	0.693448	1.402909	2.153789
15	1	0	-0.667409	0.247951	0.825302
16	6	0	-3.254724	-0.087999	-0.287027
17	6	0	-4.459982	-0.441649	-0.712276
18	1	0	-3.065377	0.830443	0.253667
19	1	0	-5.298775	0.215093	-0.526122
20	1	0	-4.662682	-1.364547	-1.241448
21	8	0	3.263409	0.074297	0.344703
22	1	0	2.860516	0.599043	1.066742

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.358613	0.000000			
3	N	2.205646	1.390115	0.000000		
4	C	2.212317	2.225423	1.349492	0.000000	
5	N	1.384480	2.211933	2.174422	1.334105	0.000000

6	C	2.572747	3.656373	3.598660	2.478644	1.480949
7	C	3.538314	4.502188	4.315786	3.179028	2.508265
8	H	1.076446	2.213912	3.265008	3.229938	2.158420
9	H	2.212776	1.074988	2.169838	3.246641	3.268580
10	H	3.307054	4.222580	3.910031	2.664870	2.076907
11	H	2.680742	3.965263	4.241783	3.318029	2.087055
12	H	3.676361	4.730193	4.812078	3.868239	3.005712
13	H	3.590499	4.260114	3.841002	2.766280	2.533899
14	Br	5.170754	5.476958	4.442324	3.253215	3.825384
15	H	3.270155	3.307023	2.217877	1.106344	2.146283
16	C	3.595130	2.530809	1.420903	2.434489	3.535526
17	C	4.327170	3.038938	2.430584	3.654603	4.596056
18	H	4.266691	3.409047	2.090248	2.579972	3.869816
19	H	5.389315	4.114707	3.396565	4.511324	5.564522
20	H	4.177357	2.827807	2.742770	4.075739	4.759998
21	O	4.814097	5.794605	5.482828	4.223543	3.674674
22	H	5.070320	5.905510	5.375166	4.054549	3.784859

		6	7	8	9	10
6	C	0.000000				
7	C	1.548537	0.000000			
8	H	2.874173	3.813548	0.000000		
9	H	4.683484	5.499189	2.754078	0.000000	
10	H	1.089971	2.152632	3.722600	5.274622	0.000000
11	H	1.090483	2.213165	2.566787	4.887471	1.782360
12	H	2.184615	1.093494	3.695904	5.622021	3.028497
13	H	2.157139	1.096889	4.099916	5.239438	2.652536
14	Br	3.551707	3.500498	5.966412	6.495340	2.917882
15	H	2.765858	3.211567	4.236374	4.292523	2.607400
16	C	4.883937	5.472565	4.628634	2.863294	5.044977
17	C	6.022410	6.673681	5.250294	2.884937	6.235667
18	H	5.028441	5.451433	5.337057	3.889399	5.038472
19	H	6.949349	7.528096	6.326962	3.932672	7.088235
20	H	6.234896	6.989490	4.952649	2.315367	6.554587
21	O	2.425884	1.399638	5.047009	6.822275	2.495382
22	H	2.680212	1.920690	5.472097	6.964898	2.402041

		11	12	13	14	15
11	H	0.000000				
12	H	2.419583	0.000000			
13	H	3.044722	1.777015	0.000000		
14	Br	4.566602	4.574948	3.105732	0.000000	
15	H	3.770557	4.106321	2.672924	2.225026	0.000000
16	C	5.610120	6.033748	4.823701	4.875290	2.836254
17	C	6.635324	7.140789	6.048689	6.178557	4.150097
18	H	5.897151	6.137517	4.692951	4.250523	2.533045

19	H	7.623757	8.041056	6.823589	6.670799	4.824622
20	H	6.690912	7.337720	6.473713	6.919146	4.778474
21	O	2.940430	2.019597	2.073785	3.412141	3.963895
22	H	3.406096	2.807667	2.219360	2.554223	3.553563

		16	17	18	19	20
16	C	0.000000				
17	C	1.326104	0.000000			
18	H	1.082468	2.120421	0.000000		
19	H	2.080186	1.081452	2.444339	0.000000	
20	H	2.126697	1.082982	3.099150	1.847043	0.000000
21	O	6.550686	7.812437	6.374447	8.607506	8.210303
22	H	6.300863	7.605106	5.985887	8.322179	8.110606

		21	22
21	O	0.000000	
22	H	0.979297	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.827528	-2.004908	0.360888
2	6	0	-2.832395	-1.128189	0.101205
3	7	0	-2.242582	0.120564	-0.057405
4	6	0	-0.908680	-0.009337	0.100579
5	7	0	-0.641929	-1.289970	0.362612
6	6	0	0.729832	-1.810557	0.563788
7	6	0	1.524094	-1.863932	-0.764469
8	1	0	-1.854725	-3.067482	0.530985
9	1	0	-3.890761	-1.289383	0.003858
10	1	0	1.235722	-1.114433	1.232759
11	1	0	0.644139	-2.785259	1.045209
12	1	0	1.367123	-2.824167	-1.263505
13	1	0	1.147211	-1.067583	-1.417886
14	35	0	1.979808	1.486819	0.140120
15	1	0	-0.124409	0.769321	0.049523
16	6	0	-2.871707	1.366100	-0.325373
17	6	0	-4.182601	1.564684	-0.299444
18	1	0	-2.160527	2.148413	-0.557638

19	1	0	-4.572024	2.546821	-0.530300
20	1	0	-4.901691	0.792811	-0.054555
21	8	0	2.896629	-1.732003	-0.524206
22	1	0	3.049114	-0.789005	-0.308509

Rotational constants (GHZ): 0.9913596 0.4504084 0.3215160

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 854.3598721077 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 5.58D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Initial guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999947 0.003949 0.000035 -0.009476 Ang= 1.18 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Keep R1 ints in memory in canonical form, NReq=1804729152.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3032.34287130 A.U. after 11 cycles

NFock= 11 Conv=0.87D-08 -V/T= 2.0016

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000194232	0.000344514	-0.000514924
2	6	0.000398153	-0.000691091	-0.000414139
3	7	0.002371126	-0.000368526	0.000522907
4	6	-0.002144890	-0.001843701	-0.001056633
5	7	-0.000284012	-0.000391323	-0.000318477
6	6	-0.001477253	0.000666523	0.000698785
7	6	-0.001296797	-0.001130131	-0.002392365
8	1	-0.000067951	-0.000163290	0.000380055
9	1	0.000137710	0.000068245	0.000211080
10	1	0.000088682	-0.000341989	-0.000229676
11	1	-0.000237926	0.000216790	-0.000173983
12	1	0.000375223	0.000115315	-0.000108255
13	1	0.001108730	0.000402756	0.000469112
14	35	0.001315375	0.001769730	0.001927240
15	1	0.000113500	0.000307175	0.000243138
16	6	-0.000191957	0.000234195	-0.000389260
17	6	-0.001100284	0.000259141	-0.000346294
18	1	0.000286899	-0.000274792	0.000390172
19	1	0.000122687	-0.000160395	0.000100228
20	1	0.000213899	0.000245050	0.000129174
21	8	0.000372182	0.001174615	0.002324191
22	1	0.000091135	-0.000438812	-0.001452073

Cartesian Forces: Max 0.002392365 RMS 0.000878519

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.004928874 RMS 0.001335528

Search for a local minimum.

Step number 62 out of a maximum of 116

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 60 61 62

DE= -7.16D-05 DEPred=-2.49D-04 R= 2.87D-01

Trust test= 2.87D-01 RLast= 2.65D-01 DXMaxT set to 9.74D-01

ITU= 0 1 1 1 1 0 1 1 0 1 1 0 -1 1 1 1 -1 1 0 -1

ITU= 1 0 -1 0 -1 0 0 1 -1 0 1 1 1 1 1 1 0 -1 1 1

ITU= 1 1 1 0 -1 1 1 1 1 1 1 1 1 1 1 1 0 0 -1

ITU= 0 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00157	0.00348	0.00377	0.00717	0.00983
Eigenvalues ---	0.01380	0.01508	0.01878	0.02151	0.02249
Eigenvalues ---	0.02504	0.03033	0.03183	0.03776	0.03968
Eigenvalues ---	0.04477	0.04916	0.05356	0.05834	0.08167
Eigenvalues ---	0.08679	0.09192	0.12048	0.13668	0.14371
Eigenvalues ---	0.14945	0.15033	0.15913	0.16033	0.16176
Eigenvalues ---	0.17260	0.19025	0.22010	0.23126	0.23828
Eigenvalues ---	0.25040	0.25757	0.26148	0.29689	0.32938
Eigenvalues ---	0.33771	0.33862	0.33941	0.34200	0.34324
Eigenvalues ---	0.34783	0.35004	0.35697	0.36314	0.36406
Eigenvalues ---	0.38828	0.43181	0.43691	0.45915	0.49076
Eigenvalues ---	0.53676	0.56045	0.57490	0.60927	0.93476

RFO step: Lambda=-2.33890563D-04 EMin= 1.56550809D-03

Quartic linear search produced a step of -0.41705.

Iteration 1 RMS(Cart)= 0.02660108 RMS(Int)= 0.00034219

Iteration 2 RMS(Cart)= 0.00057186 RMS(Int)= 0.00001054

Iteration 3 RMS(Cart)= 0.00000020 RMS(Int)= 0.00001054

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56741	-0.00101	0.00011	-0.00042	-0.00030	2.56710
R2	2.61629	0.00021	-0.00017	-0.00049	-0.00066	2.61563
R3	2.03419	-0.00007	0.00002	-0.00011	-0.00009	2.03410
R4	2.62694	-0.00003	-0.00003	-0.00006	-0.00008	2.62685
R5	2.03143	-0.00025	-0.00002	-0.00031	-0.00032	2.03111
R6	2.55017	-0.00132	-0.00027	-0.00041	-0.00068	2.54949
R7	2.68512	0.00069	0.00031	0.00176	0.00208	2.68720
R8	2.52109	-0.00077	0.00001	0.00001	0.00001	2.52111
R9	2.09069	0.00041	0.00173	-0.00412	-0.00239	2.08830
R10	2.79859	0.00066	0.00086	-0.00240	-0.00154	2.79705
R11	2.92631	0.00209	-0.00048	0.00336	0.00288	2.92919
R12	2.05975	-0.00028	-0.00031	0.00043	0.00012	2.05986
R13	2.06071	-0.00026	0.00009	-0.00052	-0.00043	2.06029
R14	2.06640	0.00021	-0.00010	-0.00005	-0.00015	2.06626
R15	2.07282	-0.00036	-0.00081	0.00084	0.00003	2.07285
R16	2.64493	0.00108	0.00014	-0.00082	-0.00068	2.64425
R17	5.86898	0.00194	-0.07507	0.11443	0.03936	5.90834
R18	2.50597	0.00065	-0.00032	0.00100	0.00068	2.50665
R19	2.04557	0.00001	0.00004	0.00018	0.00022	2.04579
R20	2.04365	-0.00018	0.00003	-0.00006	-0.00003	2.04362
R21	2.04654	-0.00031	0.00006	-0.00024	-0.00018	2.04636
R22	1.85060	-0.00134	0.00092	-0.00031	0.00062	1.85122

A1	1.87589	0.00029	0.00006	-0.00019	-0.00015	1.87574
A2	2.27641	-0.00005	-0.00060	0.00210	0.00146	2.27787
A3	2.13079	-0.00023	0.00044	-0.00162	-0.00122	2.12957
A4	1.86259	-0.00053	-0.00008	0.00022	0.00015	1.86274
A5	2.27672	0.00029	-0.00146	0.00377	0.00229	2.27901
A6	2.14373	0.00024	0.00153	-0.00386	-0.00234	2.14139
A7	1.89606	0.00047	-0.00001	-0.00012	-0.00014	1.89592
A8	2.24094	0.00034	0.00101	-0.00212	-0.00113	2.23981
A9	2.14612	-0.00081	-0.00102	0.00236	0.00133	2.14745
A10	1.88918	0.00008	0.00013	-0.00013	0.00001	1.88919
A11	2.24919	-0.00002	-0.00021	0.00068	0.00049	2.24968
A12	2.14471	-0.00006	-0.00002	-0.00046	-0.00046	2.14425
A13	1.90099	-0.00030	-0.00010	0.00020	0.00011	1.90110
A14	2.22920	-0.00294	0.00211	-0.00267	-0.00055	2.22865
A15	2.15235	0.00324	-0.00183	0.00240	0.00059	2.15294
A16	1.95055	0.00363	-0.00266	0.00915	0.00649	1.95704
A17	1.86375	0.00048	0.00049	0.00027	0.00076	1.86451
A18	1.87694	-0.00277	0.00041	-0.00434	-0.00393	1.87300
A19	1.88641	-0.00031	0.00154	-0.00393	-0.00240	1.88401
A20	1.96944	-0.00136	0.00167	-0.00238	-0.00070	1.96874
A21	1.91386	0.00041	-0.00155	0.00139	-0.00016	1.91370
A22	1.92633	-0.00258	0.00069	0.00161	0.00230	1.92863
A23	1.88568	0.00344	-0.00114	-0.00437	-0.00548	1.88020
A24	1.93103	0.00129	-0.00101	0.00293	0.00194	1.93297
A25	1.89268	0.00079	0.00409	-0.00143	0.00266	1.89534
A26	1.87746	0.00063	0.00323	-0.00513	-0.00191	1.87555
A27	1.95063	-0.00368	-0.00577	0.00641	0.00065	1.95128
A28	1.77846	-0.00164	0.01568	-0.03005	-0.01437	1.76410
A29	2.17155	0.00092	0.00101	-0.00050	0.00051	2.17206
A30	1.96393	-0.00083	-0.00095	0.00050	-0.00045	1.96348
A31	2.14770	-0.00009	-0.00007	0.00001	-0.00006	2.14764
A32	2.08035	0.00009	0.00002	0.00011	0.00013	2.08047
A33	2.15804	-0.00020	0.00109	-0.00262	-0.00153	2.15650
A34	2.04480	0.00012	-0.00111	0.00252	0.00141	2.04620
A35	1.85591	-0.00104	-0.00495	0.00077	-0.00418	1.85173
D1	0.00289	-0.00012	-0.00116	0.00251	0.00136	0.00425
D2	3.12634	0.00000	-0.00137	0.01063	0.00928	3.13562
D3	-3.12428	-0.00021	0.00427	-0.02009	-0.01583	-3.14010
D4	-0.00082	-0.00008	0.00406	-0.01198	-0.00791	-0.00873
D5	-0.00823	0.00021	0.00114	-0.00342	-0.00228	-0.01050
D6	-3.11185	0.00003	-0.00565	-0.00147	-0.00709	-3.11895
D7	3.12041	0.00029	-0.00376	0.01693	0.01316	3.13357
D8	0.01678	0.00011	-0.01055	0.01888	0.00834	0.02512
D9	0.00334	-0.00001	0.00079	-0.00078	0.00000	0.00335

D10	-3.12620	-0.00001	0.00203	-0.01125	-0.00922	-3.13542
D11	-3.12182	-0.00012	0.00101	-0.00822	-0.00720	-3.12902
D12	0.03182	-0.00012	0.00226	-0.01869	-0.01642	0.01539
D13	-0.00850	0.00014	-0.00008	-0.00134	-0.00142	-0.00992
D14	-3.13521	-0.00006	0.00492	-0.00868	-0.00375	-3.13896
D15	3.12184	0.00015	-0.00123	0.00840	0.00719	3.12903
D16	-0.00487	-0.00005	0.00378	0.00107	0.00486	-0.00001
D17	0.16031	-0.00021	0.00255	-0.03877	-0.03623	0.12408
D18	-2.98011	-0.00037	0.00136	-0.03980	-0.03843	-3.01854
D19	-2.96768	-0.00022	0.00394	-0.05058	-0.04664	-3.01432
D20	0.17509	-0.00038	0.00276	-0.05160	-0.04885	0.12624
D21	0.01033	-0.00022	-0.00065	0.00293	0.00228	0.01261
D22	3.11599	-0.00020	0.00584	0.00095	0.00682	3.12280
D23	3.13812	-0.00004	-0.00529	0.00975	0.00445	-3.14061
D24	-0.03941	-0.00002	0.00119	0.00777	0.00898	-0.03042
D25	1.83742	-0.00122	0.02371	-0.01032	0.01339	1.85081
D26	-2.38628	0.00072	0.02441	-0.00985	0.01456	-2.37172
D27	-0.33319	0.00005	0.02306	-0.01028	0.01278	-0.32041
D28	-1.26119	-0.00133	0.01600	-0.00805	0.00795	-1.25325
D29	0.79830	0.00060	0.01669	-0.00757	0.00912	0.80742
D30	2.85139	-0.00007	0.01534	-0.00801	0.00734	2.85873
D31	-1.55321	0.00205	0.00278	-0.03690	-0.03412	-1.58734
D32	0.51351	0.00359	0.00745	-0.04033	-0.03288	0.48064
D33	2.65400	0.00209	-0.00103	-0.03341	-0.03445	2.61955
D34	2.68409	-0.00043	0.00276	-0.04005	-0.03729	2.64680
D35	-1.53237	0.00111	0.00743	-0.04347	-0.03604	-1.56841
D36	0.60811	-0.00039	-0.00105	-0.03656	-0.03761	0.57050
D37	0.56470	0.00013	0.00257	-0.03755	-0.03498	0.52971
D38	2.63142	0.00167	0.00724	-0.04098	-0.03374	2.59769
D39	-1.51128	0.00017	-0.00124	-0.03406	-0.03531	-1.54659
D40	1.14418	0.00493	0.02060	0.02283	0.04342	1.18760
D41	-3.05092	0.00425	0.02309	0.02147	0.04455	-3.00637
D42	-0.98427	0.00333	0.02619	0.01806	0.04427	-0.94000
D43	-1.29865	-0.00185	-0.02028	0.02282	0.00255	-1.29609
D44	2.87921	0.00014	-0.02254	0.02232	-0.00021	2.87900
D45	0.80352	0.00092	-0.02619	0.02358	-0.00263	0.80089
D46	-3.12771	-0.00021	-0.00019	-0.00514	-0.00533	-3.13304
D47	0.01715	-0.00012	0.00001	-0.00531	-0.00531	0.01184
D48	0.01258	-0.00003	0.00112	-0.00401	-0.00289	0.00969
D49	-3.12574	0.00006	0.00131	-0.00418	-0.00287	-3.12862

Item	Value	Threshold	Converged?
Maximum Force	0.004929	0.000450	NO
RMS Force	0.001336	0.000300	NO
Maximum Displacement	0.098808	0.001800	NO

RMS Displacement 0.026749 0.001200 NO

Predicted change in Energy=-1.956715D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.615028	-2.380731	-1.127994
2	6	0	-1.910822	-1.996339	-1.264202
3	7	0	-2.078452	-0.866690	-0.471680
4	6	0	-0.902312	-0.579494	0.123608
5	7	0	-0.007817	-1.493530	-0.256223
6	6	0	1.405204	-1.481575	0.184266
7	6	0	2.213727	-0.337020	-0.478284
8	1	0	-0.079277	-3.202709	-1.570663
9	1	0	-2.706829	-2.416932	-1.851319
10	1	0	1.398801	-1.308892	1.260515
11	1	0	1.819083	-2.468003	-0.026264
12	1	0	2.674083	-0.681866	-1.408183
13	1	0	1.513299	0.473464	-0.714321
14	35	0	0.736251	1.449691	2.152481
15	1	0	-0.660139	0.242760	0.821071
16	6	0	-3.257131	-0.096816	-0.271434
17	6	0	-4.457101	-0.429038	-0.728826
18	1	0	-3.072186	0.802205	0.302628
19	1	0	-5.295972	0.224792	-0.533104
20	1	0	-4.653553	-1.331772	-1.293735
21	8	0	3.243415	0.095124	0.364911
22	1	0	2.813109	0.616494	1.073905

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.358452	0.000000			
3	N	2.205601	1.390071	0.000000		
4	C	2.212124	2.224985	1.349130	0.000000	
5	N	1.384130	2.211395	2.174138	1.334112	0.000000
6	C	2.571351	3.655006	3.597805	2.478318	1.480135
7	C	3.549751	4.514744	4.324742	3.182886	2.514375
8	H	1.076398	2.214454	3.265187	3.229426	2.157348
9	H	2.213626	1.074817	2.168297	3.245427	3.268282
10	H	3.302926	4.219050	3.909901	2.668277	2.076815

11	H	2.673261	3.958175	4.237142	3.315859	2.083277
12	H	3.712533	4.771784	4.847451	3.891974	3.029587
13	H	3.584317	4.257570	3.841296	2.765144	2.528381
14	Br	5.221074	5.527734	4.491592	3.304362	3.875312
15	H	3.268577	3.305471	2.216686	1.105081	2.144945
16	C	3.595925	2.531072	1.422003	2.436023	3.536818
17	C	4.327813	3.037531	2.432208	3.658662	4.599198
18	H	4.267949	3.411095	2.090998	2.578661	3.869505
19	H	5.390165	4.114264	3.398168	4.514687	5.567214
20	H	4.175820	2.822250	2.742850	4.080024	4.762926
21	O	4.821432	5.796066	5.472406	4.207183	3.671530
22	H	5.058047	5.882956	5.340041	4.017189	3.765510

		6	7	8	9	10
6	C	0.000000				
7	C	1.550061	0.000000			
8	H	2.871543	3.829273	0.000000		
9	H	4.682661	5.515717	2.756854	0.000000	
10	H	1.090033	2.152222	3.713061	5.269484	0.000000
11	H	1.090256	2.213855	2.555138	4.880299	1.782127
12	H	2.187574	1.093416	3.736582	5.671070	3.023483
13	H	2.154372	1.096903	4.096812	5.239907	2.662682
14	Br	3.593563	3.506594	6.014293	6.544921	2.973947
15	H	2.764867	3.206801	4.234270	4.290055	2.615333
16	C	4.884935	5.480034	4.629614	2.860386	5.049129
17	C	6.025627	6.676165	5.250455	2.876658	6.246856
18	H	5.027592	5.463381	5.339106	3.890477	5.036269
19	H	6.952127	7.530884	6.327574	3.926838	7.098538
20	H	6.238226	6.986704	4.949858	2.297435	6.569301
21	O	2.428504	1.399279	5.065810	6.828433	2.485149
22	H	2.678721	1.917743	5.472289	6.944662	2.396289

		11	12	13	14	15
11	H	0.000000				
12	H	2.414748	0.000000			
13	H	3.036306	1.778665	0.000000		
14	Br	4.611701	4.580072	3.126560	0.000000	
15	H	3.769981	4.116010	2.671046	2.275794	0.000000
16	C	5.608083	6.067436	4.824766	4.920788	2.837825
17	C	6.636374	7.167931	6.038244	6.229163	4.155769
18	H	5.892957	6.176484	4.708389	4.283152	2.529770
19	H	7.624437	8.069050	6.816220	6.715688	4.829603
20	H	6.692722	7.357291	6.451718	6.975882	4.785281
21	O	2.958269	2.017848	2.073929	3.363946	3.932888
22	H	3.422364	2.804608	2.215337	2.484127	3.502435

		16	17	18	19	20

16	C	0.000000				
17	C	1.326464	0.000000			
18	H	1.082585	2.120813	0.000000		
19	H	2.080571	1.081437	2.444806	0.000000	
20	H	2.126079	1.082886	3.098863	1.847742	0.000000
21	O	6.534438	7.795444	6.355365	8.587455	8.194464
22	H	6.258320	7.562998	5.938523	8.276056	8.071710

		21	22
21	O	0.000000	
22	H	0.979624	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.876110	-1.989683	0.346460
2	6	0	-2.866652	-1.092606	0.102594
3	7	0	-2.256428	0.148133	-0.040552
4	6	0	-0.924779	-0.006505	0.110942
5	7	0	-0.679124	-1.294734	0.355836
6	6	0	0.682508	-1.840238	0.553784
7	6	0	1.492749	-1.881478	-0.767010
8	1	0	-1.920571	-3.051932	0.514634
9	1	0	-3.928712	-1.231052	0.012628
10	1	0	1.195111	-1.167477	1.241391
11	1	0	0.574743	-2.822619	1.014189
12	1	0	1.355062	-2.842037	-1.270922
13	1	0	1.109846	-1.086564	-1.418696
14	35	0	2.034733	1.462994	0.136847
15	1	0	-0.127808	0.757653	0.065070
16	6	0	-2.866372	1.406374	-0.299178
17	6	0	-4.176052	1.616034	-0.316136
18	1	0	-2.140790	2.188553	-0.482800
19	1	0	-4.548825	2.608261	-0.530685
20	1	0	-4.908668	0.842520	-0.122246
21	8	0	2.860892	-1.732270	-0.514214
22	1	0	2.994950	-0.787127	-0.294224

```
 Rotational constants (GHZ):           0.9940586           0.4439376           0.3182065
 Standard basis: 6-311++G(d,p) (5D, 7F)
 There are      358 symmetry adapted cartesian basis functions of A      symmetry.
 There are      345 symmetry adapted basis functions of A      symmetry.
    345 basis functions,      553 primitive gaussians,      358 cartesian basis functions
     55 alpha electrons              55 beta electrons
          nuclear repulsion energy              852.1929943195 Hartrees.
 NAtoms=       22 NActive=       22 NUniq=       22 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      345 RedAO= T EigKep=    5.25D-06    NBF=      345
 NBsUse=      345 1.00D-06 EigRej= -1.00D+00 NBFU=      345
 Initial guess from the checkpoint file:    "."
 B after Tr=          0.000000        0.000000        0.000000
             Rot=        0.999971      -0.001376      -0.000103        0.007430 Ang=    -0.87 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn=                5 AccDes=
0.00D+00
 Harris functional with IExCor=    402 and IRadAn=             5 diagonalized for initial guess.
 HarFok:    IExCor=    402 AccDes= 0.00D+00 IRadAn=                5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=    3500011 ScaDFX=    1.000000    1.000000    1.000000    1.000000
 FoFCou: FMM=F IPFlag=                  0 FMFlag=           100000 FMFlg1=                  0
             NFxFlg=                   0 DoJE=T BraDBF=F KetDBF=T FulRan=T
             wScrn=      0.000000  ICntrl=             500  IOpCl=      0  I1Cent=        200000004  NGrid=
0
             NMat0=         1 NMatS0=            1 NMatT0=         0 NMatD0=         1 NMtDS0=         0
NMtDT0=         0
 Petite list used in FoFCou.
 Keep R1 ints in memory in canonical form, NReq=1804729152.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                      energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3032.34307940          A.U. after      11 cycles
                   NFock= 11    Conv=0.63D-08         -V/T= 2.0017
 Calling FoFJK, ICntrl=             2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center         Atomic                             Forces (Hartrees/Bohr)
 Number          Number                       X                      Y                      Z
 -------------------------------------------------------------------
```

1	6	-0.000275935	-0.000118924	0.000125068
2	6	0.000192460	-0.000416933	-0.000264280
3	7	0.001624246	0.000504441	0.000192449
4	6	-0.001083181	-0.001428004	-0.000165213
5	7	-0.000369450	0.000217059	-0.000407859
6	6	-0.000523021	0.000329382	0.001091291
7	6	-0.001077786	-0.000809005	-0.002170124
8	1	-0.000055564	0.000018532	0.000018501
9	1	0.000296175	-0.000091293	0.000006510
10	1	0.000104405	-0.000464947	-0.000234822
11	1	-0.000040296	0.000050122	0.000151286
12	1	-0.000158984	-0.000014347	-0.000218885
13	1	0.001354652	0.000852349	0.000089954
14	35	-0.000054299	0.000227492	0.000530648
15	1	-0.000025348	0.000520142	0.000355351
16	6	-0.000107010	-0.000044970	-0.000145500
17	6	-0.000386367	0.000246481	-0.000098879
18	1	0.000315112	-0.000280333	0.000216873
19	1	0.000143833	-0.000167154	0.000001059
20	1	-0.000029716	0.000266768	0.000119060
21	8	0.000100023	0.000003366	0.001000295
22	1	0.000056050	0.000599777	-0.000192784

Cartesian Forces: Max 0.002170124 RMS 0.000561591

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.001809437 RMS 0.000449536
Search for a local minimum.
Step number 63 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Update second derivatives using D2CorX and points 60 61 62 63
DE= -2.08D-04 DEPred=-1.96D-04 R= 1.06D+00
TightC=F SS= 1.41D+00 RLast= 1.69D-01 DXNew= 1.6377D+00 5.0602D-01
Trust test= 1.06D+00 RLast= 1.69D-01 DXMaxT set to 9.74D-01
ITU= 1 0 1 1 1 1 0 1 1 0 1 1 0 -1 1 1 1 -1 1 0
ITU= -1 1 0 -1 0 -1 0 0 1 -1 0 1 1 1 1 1 1 0 -1 1
ITU= 1 1 1 1 0 -1 1 1 1 1 1 1 1 1 1 1 1 1 0 0
ITU= -1 0 0
Use linear search instead of GDIIS.
Eigenvalues --- 0.00195 0.00282 0.00376 0.00707 0.00970

Eigenvalues ---	0.01365	0.01484	0.01844	0.02147	0.02300
Eigenvalues ---	0.02513	0.03031	0.03182	0.03847	0.04086
Eigenvalues ---	0.04577	0.04939	0.05357	0.05810	0.08231
Eigenvalues ---	0.08895	0.09393	0.12068	0.13831	0.14386
Eigenvalues ---	0.14956	0.15165	0.16013	0.16051	0.16428
Eigenvalues ---	0.17408	0.19117	0.22204	0.23114	0.23680
Eigenvalues ---	0.25089	0.26005	0.28412	0.29674	0.32907
Eigenvalues ---	0.33778	0.33850	0.33955	0.34231	0.34418
Eigenvalues ---	0.34611	0.34916	0.35784	0.36317	0.36413
Eigenvalues ---	0.39489	0.43150	0.43594	0.46125	0.48880
Eigenvalues ---	0.53689	0.56794	0.57419	0.60982	0.80910

RFO step: Lambda=-1.35463988D-04 EMin= 1.95462594D-03

Quartic linear search produced a step of 0.03811.

Iteration 1 RMS(Cart)= 0.02808091 RMS(Int)= 0.00057240

Iteration 2 RMS(Cart)= 0.00081950 RMS(Int)= 0.00000474

Iteration 3 RMS(Cart)= 0.00000033 RMS(Int)= 0.00000473

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56710	-0.00055	-0.00001	-0.00048	-0.00049	2.56661
R2	2.61563	-0.00001	-0.00003	-0.00019	-0.00021	2.61542
R3	2.03410	-0.00005	0.00000	-0.00012	-0.00012	2.03397
R4	2.62685	0.00042	0.00000	0.00053	0.00053	2.62738
R5	2.03111	-0.00019	-0.00001	-0.00034	-0.00036	2.03075
R6	2.54949	-0.00137	-0.00003	-0.00121	-0.00124	2.54825
R7	2.68720	0.00008	0.00008	-0.00046	-0.00038	2.68682
R8	2.52111	-0.00072	0.00000	-0.00092	-0.00092	2.52018
R9	2.08830	0.00061	-0.00009	-0.00030	-0.00039	2.08792
R10	2.79705	-0.00021	-0.00006	-0.00230	-0.00236	2.79469
R11	2.92919	0.00117	0.00011	0.00231	0.00242	2.93161
R12	2.05986	-0.00030	0.00000	-0.00041	-0.00040	2.05946
R13	2.06029	-0.00009	-0.00002	-0.00014	-0.00016	2.06013
R14	2.06626	0.00013	-0.00001	0.00010	0.00009	2.06635
R15	2.07285	-0.00016	0.00000	-0.00075	-0.00075	2.07210
R16	2.64425	0.00079	-0.00003	0.00232	0.00230	2.64655
R17	5.90834	0.00057	0.00150	0.04321	0.04472	5.95306
R18	2.50665	0.00015	0.00003	0.00061	0.00063	2.50729
R19	2.04579	-0.00006	0.00001	-0.00003	-0.00003	2.04576
R20	2.04362	-0.00021	0.00000	-0.00032	-0.00032	2.04330
R21	2.04636	-0.00028	-0.00001	-0.00042	-0.00042	2.04594
R22	1.85122	0.00015	0.00002	-0.00143	-0.00140	1.84982
A1	1.87574	-0.00014	-0.00001	-0.00013	-0.00014	1.87560
A2	2.27787	0.00004	0.00006	0.00104	0.00108	2.27895
A3	2.12957	0.00010	-0.00005	-0.00094	-0.00100	2.12857
A4	1.86274	-0.00036	0.00001	-0.00040	-0.00040	1.86234

A5	2.27901	-0.00007	0.00009	0.00094	0.00102	2.28004
A6	2.14139	0.00043	-0.00009	-0.00049	-0.00059	2.14080
A7	1.89592	0.00030	-0.00001	0.00022	0.00022	1.89614
A8	2.23981	0.00086	-0.00004	0.00202	0.00198	2.24179
A9	2.14745	-0.00116	0.00005	-0.00224	-0.00219	2.14525
A10	1.88919	0.00001	0.00000	0.00002	0.00001	1.88920
A11	2.24968	-0.00019	0.00002	-0.00060	-0.00060	2.24908
A12	2.14425	0.00018	-0.00002	0.00068	0.00065	2.14490
A13	1.90110	0.00019	0.00000	0.00031	0.00032	1.90142
A14	2.22865	-0.00035	-0.00002	-0.00180	-0.00182	2.22683
A15	2.15294	0.00016	0.00002	0.00137	0.00139	2.15433
A16	1.95704	0.00068	0.00025	0.00386	0.00410	1.96115
A17	1.86451	0.00000	0.00003	0.00122	0.00125	1.86576
A18	1.87300	-0.00042	-0.00015	-0.00097	-0.00111	1.87189
A19	1.88401	0.00029	-0.00009	-0.00139	-0.00149	1.88252
A20	1.96874	-0.00043	-0.00003	-0.00228	-0.00231	1.96643
A21	1.91370	-0.00011	-0.00001	-0.00028	-0.00029	1.91341
A22	1.92863	-0.00058	0.00009	0.00269	0.00278	1.93141
A23	1.88020	0.00181	-0.00021	0.00379	0.00357	1.88377
A24	1.93297	-0.00035	0.00007	-0.00297	-0.00290	1.93007
A25	1.89534	-0.00015	0.00010	0.00071	0.00080	1.89614
A26	1.87555	0.00053	-0.00007	0.00190	0.00183	1.87738
A27	1.95128	-0.00130	0.00002	-0.00604	-0.00602	1.94526
A28	1.76410	-0.00008	-0.00055	-0.01003	-0.01058	1.75352
A29	2.17206	0.00102	0.00002	0.00357	0.00359	2.17565
A30	1.96348	-0.00091	-0.00002	-0.00204	-0.00206	1.96142
A31	2.14764	-0.00011	0.00000	-0.00153	-0.00153	2.14611
A32	2.08047	-0.00003	0.00000	-0.00060	-0.00059	2.07988
A33	2.15650	0.00011	-0.00006	-0.00018	-0.00024	2.15626
A34	2.04620	-0.00007	0.00005	0.00078	0.00084	2.04704
A35	1.85173	0.00013	-0.00016	0.00280	0.00264	1.85436
D1	0.00425	-0.00015	0.00005	0.00037	0.00042	0.00467
D2	3.13562	-0.00013	0.00035	0.00597	0.00633	-3.14123
D3	-3.14010	0.00004	-0.00060	-0.00866	-0.00927	3.13381
D4	-0.00873	0.00007	-0.00030	-0.00306	-0.00336	-0.01209
D5	-0.01050	0.00029	-0.00009	0.00057	0.00048	-0.01002
D6	-3.11895	0.00023	-0.00027	0.00446	0.00419	-3.11476
D7	3.13357	0.00012	0.00050	0.00866	0.00916	-3.14046
D8	0.02512	0.00005	0.00032	0.01256	0.01287	0.03798
D9	0.00335	-0.00004	0.00000	-0.00117	-0.00117	0.00217
D10	-3.13542	0.00002	-0.00035	-0.00249	-0.00284	-3.13826
D11	-3.12902	-0.00006	-0.00027	-0.00624	-0.00651	-3.13553
D12	0.01539	0.00001	-0.00063	-0.00755	-0.00818	0.00722
D13	-0.00992	0.00022	-0.00005	0.00154	0.00149	-0.00843

D14	-3.13896	-0.00004	-0.00014	-0.00635	-0.00649	3.13774
D15	3.12903	0.00016	0.00027	0.00278	0.00305	3.13208
D16	-0.00001	-0.00010	0.00019	-0.00511	-0.00493	-0.00493
D17	0.12408	-0.00018	-0.00138	-0.05298	-0.05436	0.06972
D18	-3.01854	-0.00027	-0.00146	-0.05300	-0.05446	-3.07300
D19	-3.01432	-0.00012	-0.00178	-0.05447	-0.05625	-3.07057
D20	0.12624	-0.00020	-0.00186	-0.05449	-0.05635	0.06990
D21	0.01261	-0.00031	0.00009	-0.00131	-0.00122	0.01139
D22	3.12280	-0.00027	0.00026	-0.00507	-0.00482	3.11799
D23	-3.14061	-0.00008	0.00017	0.00599	0.00616	-3.13445
D24	-0.03042	-0.00003	0.00034	0.00223	0.00257	-0.02785
D25	1.85081	-0.00055	0.00051	-0.01779	-0.01728	1.83353
D26	-2.37172	0.00018	0.00055	-0.01657	-0.01601	-2.38773
D27	-0.32041	-0.00016	0.00049	-0.01676	-0.01627	-0.33668
D28	-1.25325	-0.00062	0.00030	-0.01335	-0.01305	-1.26629
D29	0.80742	0.00011	0.00035	-0.01213	-0.01178	0.79564
D30	2.85873	-0.00023	0.00028	-0.01231	-0.01203	2.84669
D31	-1.58734	0.00027	-0.00130	-0.00582	-0.00713	-1.59446
D32	0.48064	0.00085	-0.00125	-0.00117	-0.00242	0.47822
D33	2.61955	0.00021	-0.00131	-0.00801	-0.00933	2.61022
D34	2.64680	-0.00030	-0.00142	-0.00866	-0.01008	2.63672
D35	-1.56841	0.00028	-0.00137	-0.00401	-0.00538	-1.57379
D36	0.57050	-0.00037	-0.00143	-0.01085	-0.01228	0.55822
D37	0.52971	-0.00009	-0.00133	-0.00591	-0.00725	0.52247
D38	2.59769	0.00049	-0.00129	-0.00125	-0.00254	2.59515
D39	-1.54659	-0.00016	-0.00135	-0.00810	-0.00945	-1.55603
D40	1.18760	0.00010	0.00165	-0.01163	-0.00998	1.17763
D41	-3.00637	0.00036	0.00170	-0.00585	-0.00416	-3.01052
D42	-0.94000	0.00014	0.00169	-0.00668	-0.00499	-0.94499
D43	-1.29609	-0.00095	0.00010	-0.00773	-0.00764	-1.30374
D44	2.87900	-0.00037	-0.00001	-0.01046	-0.01046	2.86854
D45	0.80089	0.00023	-0.00010	-0.00901	-0.00910	0.79179
D46	-3.13304	-0.00009	-0.00020	-0.00420	-0.00440	-3.13745
D47	0.01184	-0.00006	-0.00020	-0.00514	-0.00535	0.00649
D48	0.00969	0.00000	-0.00011	-0.00418	-0.00429	0.00539
D49	-3.12862	0.00003	-0.00011	-0.00513	-0.00524	-3.13385

Item	Value	Threshold	Converged?
Maximum Force	0.001809	0.000450	NO
RMS Force	0.000450	0.000300	NO
Maximum Displacement	0.150015	0.001800	NO
RMS Displacement	0.028123	0.001200	NO

Predicted change in Energy=-6.998713D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.613196	-2.383204	-1.120906
2	6	0	-1.911015	-2.005083	-1.252739
3	7	0	-2.082107	-0.878902	-0.455546
4	6	0	-0.906916	-0.588950	0.138792
5	7	0	-0.008877	-1.496257	-0.247046
6	6	0	1.405423	-1.477751	0.184830
7	6	0	2.214350	-0.339879	-0.491588
8	1	0	-0.075211	-3.204886	-1.561248
9	1	0	-2.707964	-2.429699	-1.835318
10	1	0	1.406221	-1.295309	1.259270
11	1	0	1.818731	-2.465689	-0.019214
12	1	0	2.678323	-0.693489	-1.416442
13	1	0	1.517267	0.470270	-0.736673
14	35	0	0.734573	1.446195	2.154497
15	1	0	-0.666568	0.235081	0.834463
16	6	0	-3.261632	-0.112023	-0.250261
17	6	0	-4.452193	-0.409336	-0.754804
18	1	0	-3.085946	0.755633	0.372850
19	1	0	-5.290781	0.240028	-0.544475
20	1	0	-4.639957	-1.278007	-1.373119
21	8	0	3.239665	0.104403	0.352643
22	1	0	2.808160	0.639976	1.049186

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.358193	0.000000			
3	N	2.205296	1.390351	0.000000		
4	C	2.211890	2.224861	1.348474	0.000000	
5	N	1.384018	2.210984	2.173220	1.333623	0.000000
6	C	2.568971	3.652868	3.596049	2.477700	1.478886
7	C	3.544888	4.513412	4.330287	3.194012	2.517886
8	H	1.076332	2.214696	3.265029	3.228775	2.156604
9	H	2.213730	1.074628	2.168051	3.244880	3.267873
10	H	3.305571	4.221140	3.909274	2.665524	2.076505
11	H	2.671104	3.955344	4.233771	3.313045	2.081311
12	H	3.711680	4.775887	4.859979	3.909427	3.038580
13	H	3.581734	4.259907	3.854191	2.786584	2.536943
14	Br	5.216229	5.524465	4.489107	3.301419	3.870162

15	H	3.268292	3.305057	2.215588	1.104877	2.144703
16	C	3.595900	2.532352	1.421803	2.433826	3.535043
17	C	4.332214	3.041699	2.434615	3.660568	4.602420
18	H	4.265922	3.412412	2.089410	2.571159	3.863112
19	H	5.393831	4.118857	3.399338	4.513571	5.567913
20	H	4.183285	2.826704	2.746602	4.086106	4.771014
21	O	4.817061	5.792814	5.471866	4.209586	3.670799
22	H	5.055154	5.879269	5.337220	4.017570	3.765555

		6	7	8	9	10
6	C	0.000000				
7	C	1.551340	0.000000			
8	H	2.867763	3.820279	0.000000		
9	H	4.680509	5.513813	2.758155	0.000000	
10	H	1.089820	2.152074	3.714357	5.271607	0.000000
11	H	1.090174	2.213305	2.551725	4.877551	1.781706
12	H	2.190756	1.093466	3.729616	5.674678	3.023221
13	H	2.157884	1.096509	4.089338	5.241128	2.667094
14	Br	3.588745	3.518744	6.007917	6.541578	2.961147
15	H	2.765676	3.223147	4.233499	4.289066	2.611323
16	C	4.882204	5.486030	4.630094	2.861918	5.046554
17	C	6.027942	6.672098	5.255799	2.879533	6.257991
18	H	5.019537	5.480924	5.337693	3.894254	5.017138
19	H	6.951388	7.527687	6.332727	3.932513	7.103562
20	H	6.246096	6.974145	4.958342	2.296218	6.594395
21	O	2.428131	1.400494	5.059919	6.825185	2.478444
22	H	2.683197	1.920080	5.469109	6.940525	2.398936

		11	12	13	14	15
11	H	0.000000				
12	H	2.414919	0.000000			
13	H	3.037348	1.778897	0.000000		
14	Br	4.604699	4.594346	3.150222	0.000000	
15	H	3.768240	4.137283	2.700540	2.274309	0.000000
16	C	5.603857	6.081212	4.838753	4.917373	2.833984
17	C	6.640344	7.166781	6.033944	6.229732	4.155960
18	H	5.881027	6.207118	4.743631	4.271710	2.517429
19	H	7.625087	8.070836	6.814650	6.711496	4.825437
20	H	6.705095	7.341713	6.432180	6.982186	4.790686
21	O	2.960187	2.020248	2.070537	3.364903	3.938005
22	H	3.430102	2.806120	2.210089	2.484243	3.504822

		16	17	18	19	20
16	C	0.000000				
17	C	1.326798	0.000000			
18	H	1.082571	2.120233	0.000000		
19	H	2.080372	1.081269	2.443078	0.000000	

20	H	2.126054	1.082662	3.098233	1.847878	0.000000
21	O	6.532779	7.788135	6.359077	8.578562	8.183994
22	H	6.252714	7.554346	5.933910	8.263931	8.063539

		21	22
21	O	0.000000	
22	H	0.978880	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.870863	-1.989393	0.352316
2	6	0	-2.863868	-1.093906	0.114129
3	7	0	-2.256378	0.149001	-0.024490
4	6	0	-0.924909	-0.002890	0.125524
5	7	0	-0.675852	-1.291299	0.363272
6	6	0	0.685785	-1.836693	0.551940
7	6	0	1.488813	-1.891287	-0.774266
8	1	0	-1.911929	-3.051244	0.523420
9	1	0	-3.926150	-1.232789	0.029908
10	1	0	1.206448	-1.161171	1.230385
11	1	0	0.579977	-2.815740	1.019647
12	1	0	1.353810	-2.857784	-1.267546
13	1	0	1.104696	-1.104314	-1.434161
14	35	0	2.032891	1.463624	0.136843
15	1	0	-0.129923	0.762848	0.076579
16	6	0	-2.866501	1.407657	-0.279551
17	6	0	-4.175551	1.609771	-0.356567
18	1	0	-2.139724	2.199991	-0.405888
19	1	0	-4.543961	2.605978	-0.559021
20	1	0	-4.910694	0.825932	-0.224961
21	8	0	2.858003	-1.730114	-0.527840
22	1	0	2.990418	-0.781088	-0.327782

Rotational constants (GHZ): 0.9924015 0.4442481 0.3184998
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 358 symmetry adapted cartesian basis functions of A symmetry.
There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 852.2053397706 Hartrees.
NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 345 RedAO= T EigKep= 4.93D-06 NBF= 345
NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345
Initial guess from the checkpoint file: "."
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 0.000479 -0.000141 -0.000224 Ang= 0.06 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.34317224 A.U. after 10 cycles
NFock= 10 Conv=0.49D-08 -V/T= 2.0016
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000295487	-0.000311085	0.000293109
2	6	-0.000082396	-0.000123832	-0.000198933
3	7	0.000872891	0.000334587	-0.000094430
4	6	-0.000837825	-0.001046589	-0.000172714

5	7	-0.000158514	0.000236223	-0.000593187
6	6	0.000341746	0.000360069	0.000810246
7	6	-0.001094793	-0.000144166	-0.000715696
8	1	-0.000061406	0.000078577	-0.000214734
9	1	0.000253044	-0.000230228	-0.000061729
10	1	0.000009507	-0.000396145	-0.000181069
11	1	0.000044087	-0.000045352	0.000204392
12	1	-0.000137920	-0.000087645	0.000014748
13	1	0.000677455	0.000532779	-0.000284589
14	35	-0.000020892	0.000429224	0.000453027
15	1	0.000084226	0.000434244	0.000490558
16	6	-0.000424834	0.000109928	-0.000076011
17	6	0.000290154	0.000083611	0.000083738
18	1	0.000300166	-0.000176384	0.000119581
19	1	0.000061756	-0.000113083	-0.000052311
20	1	-0.000154508	0.000150274	0.000038655
21	8	0.000773025	-0.000479078	-0.000215366
22	1	-0.000439481	0.000404070	0.000352714

Cartesian Forces: Max 0.001094793 RMS 0.000390260

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.001516860 RMS 0.000348531
Search for a local minimum.
Step number 64 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 61 62 63 64
DE= -9.28D-05 DEPred=-7.00D-05 R= 1.33D+00
TightC=F SS= 1.41D+00 RLast= 1.32D-01 DXNew= 1.6377D+00 3.9732D-01
Trust test= 1.33D+00 RLast= 1.32D-01 DXMaxT set to 9.74D-01
ITU= 1 1 0 1 1 1 1 0 1 1 0 1 1 0 -1 1 1 1 -1 1
ITU= 0 -1 1 0 -1 0 -1 0 0 1 -1 0 1 1 1 1 1 1 0 -1
ITU= 1 1 1 1 1 0 -1 1 1 1 1 1 1 1 1 1 1 1 1 0
ITU= 0 -1 0 0
Eigenvalues --- 0.00188 0.00232 0.00373 0.00689 0.00990
Eigenvalues --- 0.01318 0.01512 0.01851 0.02157 0.02306
Eigenvalues --- 0.02508 0.03028 0.03189 0.03803 0.04068
Eigenvalues --- 0.04379 0.04840 0.05391 0.05791 0.08623
Eigenvalues --- 0.08953 0.09451 0.12715 0.13946 0.14396

Eigenvalues --- 0.14885 0.15372 0.16009 0.16056 0.16412
Eigenvalues --- 0.17490 0.18675 0.21692 0.23119 0.23425
Eigenvalues --- 0.24819 0.26076 0.28567 0.29928 0.32779
Eigenvalues --- 0.33797 0.33843 0.33970 0.34243 0.34482
Eigenvalues --- 0.34622 0.34964 0.36316 0.36342 0.36418
Eigenvalues --- 0.39489 0.43007 0.43908 0.45729 0.48873
Eigenvalues --- 0.53563 0.55386 0.58040 0.61169 0.75057
En-DIIS/RFO-DIIS IScMMF= 0 using points: 64 63
RFO step: Lambda=-2.55628953D-05.
DidBck=F Rises=F RFO-DIIS coefs: 1.57408 -0.57408
Iteration 1 RMS(Cart)= 0.03611487 RMS(Int)= 0.00094493
Iteration 2 RMS(Cart)= 0.00136026 RMS(Int)= 0.00000583
Iteration 3 RMS(Cart)= 0.00000099 RMS(Int)= 0.00000578

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56661	-0.00026	-0.00028	-0.00025	-0.00053	2.56608
R2	2.61542	0.00024	-0.00012	0.00049	0.00037	2.61578
R3	2.03397	0.00000	-0.00007	0.00001	-0.00006	2.03391
R4	2.62738	0.00032	0.00030	0.00070	0.00101	2.62839
R5	2.03075	-0.00006	-0.00021	-0.00014	-0.00034	2.03041
R6	2.54825	-0.00070	-0.00071	-0.00125	-0.00196	2.54629
R7	2.68682	-0.00002	-0.00022	0.00002	-0.00020	2.68662
R8	2.52018	-0.00037	-0.00053	-0.00037	-0.00090	2.51928
R9	2.08792	0.00065	-0.00022	0.00069	0.00047	2.08838
R10	2.79469	0.00028	-0.00136	0.00079	-0.00057	2.79412
R11	2.93161	0.00054	0.00139	0.00047	0.00185	2.93346
R12	2.05946	-0.00024	-0.00023	-0.00050	-0.00074	2.05873
R13	2.06013	0.00002	-0.00009	0.00005	-0.00004	2.06009
R14	2.06635	-0.00004	0.00005	-0.00040	-0.00035	2.06600
R15	2.07210	0.00026	-0.00043	-0.00026	-0.00069	2.07141
R16	2.64655	0.00030	0.00132	0.00075	0.00207	2.64862
R17	5.95306	0.00055	0.02567	0.02496	0.05063	6.00369
R18	2.50729	-0.00023	0.00036	-0.00050	-0.00013	2.50715
R19	2.04576	-0.00002	-0.00001	-0.00007	-0.00008	2.04568
R20	2.04330	-0.00013	-0.00018	-0.00023	-0.00042	2.04289
R21	2.04594	-0.00012	-0.00024	-0.00022	-0.00046	2.04547
R22	1.84982	0.00066	-0.00081	0.00089	0.00009	1.84990
A1	1.87560	0.00000	-0.00008	0.00009	0.00000	1.87560
A2	2.27895	-0.00013	0.00062	-0.00093	-0.00032	2.27863
A3	2.12857	0.00013	-0.00058	0.00085	0.00026	2.12882
A4	1.86234	-0.00026	-0.00023	-0.00036	-0.00059	1.86175
A5	2.28004	-0.00022	0.00059	-0.00210	-0.00153	2.27851
A6	2.14080	0.00048	-0.00034	0.00248	0.00213	2.14292
A7	1.89614	0.00021	0.00013	0.00013	0.00026	1.89640

A8	2.24179	0.00062	0.00113	0.00276	0.00389	2.24568
A9	2.14525	-0.00083	-0.00126	-0.00289	-0.00415	2.14111
A10	1.88920	0.00007	0.00001	0.00048	0.00047	1.88967
A11	2.24908	-0.00007	-0.00034	0.00027	-0.00011	2.24897
A12	2.14490	0.00000	0.00037	-0.00072	-0.00038	2.14452
A13	1.90142	-0.00001	0.00018	-0.00030	-0.00011	1.90131
A14	2.22683	-0.00009	-0.00105	0.00136	0.00030	2.22713
A15	2.15433	0.00011	0.00080	-0.00109	-0.00031	2.15402
A16	1.96115	0.00011	0.00236	-0.00042	0.00193	1.96308
A17	1.86576	0.00011	0.00072	0.00006	0.00077	1.86653
A18	1.87189	-0.00020	-0.00064	0.00012	-0.00051	1.87138
A19	1.88252	0.00041	-0.00086	0.00265	0.00178	1.88430
A20	1.96643	-0.00025	-0.00133	-0.00018	-0.00150	1.96493
A21	1.91341	-0.00017	-0.00016	-0.00232	-0.00249	1.91093
A22	1.93141	-0.00072	0.00159	-0.00190	-0.00032	1.93109
A23	1.88377	0.00152	0.00205	0.00006	0.00210	1.88587
A24	1.93007	-0.00021	-0.00166	-0.00010	-0.00177	1.92830
A25	1.89614	-0.00024	0.00046	0.00083	0.00128	1.89741
A26	1.87738	0.00028	0.00105	-0.00114	-0.00009	1.87729
A27	1.94526	-0.00067	-0.00345	0.00226	-0.00119	1.94407
A28	1.75352	0.00082	-0.00607	0.00694	0.00087	1.75439
A29	2.17565	0.00049	0.00206	0.00239	0.00445	2.18010
A30	1.96142	-0.00059	-0.00118	-0.00330	-0.00448	1.95694
A31	2.14611	0.00011	-0.00088	0.00092	0.00004	2.14615
A32	2.07988	-0.00004	-0.00034	-0.00080	-0.00114	2.07874
A33	2.15626	0.00021	-0.00014	0.00179	0.00165	2.15792
A34	2.04704	-0.00017	0.00048	-0.00099	-0.00051	2.04653
A35	1.85436	-0.00032	0.00151	-0.00249	-0.00098	1.85339
D1	0.00467	-0.00011	0.00024	-0.00047	-0.00023	0.00444
D2	-3.14123	-0.00011	0.00363	0.00285	0.00648	-3.13475
D3	3.13381	0.00013	-0.00532	0.00016	-0.00517	3.12864
D4	-0.01209	0.00013	-0.00193	0.00348	0.00154	-0.01055
D5	-0.01002	0.00023	0.00028	0.00158	0.00186	-0.00816
D6	-3.11476	0.00017	0.00241	0.00281	0.00522	-3.10954
D7	-3.14046	0.00001	0.00526	0.00103	0.00629	-3.13418
D8	0.03798	-0.00004	0.00739	0.00227	0.00965	0.04763
D9	0.00217	-0.00005	-0.00067	-0.00078	-0.00145	0.00072
D10	-3.13826	0.00001	-0.00163	0.00089	-0.00074	-3.13900
D11	-3.13553	-0.00004	-0.00374	-0.00377	-0.00751	3.14014
D12	0.00722	0.00002	-0.00469	-0.00209	-0.00679	0.00042
D13	-0.00843	0.00019	0.00085	0.00177	0.00262	-0.00581
D14	3.13774	0.00003	-0.00372	-0.00481	-0.00853	3.12920
D15	3.13208	0.00013	0.00175	0.00022	0.00196	3.13404
D16	-0.00493	-0.00002	-0.00283	-0.00636	-0.00919	-0.01413

D17	0.06972	-0.00011	-0.03121	-0.03539	-0.06659	0.00313
D18	-3.07300	-0.00014	-0.03127	-0.03329	-0.06455	-3.13756
D19	-3.07057	-0.00004	-0.03229	-0.03350	-0.06579	-3.13636
D20	0.06990	-0.00007	-0.03235	-0.03140	-0.06375	0.00615
D21	0.01139	-0.00026	-0.00070	-0.00207	-0.00277	0.00862
D22	3.11799	-0.00021	-0.00276	-0.00318	-0.00594	3.11204
D23	-3.13445	-0.00011	0.00354	0.00403	0.00757	-3.12688
D24	-0.02785	-0.00006	0.00147	0.00293	0.00440	-0.02345
D25	1.83353	-0.00051	-0.00992	-0.01836	-0.02828	1.80524
D26	-2.38773	0.00012	-0.00919	-0.01534	-0.02453	-2.41225
D27	-0.33668	-0.00012	-0.00934	-0.01794	-0.02728	-0.36396
D28	-1.26629	-0.00057	-0.00749	-0.01699	-0.02448	-1.29077
D29	0.79564	0.00006	-0.00676	-0.01397	-0.02072	0.77492
D30	2.84669	-0.00018	-0.00691	-0.01657	-0.02348	2.82321
D31	-1.59446	0.00028	-0.00409	0.00051	-0.00358	-1.59804
D32	0.47822	0.00050	-0.00139	0.00045	-0.00093	0.47728
D33	2.61022	0.00052	-0.00535	0.00321	-0.00214	2.60808
D34	2.63672	-0.00018	-0.00579	-0.00099	-0.00678	2.62994
D35	-1.57379	0.00004	-0.00309	-0.00105	-0.00413	-1.57792
D36	0.55822	0.00007	-0.00705	0.00171	-0.00534	0.55288
D37	0.52247	-0.00008	-0.00416	0.00023	-0.00393	0.51853
D38	2.59515	0.00013	-0.00146	0.00017	-0.00128	2.59386
D39	-1.55603	0.00016	-0.00542	0.00293	-0.00249	-1.55853
D40	1.17763	0.00066	-0.00573	0.00076	-0.00497	1.17266
D41	-3.01052	0.00054	-0.00239	-0.00102	-0.00340	-3.01392
D42	-0.94499	0.00033	-0.00287	-0.00055	-0.00342	-0.94841
D43	-1.30374	-0.00077	-0.00439	0.00554	0.00115	-1.30259
D44	2.86854	0.00005	-0.00601	0.00864	0.00263	2.87117
D45	0.79179	0.00056	-0.00522	0.00704	0.00182	0.79361
D46	-3.13745	-0.00002	-0.00253	-0.00036	-0.00289	-3.14033
D47	0.00649	-0.00003	-0.00307	-0.00272	-0.00579	0.00071
D48	0.00539	0.00001	-0.00246	-0.00267	-0.00514	0.00025
D49	-3.13385	0.00000	-0.00301	-0.00503	-0.00804	3.14129

Item	Value	Threshold	Converged?
Maximum Force	0.001517	0.000450	NO
RMS Force	0.000349	0.000300	NO
Maximum Displacement	0.173234	0.001800	NO
RMS Displacement	0.036304	0.001200	NO

Predicted change in Energy=-5.086591D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-0.608579	-2.384553	-1.118766
2	6	0	-1.908638	-2.013704	-1.246207
3	7	0	-2.085888	-0.896147	-0.437379
4	6	0	-0.913438	-0.606063	0.159947
5	7	0	-0.009399	-1.501999	-0.236652
6	6	0	1.405992	-1.474365	0.190107
7	6	0	2.213552	-0.345626	-0.505232
8	1	0	-0.066833	-3.200902	-1.564304
9	1	0	-2.703308	-2.442100	-1.828796
10	1	0	1.410691	-1.279490	1.261956
11	1	0	1.820233	-2.464407	-0.001357
12	1	0	2.678486	-0.713943	-1.423623
13	1	0	1.517438	0.461077	-0.762502
14	35	0	0.717312	1.483477	2.137140
15	1	0	-0.676094	0.216737	0.858491
16	6	0	-3.266800	-0.134760	-0.220663
17	6	0	-4.443905	-0.383495	-0.779914
18	1	0	-3.101578	0.688195	0.462942
19	1	0	-5.282028	0.259081	-0.549022
20	1	0	-4.621243	-1.202714	-1.464791
21	8	0	3.238833	0.112139	0.333641
22	1	0	2.805542	0.656686	1.022136

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.357911	0.000000			
3	N	2.205013	1.390883	0.000000		
4	C	2.211577	2.224667	1.347437	0.000000	
5	N	1.384213	2.210917	2.172362	1.333146	0.000000
6	C	2.569064	3.652487	3.594622	2.476815	1.478587
7	C	3.535261	4.508212	4.335074	3.207546	2.520088
8	H	1.076299	2.214243	3.264727	3.228462	2.156903
9	H	2.212543	1.074446	2.169613	3.244960	3.267394
10	H	3.311564	4.224677	3.906502	2.658853	2.076533
11	H	2.674716	3.956925	4.231706	3.309443	2.080659
12	H	3.699821	4.771012	4.868792	3.926990	3.042147
13	H	3.569941	4.253999	3.864159	2.810490	2.541931
14	Br	5.226908	5.529279	4.488729	3.306784	3.882791
15	H	3.268152	3.305116	2.214794	1.105123	2.144265
16	C	3.596428	2.535109	1.421699	2.430083	3.532741
17	C	4.339214	3.050015	2.437290	3.660201	4.605543

18	H	4.261293	3.412412	2.086226	2.560247	3.853304
19	H	5.399494	4.126909	3.400342	4.509511	5.567728
20	H	4.197375	2.839668	2.752741	4.091893	4.781946
21	O	4.810980	5.788919	5.473917	4.217503	3.671741
22	H	5.048646	5.873658	5.335501	4.021035	3.764088

		6	7	8	9	10
6	C	0.000000				
7	C	1.552321	0.000000			
8	H	2.868467	3.804522	0.000000		
9	H	4.679619	5.506591	2.756218	0.000000	
10	H	1.089431	2.153983	3.723258	5.275358	0.000000
11	H	1.090154	2.213102	2.558563	4.878776	1.779807
12	H	2.191257	1.093282	3.706957	5.666957	3.023158
13	H	2.160051	1.096144	4.069753	5.232602	2.671965
14	Br	3.607499	3.544923	6.021543	6.545186	2.980051
15	H	2.764353	3.244386	4.233367	4.289584	2.599259
16	C	4.878346	5.491785	4.631025	2.868351	5.038599
17	C	6.029281	6.663228	5.264201	2.892695	6.264848
18	H	5.006924	5.500613	5.333336	3.899926	4.987060
19	H	6.948436	7.520060	6.340390	3.947657	7.102065
20	H	6.256201	6.954839	4.974466	2.312369	6.620066
21	O	2.428353	1.401590	5.050333	6.819774	2.478004
22	H	2.681863	1.920400	5.460879	6.933811	2.398312

		11	12	13	14	15
11	H	0.000000				
12	H	2.413206	0.000000			
13	H	3.038006	1.779266	0.000000		
14	Br	4.623352	4.621028	3.177016	0.000000	
15	H	3.762913	4.162621	2.738412	2.276215	0.000000
16	C	5.599397	6.093356	4.851550	4.904190	2.828406
17	C	6.646485	7.159051	6.020898	6.215541	4.152234
18	H	5.863334	6.239732	4.784203	4.244919	2.502340
19	H	7.626233	8.067310	6.805814	6.686306	4.816380
20	H	6.725037	7.316190	6.398814	6.977801	4.793400
21	O	2.960276	2.020984	2.070383	3.389874	3.951336
22	H	3.429226	2.806512	2.209617	2.507493	3.513136

		16	17	18	19	20
16	C	0.000000				
17	C	1.326728	0.000000			
18	H	1.082528	2.120153	0.000000		
19	H	2.079441	1.081049	2.441838	0.000000	
20	H	2.126711	1.082417	3.098560	1.847191	0.000000
21	O	6.533871	7.778824	6.367838	8.567715	8.169699
22	H	6.248542	7.542138	5.933613	8.248358	8.049803

		21	22
21	O	0.000000	
22	H	0.978927	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.874468	-1.993102	0.340862
2	6	0	-2.865017	-1.093327	0.110342
3	7	0	-2.254935	0.151491	-0.002720
4	6	0	-0.925976	-0.003770	0.156494
5	7	0	-0.679038	-1.295960	0.372237
6	6	0	0.681335	-1.845451	0.555717
7	6	0	1.479331	-1.910781	-0.774183
8	1	0	-1.918077	-3.056988	0.497909
9	1	0	-3.926899	-1.230960	0.021469
10	1	0	1.207677	-1.171389	1.230597
11	1	0	0.573951	-2.822152	1.027902
12	1	0	1.341136	-2.880715	-1.259358
13	1	0	1.096775	-1.127458	-1.438704
14	35	0	2.033137	1.471949	0.129650
15	1	0	-0.129239	0.761186	0.119760
16	6	0	-2.856660	1.417195	-0.241779
17	6	0	-4.158052	1.621630	-0.399228
18	1	0	-2.125803	2.214660	-0.283788
19	1	0	-4.514602	2.626363	-0.578252
20	1	0	-4.898073	0.832690	-0.359614
21	8	0	2.850494	-1.750731	-0.531793
22	1	0	2.984243	-0.800688	-0.337298

Rotational constants (GHZ): 0.9806942 0.4455882 0.3180555
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 358 symmetry adapted cartesian basis functions of A symmetry.
There are 345 symmetry adapted basis functions of A symmetry.
345 basis functions, 553 primitive gaussians, 358 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 851.1286154922 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 4.73D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Initial guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999999 0.000560 0.000023 0.000978 Ang= 0.13 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Keep R1 ints in memory in canonical form, NReq=1804729152.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3032.34322828 A.U. after 11 cycles

NFock= 11 Conv=0.60D-08 -V/T= 2.0017

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000005778	-0.000303803	0.000291519
2	6	-0.000158959	0.000215667	-0.000076475
3	7	-0.000074450	-0.000045176	-0.000363710
4	6	-0.000070735	-0.000715323	0.000189125
5	7	0.000120175	0.000003273	-0.000549460
6	6	0.000664961	0.000221116	0.000355376
7	6	-0.001038370	-0.000341882	0.000142749

8	1	-0.000005372	0.000107613	-0.000286912
9	1	-0.000027839	-0.000151137	-0.000041133
10	1	-0.000064258	-0.000113623	-0.000029107
11	1	0.000111460	-0.000084577	0.000171975
12	1	-0.000113581	-0.000027362	-0.000033696
13	1	0.000400315	0.000525194	-0.000394101
14	35	0.000159604	-0.000053692	-0.000046969
15	1	0.000049391	0.000551059	0.000469184
16	6	-0.000302189	0.000343043	0.000038359
17	6	0.000510496	-0.000103059	0.000089467
18	1	0.000047415	0.000036473	0.000026186
19	1	-0.000066971	-0.000013512	-0.000026289
20	1	-0.000056620	-0.000062322	-0.000040302
21	8	0.000062938	-0.000288108	-0.000122197
22	1	-0.000141631	0.000300139	0.000236409

Cartesian Forces: Max 0.001038370 RMS 0.000281276

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000969693 RMS 0.000207568
Search for a local minimum.
Step number 65 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 61 62 63 64 65
DE= -5.60D-05 DEPred=-5.09D-05 R= 1.10D+00
TightC=F SS= 1.41D+00 RLast= 1.56D-01 DXNew= 1.6377D+00 4.6830D-01
Trust test= 1.10D+00 RLast= 1.56D-01 DXMaxT set to 9.74D-01
ITU= 1 1 1 0 1 1 1 1 0 1 1 0 1 1 0 -1 1 1 1 -1
ITU= 1 0 -1 1 0 -1 0 -1 0 0 1 -1 0 1 1 1 1 1 1 0
ITU= -1 1 1 1 1 1 0 -1 1 1 1 1 1 1 1 1 1 1 1 1
ITU= 0 0 -1 0 0

Eigenvalues ---	0.00162	0.00231	0.00386	0.00670	0.00974
Eigenvalues ---	0.01315	0.01507	0.01857	0.02159	0.02296
Eigenvalues ---	0.02505	0.03028	0.03187	0.03718	0.04041
Eigenvalues ---	0.04366	0.05003	0.05511	0.05869	0.08623
Eigenvalues ---	0.08937	0.09568	0.13490	0.14072	0.14399
Eigenvalues ---	0.15008	0.15330	0.15994	0.16080	0.16362
Eigenvalues ---	0.17457	0.19426	0.21372	0.23212	0.23293
Eigenvalues ---	0.24634	0.26730	0.27374	0.30133	0.32717

Eigenvalues --- 0.33812 0.33859 0.33956 0.34251 0.34397
Eigenvalues --- 0.34813 0.35034 0.36266 0.36317 0.36528
Eigenvalues --- 0.39073 0.43036 0.43891 0.45550 0.48958
Eigenvalues --- 0.53576 0.54960 0.58453 0.61090 0.73831
En-DIIS/RFO-DIIS IScMMF= 0 using points: 65 64 63
RFO step: Lambda=-9.39492829D-06.
DidBck=F Rises=F RFO-DIIS coefs: 0.94789 0.27309 -0.22098
Iteration 1 RMS(Cart)= 0.01044381 RMS(Int)= 0.00004282
Iteration 2 RMS(Cart)= 0.00007013 RMS(Int)= 0.00000256
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000256

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56608	0.00013	-0.00008	0.00030	0.00022	2.56630
R2	2.61578	0.00017	-0.00007	0.00009	0.00002	2.61580
R3	2.03391	0.00003	-0.00002	0.00004	0.00002	2.03393
R4	2.62839	0.00002	0.00006	-0.00008	-0.00001	2.62837
R5	2.03041	0.00010	-0.00006	0.00019	0.00013	2.03054
R6	2.54629	0.00013	-0.00017	-0.00015	-0.00032	2.54596
R7	2.68662	0.00001	-0.00007	0.00097	0.00090	2.68752
R8	2.51928	0.00012	-0.00016	0.00021	0.00006	2.51934
R9	2.08838	0.00072	-0.00011	0.00172	0.00161	2.08999
R10	2.79412	0.00012	-0.00049	0.00043	-0.00006	2.79407
R11	2.93346	-0.00017	0.00044	-0.00045	-0.00002	2.93345
R12	2.05873	-0.00005	-0.00005	-0.00022	-0.00027	2.05846
R13	2.06009	0.00009	-0.00003	0.00019	0.00016	2.06025
R14	2.06600	-0.00001	0.00004	0.00000	0.00004	2.06605
R15	2.07141	0.00010	-0.00013	-0.00011	-0.00024	2.07117
R16	2.64862	0.00001	0.00040	0.00002	0.00042	2.64904
R17	6.00369	-0.00010	0.00724	0.01503	0.02227	6.02596
R18	2.50715	-0.00032	0.00015	-0.00054	-0.00039	2.50676
R19	2.04568	0.00005	0.00000	0.00019	0.00019	2.04587
R20	2.04289	0.00004	-0.00005	0.00015	0.00010	2.04298
R21	2.04547	0.00008	-0.00007	0.00022	0.00015	2.04562
R22	1.84990	0.00039	-0.00032	0.00064	0.00032	1.85022
A1	1.87560	-0.00001	-0.00003	-0.00006	-0.00010	1.87551
A2	2.27863	-0.00011	0.00026	-0.00065	-0.00041	2.27822
A3	2.12882	0.00012	-0.00024	0.00078	0.00053	2.12936
A4	1.86175	-0.00001	-0.00006	-0.00006	-0.00011	1.86164
A5	2.27851	-0.00010	0.00031	-0.00063	-0.00032	2.27818
A6	2.14292	0.00011	-0.00024	0.00068	0.00044	2.14336
A7	1.89640	0.00007	0.00004	0.00017	0.00021	1.89661
A8	2.24568	-0.00005	0.00023	-0.00023	0.00000	2.24568
A9	2.14111	-0.00002	-0.00027	0.00006	-0.00021	2.14090
A10	1.88967	-0.00005	-0.00002	-0.00003	-0.00006	1.88961

A11	2.24897	-0.00009	-0.00013	-0.00003	-0.00017	2.24880
A12	2.14452	0.00013	0.00016	0.00005	0.00020	2.14473
A13	1.90131	0.00000	0.00008	-0.00001	0.00007	1.90138
A14	2.22713	0.00019	-0.00042	0.00121	0.00079	2.22791
A15	2.15402	-0.00019	0.00032	-0.00130	-0.00099	2.15303
A16	1.96308	-0.00047	0.00081	-0.00151	-0.00070	1.96237
A17	1.86653	0.00010	0.00024	-0.00023	0.00000	1.86653
A18	1.87138	0.00019	-0.00022	0.00081	0.00059	1.87197
A19	1.88430	0.00034	-0.00042	0.00164	0.00122	1.88552
A20	1.96493	-0.00001	-0.00043	0.00011	-0.00032	1.96461
A21	1.91093	-0.00015	0.00007	-0.00088	-0.00081	1.91011
A22	1.93109	-0.00034	0.00063	-0.00107	-0.00044	1.93065
A23	1.88587	0.00097	0.00068	0.00201	0.00269	1.88856
A24	1.92830	-0.00026	-0.00055	0.00009	-0.00045	1.92785
A25	1.89741	-0.00020	0.00011	-0.00121	-0.00110	1.89632
A26	1.87729	0.00024	0.00041	-0.00043	-0.00002	1.87727
A27	1.94407	-0.00043	-0.00127	0.00053	-0.00073	1.94334
A28	1.75439	-0.00065	-0.00238	-0.00766	-0.01004	1.74435
A29	2.18010	-0.00047	0.00056	-0.00202	-0.00146	2.17865
A30	1.95694	0.00020	-0.00022	-0.00002	-0.00024	1.95670
A31	2.14615	0.00028	-0.00034	0.00204	0.00170	2.14784
A32	2.07874	0.00006	-0.00007	0.00083	0.00075	2.07950
A33	2.15792	0.00001	-0.00014	-0.00026	-0.00040	2.15752
A34	2.04653	-0.00007	0.00021	-0.00057	-0.00035	2.04617
A35	1.85339	0.00005	0.00063	-0.00051	0.00012	1.85351
D1	0.00444	-0.00003	0.00010	-0.00014	-0.00003	0.00440
D2	-3.13475	-0.00008	0.00106	-0.00084	0.00022	-3.13453
D3	3.12864	0.00018	-0.00178	0.00405	0.00227	3.13091
D4	-0.01055	0.00013	-0.00082	0.00335	0.00252	-0.00803
D5	-0.00816	0.00012	0.00001	0.00085	0.00086	-0.00730
D6	-3.10954	0.00013	0.00065	0.00366	0.00432	-3.10522
D7	-3.13418	-0.00006	0.00170	-0.00288	-0.00119	-3.13537
D8	0.04763	-0.00006	0.00234	-0.00007	0.00227	0.04990
D9	0.00072	-0.00008	-0.00018	-0.00061	-0.00079	-0.00007
D10	-3.13900	-0.00006	-0.00059	-0.00336	-0.00395	3.14023
D11	3.14014	-0.00003	-0.00105	0.00002	-0.00103	3.13912
D12	0.00042	-0.00002	-0.00145	-0.00273	-0.00418	-0.00376
D13	-0.00581	0.00015	0.00019	0.00115	0.00134	-0.00447
D14	3.12920	0.00000	-0.00099	-0.00117	-0.00216	3.12705
D15	3.13404	0.00014	0.00057	0.00370	0.00427	3.13831
D16	-0.01413	-0.00001	-0.00061	0.00138	0.00077	-0.01335
D17	0.00313	0.00003	-0.00854	0.00126	-0.00729	-0.00416
D18	-3.13756	0.00002	-0.00867	0.00087	-0.00781	3.13782
D19	-3.13636	0.00004	-0.00900	-0.00184	-0.01084	3.13599

D20	0.00615	0.00003	-0.00913	-0.00223	-0.01136	-0.00522
D21	0.00862	-0.00017	-0.00013	-0.00124	-0.00136	0.00726
D22	3.11204	-0.00017	-0.00075	-0.00384	-0.00459	3.10745
D23	-3.12688	-0.00003	0.00097	0.00092	0.00188	-3.12499
D24	-0.02345	-0.00002	0.00034	-0.00169	-0.00135	-0.02480
D25	1.80524	-0.00028	-0.00235	-0.01417	-0.01652	1.78873
D26	-2.41225	-0.00006	-0.00226	-0.01317	-0.01543	-2.42768
D27	-0.36396	-0.00009	-0.00217	-0.01390	-0.01607	-0.38003
D28	-1.29077	-0.00028	-0.00161	-0.01102	-0.01263	-1.30340
D29	0.77492	-0.00006	-0.00152	-0.01002	-0.01154	0.76338
D30	2.82321	-0.00009	-0.00144	-0.01075	-0.01219	2.81103
D31	-1.59804	0.00004	-0.00139	0.00450	0.00311	-1.59493
D32	0.47728	0.00019	-0.00049	0.00364	0.00316	0.48044
D33	2.60808	0.00012	-0.00195	0.00566	0.00371	2.61179
D34	2.62994	-0.00004	-0.00188	0.00462	0.00274	2.63267
D35	-1.57792	0.00012	-0.00097	0.00376	0.00279	-1.57513
D36	0.55288	0.00005	-0.00244	0.00577	0.00334	0.55621
D37	0.51853	-0.00007	-0.00140	0.00453	0.00313	0.52166
D38	2.59386	0.00008	-0.00049	0.00367	0.00318	2.59704
D39	-1.55853	0.00001	-0.00196	0.00569	0.00373	-1.55480
D40	1.17266	0.00018	-0.00195	-0.00474	-0.00669	1.16597
D41	-3.01392	0.00022	-0.00074	-0.00555	-0.00629	-3.02021
D42	-0.94841	0.00014	-0.00093	-0.00652	-0.00744	-0.95585
D43	-1.30259	-0.00045	-0.00175	0.00340	0.00165	-1.30094
D44	2.87117	-0.00003	-0.00245	0.00492	0.00247	2.87364
D45	0.79361	0.00031	-0.00211	0.00635	0.00425	0.79786
D46	-3.14033	0.00000	-0.00082	-0.00060	-0.00143	3.14143
D47	0.00071	0.00001	-0.00088	-0.00016	-0.00104	-0.00033
D48	0.00025	0.00000	-0.00068	-0.00017	-0.00085	-0.00060
D49	3.14129	0.00002	-0.00074	0.00027	-0.00047	3.14083

Item	Value	Threshold	Converged?
Maximum Force	0.000970	0.000450	NO
RMS Force	0.000208	0.000300	YES
Maximum Displacement	0.037225	0.001800	NO
RMS Displacement	0.010444	0.001200	NO

Predicted change in Energy=-1.429041D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.607088	-2.382285	-1.117489

2	6	0	-1.907674	-2.012887	-1.245000
3	7	0	-2.087728	-0.899558	-0.430988
4	6	0	-0.917047	-0.611027	0.170161
5	7	0	-0.010688	-1.502947	-0.230275
6	6	0	1.404862	-1.470939	0.195543
7	6	0	2.210882	-0.348220	-0.511215
8	1	0	-0.063298	-3.194634	-1.567843
9	1	0	-2.700705	-2.440132	-1.830786
10	1	0	1.409962	-1.267211	1.265598
11	1	0	1.820019	-2.462359	0.012923
12	1	0	2.672509	-0.724497	-1.428073
13	1	0	1.516747	0.458320	-0.773745
14	35	0	0.725880	1.475421	2.143185
15	1	0	-0.681722	0.210399	0.872342
16	6	0	-3.269416	-0.138155	-0.215449
17	6	0	-4.441267	-0.379674	-0.788238
18	1	0	-3.108316	0.676309	0.479376
19	1	0	-5.281880	0.259784	-0.557501
20	1	0	-4.612191	-1.190732	-1.484489
21	8	0	3.239551	0.114633	0.321063
22	1	0	2.808958	0.663511	1.008052

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.358028	0.000000			
3	N	2.205007	1.390876	0.000000		
4	C	2.211667	2.224688	1.347266	0.000000	
5	N	1.384224	2.210942	2.172202	1.333176	0.000000
6	C	2.569542	3.652639	3.594051	2.476157	1.478556
7	C	3.527881	4.502451	4.334565	3.212052	2.519463
8	H	1.076307	2.214154	3.264679	3.228710	2.157234
9	H	2.212549	1.074515	2.169918	3.245128	3.267437
10	H	3.315266	4.226802	3.904794	2.654342	2.076404
11	H	2.678636	3.959810	4.232008	3.308124	2.081131
12	H	3.687882	4.761464	4.866691	3.930920	3.039778
13	H	3.563406	4.249188	3.866982	2.820959	2.544599
14	Br	5.224049	5.530253	4.492581	3.308368	3.878985
15	H	3.269099	3.305918	2.215294	1.105973	2.145135
16	C	3.596913	2.535534	1.422173	2.430215	3.533013
17	C	4.338178	3.048788	2.436607	3.659533	4.604682
18	H	4.261586	3.412739	2.086557	2.560178	3.853318
19	H	5.398870	4.125888	3.400395	4.509942	5.567744
20	H	4.194680	2.836847	2.750920	4.089990	4.779578

21	O	4.806315	5.785570	5.474858	4.222163	3.672138
22	H	5.046203	5.872476	5.337748	4.026117	3.765289

		6	7	8	9	10
6	C	0.000000				
7	C	1.552313	0.000000			
8	H	2.869869	3.793472	0.000000		
9	H	4.679853	5.499187	2.755781	0.000000	
10	H	1.089288	2.154781	3.730126	5.278345	0.000000
11	H	1.090238	2.212934	2.565527	4.882285	1.779247
12	H	2.190944	1.093304	3.688597	5.654822	3.023976
13	H	2.161962	1.096016	4.058473	5.225443	2.673534
14	Br	3.596577	3.546369	6.016971	6.547174	2.959757
15	H	2.763835	3.254756	4.234524	4.290514	2.590970
16	C	4.877920	5.492291	4.631438	2.869119	5.036353
17	C	6.027927	6.657989	5.262926	2.891703	6.264412
18	H	5.005998	5.506795	5.333614	3.900667	4.980990
19	H	6.948021	7.517532	6.339353	3.946298	7.101842
20	H	6.253475	6.943444	4.971418	2.309697	6.620813
21	O	2.428143	1.401813	5.042621	6.814978	2.479725
22	H	2.680958	1.920798	5.456223	6.931666	2.398168

		11	12	13	14	15
11	H	0.000000				
12	H	2.413166	0.000000			
13	H	3.039931	1.778479	0.000000		
14	Br	4.608825	4.624164	3.188801	0.000000	
15	H	3.760445	4.173344	2.757595	2.279620	0.000000
16	C	5.599681	6.092678	4.855392	4.912145	2.828593
17	C	6.647040	7.150811	6.016674	6.223666	4.152095
18	H	5.861511	6.246483	4.796774	4.255337	2.501970
19	H	7.627085	8.062196	6.804962	6.698109	4.817505
20	H	6.725519	7.299822	6.386580	6.983079	4.792328
21	O	2.958193	2.021177	2.069971	3.389752	3.960992
22	H	3.426273	2.807115	2.210592	2.507377	3.522581

		16	17	18	19	20
16	C	0.000000				
17	C	1.326520	0.000000			
18	H	1.082630	2.121015	0.000000		
19	H	2.079752	1.081100	2.443970	0.000000	
20	H	2.126365	1.082495	3.099072	1.847102	0.000000
21	O	6.535931	7.776236	6.374634	8.567832	8.161731
22	H	6.251900	7.541927	5.940858	8.250795	8.045150

		21	22
21	O	0.000000	
22	H	0.979097	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.871651	-1.990572	0.344526
2	6	0	-2.864200	-1.093023	0.113248
3	7	0	-2.257027	0.153454	0.002920
4	6	0	-0.928227	0.001748	0.165403
5	7	0	-0.678161	-1.290235	0.378958
6	6	0	0.684222	-1.835721	0.559193
7	6	0	1.472761	-1.913167	-0.775679
8	1	0	-1.913029	-3.055035	0.498290
9	1	0	-3.925598	-1.233641	0.022455
10	1	0	1.213462	-1.154610	1.224430
11	1	0	0.582078	-2.808001	1.041746
12	1	0	1.329916	-2.887200	-1.251251
13	1	0	1.088288	-1.136020	-1.446106
14	35	0	2.036748	1.469034	0.129510
15	1	0	-0.132849	0.769382	0.129520
16	6	0	-2.861204	1.417770	-0.240083
17	6	0	-4.161564	1.615446	-0.412253
18	1	0	-2.132946	2.218262	-0.270743
19	1	0	-4.522441	2.618610	-0.591718
20	1	0	-4.897285	0.821898	-0.384093
21	8	0	2.845934	-1.753171	-0.543562
22	1	0	2.982242	-0.801895	-0.356145

Rotational constants (GHZ): 0.9823818 0.4448870 0.3181115
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 358 symmetry adapted cartesian basis functions of A symmetry.
There are 345 symmetry adapted basis functions of A symmetry.
345 basis functions, 553 primitive gaussians, 358 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 851.1627138175 Hartrees.
NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.

Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 345 RedAO= T EigKep= 4.71D-06 NBF= 345
NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345
Initial guess from the checkpoint file: "."
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 0.000532 -0.000251 0.000156 Ang= 0.07 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.34324493 A.U. after 11 cycles
NFock= 11 Conv=0.18D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000054710	-0.000150183	0.000195878
2	6	-0.000047021	0.000217258	-0.000101299
3	7	-0.000395082	0.000130210	-0.000334980
4	6	0.000106282	-0.000232587	0.000457596
5	7	0.000138883	0.000039107	-0.000315584
6	6	0.000669911	0.000054989	0.000126543
7	6	-0.000740958	-0.000375739	0.000295077
8	1	0.000016544	0.000081219	-0.000198051
9	1	-0.000006469	-0.000110135	0.000006107
10	1	-0.000082226	0.000041514	0.000011080

11	1	0.000090874	-0.000047515	0.000070275
12	1	-0.000051390	-0.000026182	-0.000026121
13	1	0.000107914	0.000428075	-0.000316493
14	35	0.000071819	0.000043470	-0.000084980
15	1	0.000064108	0.000066757	0.000060281
16	6	0.000076108	0.000015540	0.000123344
17	6	0.000200573	-0.000081393	0.000065340
18	1	-0.000043143	0.000012537	-0.000073618
19	1	-0.000010545	0.000013055	-0.000040316
20	1	-0.000048652	-0.000012636	-0.000004363
21	8	0.000023311	-0.000173981	-0.000109476
22	1	-0.000086132	0.000066620	0.000193759

Cartesian Forces: Max 0.000740958 RMS 0.000199753

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000756874 RMS 0.000148338
Search for a local minimum.
Step number 66 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 61 62 63 64 65
66
DE= -1.67D-05 DEPred=-1.43D-05 R= 1.17D+00
TightC=F SS= 1.41D+00 RLast= 5.08D-02 DXNew= 1.6377D+00 1.5246D-01
Trust test= 1.17D+00 RLast= 5.08D-02 DXMaxT set to 9.74D-01
ITU= 1 1 1 1 0 1 1 1 1 0 1 1 0 1 1 0 -1 1 1 1
ITU= -1 1 0 -1 1 0 -1 0 -1 0 0 1 -1 0 1 1 1 1 1 1
ITU= 0 -1 1 1 1 1 1 0 -1 1 1 1 1 1 1 1 1 1 1 1
ITU= 1 0 0 -1 0 0

Eigenvalues ---	0.00146	0.00227	0.00382	0.00597	0.01044
Eigenvalues ---	0.01335	0.01608	0.01854	0.02154	0.02227
Eigenvalues ---	0.02522	0.03032	0.03189	0.03747	0.04114
Eigenvalues ---	0.04334	0.05009	0.05418	0.05830	0.08614
Eigenvalues ---	0.08879	0.09680	0.13292	0.13864	0.14575
Eigenvalues ---	0.15019	0.15525	0.15973	0.16059	0.16541
Eigenvalues ---	0.17563	0.19473	0.20248	0.22776	0.23291
Eigenvalues ---	0.23821	0.25325	0.27317	0.29847	0.32701
Eigenvalues ---	0.33764	0.33855	0.33953	0.34132	0.34307
Eigenvalues ---	0.34747	0.34844	0.36059	0.36324	0.36410

Eigenvalues --- 0.42017 0.43038 0.43730 0.45794 0.48886

Eigenvalues --- 0.54091 0.55334 0.57896 0.60870 0.73792

En-DIIS/RFO-DIIS IScMMF= 0 using points: 66 65 64 63

RFO step: Lambda=-6.14033699D-06.

DidBck=F Rises=F RFO-DIIS coefs: 1.65000 -0.45369 -0.29679 0.10048

Iteration 1 RMS(Cart)= 0.01902275 RMS(Int)= 0.00013651

Iteration 2 RMS(Cart)= 0.00021170 RMS(Int)= 0.00000646

Iteration 3 RMS(Cart)= 0.00000002 RMS(Int)= 0.00000646

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56630	0.00010	0.00009	0.00014	0.00022	2.56652
R2	2.61580	0.00008	0.00011	-0.00005	0.00005	2.61586
R3	2.03393	0.00003	0.00001	0.00005	0.00006	2.03398
R4	2.62837	0.00000	0.00014	-0.00014	-0.00001	2.62837
R5	2.03054	0.00004	0.00005	0.00001	0.00007	2.03060
R6	2.54596	0.00029	-0.00047	0.00030	-0.00016	2.54580
R7	2.68752	-0.00016	0.00058	-0.00045	0.00013	2.68765
R8	2.51934	0.00005	-0.00005	-0.00002	-0.00006	2.51927
R9	2.08999	0.00010	0.00117	0.00047	0.00164	2.09163
R10	2.79407	0.00005	0.00009	-0.00021	-0.00012	2.79395
R11	2.93345	-0.00036	0.00011	-0.00095	-0.00084	2.93260
R12	2.05846	0.00002	-0.00028	-0.00008	-0.00036	2.05810
R13	2.06025	0.00007	0.00011	0.00010	0.00021	2.06046
R14	2.06605	0.00001	-0.00005	0.00027	0.00022	2.06626
R15	2.07117	0.00033	-0.00022	0.00029	0.00007	2.07124
R16	2.64904	-0.00003	0.00045	0.00055	0.00100	2.65004
R17	6.02596	-0.00008	0.01992	-0.00563	0.01429	6.04025
R18	2.50676	-0.00012	-0.00034	-0.00001	-0.00035	2.50641
R19	2.04587	-0.00004	0.00011	-0.00035	-0.00024	2.04563
R20	2.04298	0.00001	0.00001	-0.00007	-0.00006	2.04293
R21	2.04562	0.00002	0.00005	-0.00016	-0.00011	2.04551
R22	1.85022	0.00021	0.00037	-0.00008	0.00029	1.85051
A1	1.87551	0.00002	-0.00005	-0.00009	-0.00014	1.87537
A2	2.27822	-0.00007	-0.00044	-0.00020	-0.00064	2.27759
A3	2.12936	0.00005	0.00050	0.00033	0.00083	2.13019
A4	1.86164	0.00004	-0.00015	0.00024	0.00009	1.86172
A5	2.27818	-0.00009	-0.00061	-0.00041	-0.00103	2.27716
A6	2.14336	0.00005	0.00076	0.00017	0.00094	2.14430
A7	1.89661	-0.00005	0.00016	-0.00027	-0.00010	1.89650
A8	2.24568	-0.00001	0.00057	0.00031	0.00087	2.24655
A9	2.14090	0.00006	-0.00073	-0.00004	-0.00077	2.14013
A10	1.88961	0.00000	0.00005	0.00014	0.00019	1.88980
A11	2.24880	0.00004	-0.00007	-0.00048	-0.00059	2.24822
A12	2.14473	-0.00004	-0.00001	0.00026	0.00022	2.14495

A13	1.90138	-0.00001	-0.00001	-0.00002	-0.00002	1.90136
A14	2.22791	0.00024	0.00075	0.00142	0.00216	2.23007
A15	2.15303	-0.00023	-0.00084	-0.00166	-0.00252	2.15051
A16	1.96237	-0.00039	-0.00049	-0.00125	-0.00174	1.96063
A17	1.86653	0.00002	0.00003	-0.00083	-0.00080	1.86573
A18	1.87197	0.00022	0.00040	0.00155	0.00195	1.87392
A19	1.88552	0.00023	0.00129	0.00016	0.00145	1.88697
A20	1.96461	-0.00003	-0.00027	0.00058	0.00031	1.96492
A21	1.91011	-0.00006	-0.00099	-0.00029	-0.00128	1.90883
A22	1.93065	-0.00023	-0.00063	0.00017	-0.00046	1.93019
A23	1.88856	0.00076	0.00180	0.00172	0.00352	1.89208
A24	1.92785	-0.00033	-0.00035	-0.00141	-0.00176	1.92609
A25	1.89632	-0.00025	-0.00054	-0.00053	-0.00108	1.89524
A26	1.87727	0.00019	-0.00021	0.00085	0.00063	1.87790
A27	1.94334	-0.00015	-0.00011	-0.00081	-0.00092	1.94242
A28	1.74435	0.00015	-0.00529	0.00264	-0.00265	1.74169
A29	2.17865	-0.00019	-0.00043	-0.00036	-0.00079	2.17785
A30	1.95670	0.00015	-0.00083	0.00040	-0.00043	1.95627
A31	2.14784	0.00004	0.00126	-0.00004	0.00122	2.14906
A32	2.07950	0.00000	0.00033	0.00023	0.00056	2.08006
A33	2.15752	0.00004	0.00009	-0.00010	-0.00001	2.15751
A34	2.04617	-0.00005	-0.00041	-0.00014	-0.00055	2.04562
A35	1.85351	0.00003	-0.00038	0.00072	0.00034	1.85385
D1	0.00440	-0.00003	-0.00011	-0.00015	-0.00026	0.00414
D2	-3.13453	-0.00003	0.00078	0.00093	0.00170	-3.13283
D3	3.13091	0.00011	0.00139	0.00326	0.00465	3.13556
D4	-0.00803	0.00011	0.00228	0.00433	0.00661	-0.00142
D5	-0.00730	0.00007	0.00088	0.00007	0.00095	-0.00635
D6	-3.10522	0.00008	0.00341	0.00653	0.00996	-3.09526
D7	-3.13537	-0.00005	-0.00046	-0.00297	-0.00344	-3.13881
D8	0.04990	-0.00005	0.00208	0.00348	0.00557	0.05547
D9	-0.00007	-0.00003	-0.00068	0.00018	-0.00051	-0.00058
D10	3.14023	-0.00001	-0.00243	-0.00030	-0.00273	3.13751
D11	3.13912	-0.00003	-0.00149	-0.00080	-0.00229	3.13683
D12	-0.00376	-0.00001	-0.00323	-0.00127	-0.00451	-0.00827
D13	-0.00447	0.00008	0.00124	-0.00013	0.00110	-0.00337
D14	3.12705	-0.00001	-0.00243	-0.00883	-0.01124	3.11580
D15	3.13831	0.00006	0.00285	0.00031	0.00316	3.14147
D16	-0.01335	-0.00003	-0.00081	-0.00839	-0.00919	-0.02254
D17	-0.00416	0.00002	-0.01235	0.00367	-0.00867	-0.01283
D18	3.13782	0.00005	-0.01227	0.00505	-0.00722	3.13060
D19	3.13599	0.00005	-0.01431	0.00314	-0.01117	3.12481
D20	-0.00522	0.00008	-0.01424	0.00452	-0.00972	-0.01494
D21	0.00726	-0.00009	-0.00131	0.00004	-0.00127	0.00599

D22	3.10745	-0.00008	-0.00367	-0.00599	-0.00964	3.09781
D23	-3.12499	-0.00002	0.00209	0.00811	0.01020	-3.11480
D24	-0.02480	0.00000	-0.00027	0.00208	0.00182	-0.02298
D25	1.78873	-0.00020	-0.01455	-0.01889	-0.03344	1.75528
D26	-2.42768	-0.00012	-0.01323	-0.01994	-0.03317	-2.46085
D27	-0.38003	-0.00007	-0.01417	-0.01991	-0.03408	-0.41411
D28	-1.30340	-0.00021	-0.01170	-0.01163	-0.02334	-1.32674
D29	0.76338	-0.00013	-0.01038	-0.01268	-0.02306	0.74032
D30	2.81103	-0.00007	-0.01132	-0.01265	-0.02397	2.78705
D31	-1.59493	-0.00006	0.00203	-0.00323	-0.00120	-1.59613
D32	0.48044	-0.00004	0.00211	-0.00273	-0.00062	0.47982
D33	2.61179	0.00006	0.00293	-0.00349	-0.00057	2.61122
D34	2.63267	-0.00001	0.00146	-0.00158	-0.00011	2.63256
D35	-1.57513	0.00001	0.00154	-0.00108	0.00046	-1.57467
D36	0.55621	0.00011	0.00235	-0.00184	0.00051	0.55673
D37	0.52166	-0.00008	0.00199	-0.00169	0.00030	0.52197
D38	2.59704	-0.00005	0.00207	-0.00119	0.00088	2.59792
D39	-1.55480	0.00005	0.00288	-0.00195	0.00093	-1.55387
D40	1.16597	0.00016	-0.00432	0.00341	-0.00090	1.16507
D41	-3.02021	0.00019	-0.00434	0.00431	-0.00003	-3.02024
D42	-0.95585	0.00017	-0.00501	0.00453	-0.00047	-0.95632
D43	-1.30094	-0.00029	0.00206	-0.00530	-0.00324	-1.30418
D44	2.87364	0.00007	0.00317	-0.00520	-0.00203	2.87161
D45	0.79786	0.00034	0.00403	-0.00461	-0.00058	0.79728
D46	3.14143	0.00005	-0.00105	0.00123	0.00018	-3.14158
D47	-0.00033	0.00003	-0.00127	0.00096	-0.00032	-0.00065
D48	-0.00060	0.00002	-0.00113	-0.00030	-0.00143	-0.00203
D49	3.14083	0.00000	-0.00136	-0.00057	-0.00192	3.13890

Item	Value	Threshold	Converged?
Maximum Force	0.000757	0.000450	NO
RMS Force	0.000148	0.000300	YES
Maximum Displacement	0.062319	0.001800	NO
RMS Displacement	0.019061	0.001200	NO

Predicted change in Energy=-1.564114D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.602610	-2.376043	-1.123414
2	6	0	-1.903215	-2.006455	-1.251417
3	7	0	-2.088737	-0.905828	-0.421523

4	6	0	-0.921501	-0.625314	0.189840
5	7	0	-0.011658	-1.509137	-0.220417
6	6	0	1.403605	-1.471637	0.205688
7	6	0	2.207708	-0.358136	-0.516689
8	1	0	-0.055201	-3.178670	-1.586704
9	1	0	-2.692630	-2.427580	-1.846509
10	1	0	1.407267	-1.253952	1.272805
11	1	0	1.820470	-2.465078	0.037867
12	1	0	2.670102	-0.747251	-1.427922
13	1	0	1.515282	0.445648	-0.792027
14	35	0	0.723017	1.501581	2.118996
15	1	0	-0.688568	0.192170	0.898753
16	6	0	-3.271229	-0.146815	-0.201566
17	6	0	-4.436595	-0.373241	-0.793017
18	1	0	-3.115341	0.651827	0.512354
19	1	0	-5.279165	0.262012	-0.557983
20	1	0	-4.600572	-1.167774	-1.509605
21	8	0	3.235545	0.116404	0.310913
22	1	0	2.804378	0.676392	0.988731

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.358143	0.000000			
3	N	2.205166	1.390871	0.000000		
4	C	2.211647	2.224531	1.347180	0.000000	
5	N	1.384253	2.210944	2.172253	1.333143	0.000000
6	C	2.570869	3.652978	3.593047	2.474395	1.478493
7	C	3.512542	4.489595	4.332257	3.219086	2.517571
8	H	1.076338	2.213969	3.264770	3.228965	2.157771
9	H	2.212171	1.074549	2.170484	3.245271	3.267312
10	H	3.322734	4.230514	3.900510	2.644080	2.075615
11	H	2.688460	3.967167	4.233697	3.305485	2.082600
12	H	3.668288	4.746786	4.866675	3.941019	3.038153
13	H	3.543618	4.232018	3.866874	2.837065	2.545481
14	Br	5.225560	5.528389	4.489522	3.309042	3.882914
15	H	3.269904	3.306441	2.215672	1.106840	2.145972
16	C	3.597331	2.536122	1.422241	2.429688	3.532858
17	C	4.338182	3.048858	2.436000	3.658612	4.604151
18	H	4.261168	3.412712	2.086224	2.558914	3.852216
19	H	5.399001	4.125995	3.400192	4.509526	5.567545
20	H	4.194372	2.836509	2.749883	4.088758	4.778773
21	O	4.795938	5.775314	5.470776	4.224432	3.670016
22	H	5.038461	5.863221	5.332429	4.026765	3.764124

		6	7	8	9	10
6	C	0.000000				
7	C	1.551868	0.000000			
8	H	2.873108	3.771087	0.000000		
9	H	4.680223	5.483094	2.754572	0.000000	
10	H	1.089099	2.155338	3.744348	5.283624	0.000000
11	H	1.090351	2.212846	2.581973	4.890843	1.778380
12	H	2.190304	1.093419	3.655720	5.635389	3.024140
13	H	2.164230	1.096054	4.029096	5.203258	2.676535
14	Br	3.600551	3.551012	6.020181	6.544477	2.962633
15	H	2.761482	3.270280	4.235708	4.291366	2.573657
16	C	4.875970	5.492059	4.631802	2.870976	5.028703
17	C	6.025930	6.650064	5.262793	2.893367	6.260511
18	H	5.002401	5.514871	5.333218	3.902008	4.966313
19	H	6.946089	7.512626	6.339272	3.947705	7.096359
20	H	6.251777	6.927775	4.970920	2.311030	6.621432
21	O	2.426715	1.402342	5.028665	6.802174	2.479054
22	H	2.681295	1.921602	5.447161	6.920283	2.399759

		11	12	13	14	15
11	H	0.000000				
12	H	2.412746	0.000000			
13	H	3.042070	1.777915	0.000000		
14	Br	4.611928	4.629148	3.196362	0.000000	
15	H	3.754646	4.192445	2.789256	2.279500	0.000000
16	C	5.599738	6.096219	4.859048	4.904714	2.827676
17	C	6.649588	7.144798	6.007947	6.214207	4.150841
18	H	5.856831	6.260467	4.815246	4.246925	2.499963
19	H	7.628687	8.060165	6.800957	6.687969	4.816693
20	H	6.731081	7.283283	6.365668	6.973722	4.790972
21	O	2.956525	2.022171	2.069827	3.391264	3.968622
22	H	3.426521	2.808025	2.210455	2.508086	3.527497

		16	17	18	19	20
16	C	0.000000				
17	C	1.326334	0.000000			
18	H	1.082503	2.121431	0.000000		
19	H	2.079899	1.081070	2.445344	0.000000	
20	H	2.126141	1.082436	3.099222	1.846716	0.000000
21	O	6.532230	7.766605	6.376599	8.560167	8.146663
22	H	6.245596	7.530475	5.938907	8.240613	8.029689

		21	22
21	O	0.000000	
22	H	0.979249	0.000000

Stoichiometry C7H11BrN2O

Framework group C1[X(C7H11BrN2O)]

Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.871063	-1.993738	0.324368
2	6	0	-2.861643	-1.093770	0.093370
3	7	0	-2.255192	0.155396	0.013844
4	6	0	-0.928932	0.002998	0.194685
5	7	0	-0.679524	-1.292141	0.388799
6	6	0	0.683331	-1.836397	0.568668
7	6	0	1.466287	-1.919892	-0.768606
8	1	0	-1.913132	-3.061256	0.455289
9	1	0	-3.921367	-1.235312	-0.014377
10	1	0	1.213166	-1.151376	1.229091
11	1	0	0.584672	-2.806105	1.057337
12	1	0	1.322621	-2.896931	-1.237989
13	1	0	1.080824	-1.147644	-1.444168
14	35	0	2.036131	1.470233	0.121348
15	1	0	-0.133155	0.772048	0.174778
16	6	0	-2.856496	1.422973	-0.219507
17	6	0	-4.152564	1.620015	-0.420864
18	1	0	-2.129469	2.224994	-0.217004
19	1	0	-4.512850	2.625164	-0.589918
20	1	0	-4.885851	0.823826	-0.427394
21	8	0	2.840331	-1.757156	-0.540393
22	1	0	2.976779	-0.804221	-0.360876

Rotational constants (GHZ): 0.9797785 0.4460499 0.3183400
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 358 symmetry adapted cartesian basis functions of A symmetry.
There are 345 symmetry adapted basis functions of A symmetry.
345 basis functions, 553 primitive gaussians, 358 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 851.1855958746 Hartrees.
NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.
NBasis= 345 RedAO= T EigKep= 4.67D-06 NBF= 345
NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345
Initial guess from the checkpoint file: "."
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 0.000178 -0.000052 0.000377 Ang= 0.05 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.34326659 A.U. after 11 cycles
NFock= 11 Conv=0.53D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000004574	0.000021203	-0.000015389
2	6	0.000040808	0.000109942	-0.000096593
3	7	-0.000364638	0.000137818	-0.000223749
4	6	0.000155654	0.000079795	0.000718431
5	7	0.000016593	0.000073029	-0.000081289
6	6	0.000384658	-0.000068878	-0.000093513
7	6	-0.000197142	-0.000185376	0.000529671
8	1	0.000020198	0.000013348	-0.000042243
9	1	-0.000045336	-0.000023130	0.000024568
10	1	-0.000019385	0.000154989	0.000032090
11	1	0.000013957	-0.000003249	-0.000031596
12	1	0.000049452	0.000009188	0.000062994

13	1	-0.000111021	0.000201406	-0.000180239
14	35	0.000056739	-0.000006042	-0.000135208
15	1	0.000007400	-0.000224954	-0.000295128
16	6	0.000218521	-0.000177218	0.000048040
17	6	-0.000040208	-0.000058911	0.000048136
18	1	-0.000102132	0.000107409	-0.000051065
19	1	-0.000002684	0.000060961	-0.000011758
20	1	-0.000023095	-0.000061198	-0.000023270
21	8	0.000024210	-0.000065715	-0.000284832
22	1	-0.000077976	-0.000094417	0.000101942

Cartesian Forces: Max 0.000718431 RMS 0.000165918

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000355412 RMS 0.000096191
Search for a local minimum.
Step number 67 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 62 63 64 65 66
67
DE= -2.17D-05 DEPred=-1.56D-05 R= 1.38D+00
TightC=F SS= 1.41D+00 RLast= 7.96D-02 DXNew= 1.6377D+00 2.3882D-01
Trust test= 1.38D+00 RLast= 7.96D-02 DXMaxT set to 9.74D-01
ITU= 1 1 1 1 1 0 1 1 1 1 0 1 1 0 1 1 0 -1 1 1
ITU= 1 -1 1 0 -1 1 0 -1 0 -1 0 0 1 -1 0 1 1 1 1 1
ITU= 1 0 -1 1 1 1 1 1 0 -1 1 1 1 1 1 1 1 1 1 1
ITU= 1 1 0 0 -1 0 0

Eigenvalues ---	0.00138	0.00239	0.00307	0.00528	0.01038
Eigenvalues ---	0.01366	0.01605	0.01853	0.02125	0.02295
Eigenvalues ---	0.02539	0.03034	0.03182	0.03778	0.04125
Eigenvalues ---	0.04364	0.04922	0.05332	0.05775	0.08588
Eigenvalues ---	0.08949	0.09743	0.13199	0.14011	0.14745
Eigenvalues ---	0.15049	0.15498	0.16007	0.16055	0.16838
Eigenvalues ---	0.17475	0.20244	0.20432	0.22719	0.23240
Eigenvalues ---	0.23640	0.25103	0.27567	0.29697	0.32788
Eigenvalues ---	0.33763	0.33845	0.33954	0.34154	0.34353
Eigenvalues ---	0.34707	0.34850	0.35737	0.36319	0.36442
Eigenvalues ---	0.42481	0.43352	0.43701	0.46051	0.48913
Eigenvalues ---	0.53933	0.54917	0.57528	0.61030	0.71289

En-DIIS/RFO-DIIS IScMMF= 0 using points: 67 66 65 64 63

RFO step: Lambda=-2.90895087D-06.

DidBck=F Rises=F RFO-DIIS coefs: 1.81556 -0.81446 -0.12670 -0.01736 0.14296

Iteration 1 RMS(Cart)= 0.01935867 RMS(Int)= 0.00013096

Iteration 2 RMS(Cart)= 0.00019041 RMS(Int)= 0.00000992

Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00000992

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56652	0.00003	0.00031	-0.00019	0.00012	2.56664
R2	2.61586	0.00003	0.00003	-0.00006	-0.00003	2.61583
R3	2.03398	0.00002	0.00007	-0.00001	0.00006	2.03405
R4	2.62837	-0.00002	-0.00021	-0.00001	-0.00023	2.62813
R5	2.03060	0.00003	0.00015	-0.00007	0.00007	2.03068
R6	2.54580	0.00036	0.00029	0.00004	0.00034	2.54614
R7	2.68765	-0.00011	0.00018	-0.00007	0.00012	2.68776
R8	2.51927	0.00009	0.00019	-0.00015	0.00005	2.51933
R9	2.09163	-0.00035	0.00134	-0.00066	0.00067	2.09230
R10	2.79395	0.00012	0.00031	0.00005	0.00036	2.79430
R11	2.93260	-0.00029	-0.00126	0.00017	-0.00109	2.93151
R12	2.05810	0.00006	-0.00014	-0.00010	-0.00024	2.05786
R13	2.06046	0.00001	0.00020	-0.00001	0.00019	2.06066
R14	2.06626	-0.00004	0.00021	-0.00005	0.00016	2.06642
R15	2.07124	0.00026	0.00025	0.00008	0.00033	2.07157
R16	2.65004	-0.00020	0.00023	-0.00024	-0.00002	2.65003
R17	6.04025	-0.00014	-0.00107	0.01061	0.00954	6.04979
R18	2.50641	0.00006	-0.00036	0.00021	-0.00015	2.50626
R19	2.04563	0.00003	-0.00018	0.00006	-0.00012	2.04551
R20	2.04293	0.00004	0.00005	-0.00004	0.00001	2.04294
R21	2.04551	0.00006	0.00003	0.00001	0.00004	2.04555
R22	1.85051	0.00005	0.00043	-0.00001	0.00041	1.85092
A1	1.87537	0.00006	-0.00009	0.00003	-0.00007	1.87530
A2	2.27759	-0.00003	-0.00063	0.00004	-0.00061	2.27698
A3	2.13019	-0.00003	0.00079	-0.00006	0.00071	2.13090
A4	1.86172	0.00006	0.00020	-0.00006	0.00014	1.86187
A5	2.27716	-0.00001	-0.00079	0.00003	-0.00076	2.27640
A6	2.14430	-0.00005	0.00058	0.00003	0.00061	2.14491
A7	1.89650	-0.00006	-0.00015	0.00007	-0.00007	1.89643
A8	2.24655	-0.00015	-0.00006	-0.00012	-0.00019	2.24636
A9	2.14013	0.00021	0.00021	0.00005	0.00025	2.14038
A10	1.88980	-0.00003	0.00009	-0.00013	-0.00005	1.88975
A11	2.24822	0.00008	-0.00038	-0.00009	-0.00052	2.24770
A12	2.14495	-0.00005	0.00013	0.00007	0.00015	2.14510
A13	1.90136	-0.00001	-0.00005	0.00010	0.00005	1.90141

A14	2.23007	-0.00004	0.00198	-0.00053	0.00141	2.23148
A15	2.15051	0.00005	-0.00222	0.00022	-0.00203	2.14849
A16	1.96063	-0.00005	-0.00225	0.00067	-0.00158	1.95905
A17	1.86573	-0.00001	-0.00093	0.00021	-0.00072	1.86501
A18	1.87392	0.00006	0.00181	-0.00038	0.00144	1.87536
A19	1.88697	0.00001	0.00118	-0.00015	0.00103	1.88800
A20	1.96492	-0.00006	0.00078	-0.00021	0.00057	1.96549
A21	1.90883	0.00005	-0.00069	-0.00014	-0.00083	1.90800
A22	1.93019	-0.00006	-0.00073	0.00012	-0.00061	1.92958
A23	1.89208	0.00022	0.00210	-0.00016	0.00194	1.89402
A24	1.92609	-0.00008	-0.00080	0.00085	0.00005	1.92614
A25	1.89524	-0.00011	-0.00115	-0.00002	-0.00117	1.89407
A26	1.87790	-0.00002	0.00026	-0.00105	-0.00079	1.87711
A27	1.94242	0.00004	0.00026	0.00025	0.00051	1.94293
A28	1.74169	0.00011	-0.00077	-0.00444	-0.00522	1.73648
A29	2.17785	-0.00007	-0.00172	0.00079	-0.00093	2.17692
A30	1.95627	0.00017	0.00051	0.00001	0.00052	1.95679
A31	2.14906	-0.00010	0.00121	-0.00080	0.00041	2.14947
A32	2.08006	-0.00004	0.00069	-0.00014	0.00055	2.08060
A33	2.15751	0.00003	-0.00018	0.00013	-0.00005	2.15746
A34	2.04562	0.00001	-0.00050	0.00001	-0.00050	2.04512
A35	1.85385	-0.00008	0.00002	-0.00068	-0.00065	1.85320
D1	0.00414	-0.00001	-0.00024	0.00004	-0.00020	0.00394
D2	-3.13283	0.00000	-0.00033	0.00055	0.00022	-3.13261
D3	3.13556	0.00002	0.00577	0.00041	0.00618	-3.14145
D4	-0.00142	0.00003	0.00568	0.00092	0.00660	0.00518
D5	-0.00635	0.00003	0.00047	0.00033	0.00080	-0.00555
D6	-3.09526	0.00002	0.00687	0.00483	0.01173	-3.08353
D7	-3.13881	0.00000	-0.00491	-0.00001	-0.00493	3.13945
D8	0.05547	-0.00001	0.00149	0.00450	0.00601	0.06148
D9	-0.00058	-0.00002	-0.00006	-0.00038	-0.00045	-0.00103
D10	3.13751	0.00000	-0.00173	-0.00032	-0.00205	3.13546
D11	3.13683	-0.00002	0.00001	-0.00084	-0.00084	3.13599
D12	-0.00827	-0.00001	-0.00166	-0.00078	-0.00243	-0.01070
D13	-0.00337	0.00003	0.00036	0.00059	0.00095	-0.00242
D14	3.11580	-0.00004	-0.00717	-0.00760	-0.01476	3.10104
D15	3.14147	0.00002	0.00190	0.00053	0.00243	-3.13928
D16	-0.02254	-0.00006	-0.00564	-0.00765	-0.01328	-0.03582
D17	-0.01283	0.00005	0.00905	0.00913	0.01818	0.00535
D18	3.13060	0.00008	0.00999	0.00891	0.01890	-3.13368
D19	3.12481	0.00007	0.00718	0.00920	0.01638	3.14120
D20	-0.01494	0.00010	0.00812	0.00898	0.01711	0.00217
D21	0.00599	-0.00004	-0.00051	-0.00057	-0.00108	0.00491
D22	3.09781	-0.00003	-0.00643	-0.00486	-0.01127	3.08654

D23	-3.11480	0.00003	0.00649	0.00703	0.01352	-3.10128
D24	-0.02298	0.00003	0.00057	0.00274	0.00333	-0.01965
D25	1.75528	-0.00010	-0.02127	-0.01859	-0.03986	1.71542
D26	-2.46085	-0.00012	-0.02170	-0.01826	-0.03995	-2.50080
D27	-0.41411	-0.00003	-0.02206	-0.01850	-0.04056	-0.45467
D28	-1.32674	-0.00011	-0.01411	-0.01348	-0.02759	-1.35433
D29	0.74032	-0.00013	-0.01453	-0.01315	-0.02768	0.71264
D30	2.78705	-0.00004	-0.01490	-0.01339	-0.02829	2.75877
D31	-1.59613	-0.00005	0.00050	-0.00283	-0.00233	-1.59846
D32	0.47982	-0.00008	-0.00004	-0.00288	-0.00292	0.47690
D33	2.61122	0.00006	0.00114	-0.00214	-0.00100	2.61022
D34	2.63256	-0.00002	0.00220	-0.00338	-0.00118	2.63138
D35	-1.57467	-0.00005	0.00167	-0.00343	-0.00177	-1.57644
D36	0.55673	0.00009	0.00285	-0.00269	0.00016	0.55688
D37	0.52197	-0.00005	0.00178	-0.00298	-0.00120	0.52077
D38	2.59792	-0.00009	0.00124	-0.00303	-0.00179	2.59613
D39	-1.55387	0.00006	0.00243	-0.00229	0.00014	-1.55373
D40	1.16507	0.00011	0.00131	-0.00063	0.00068	1.16575
D41	-3.02024	0.00011	0.00099	-0.00059	0.00040	-3.01984
D42	-0.95632	0.00004	0.00075	-0.00174	-0.00099	-0.95731
D43	-1.30418	-0.00004	-0.00169	0.00556	0.00387	-1.30031
D44	2.87161	0.00009	-0.00049	0.00556	0.00508	2.87669
D45	0.79728	0.00021	0.00060	0.00609	0.00669	0.80397
D46	-3.14158	0.00006	0.00113	0.00095	0.00208	-3.13950
D47	-0.00065	0.00004	0.00123	0.00080	0.00203	0.00138
D48	-0.00203	0.00003	0.00009	0.00119	0.00128	-0.00074
D49	3.13890	0.00000	0.00019	0.00104	0.00123	3.14013

Item	Value	Threshold	Converged?
Maximum Force	0.000355	0.000450	YES
RMS Force	0.000096	0.000300	YES
Maximum Displacement	0.056608	0.001800	NO
RMS Displacement	0.019383	0.001200	NO

Predicted change in Energy=-1.094945D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.596796	-2.362780	-1.134529
2	6	0	-1.896483	-1.990942	-1.265960
3	7	0	-2.089121	-0.906359	-0.416988
4	6	0	-0.926945	-0.637626	0.209510

5	7	0	-0.013358	-1.512900	-0.210727
6	6	0	1.401027	-1.472708	0.218691
7	6	0	2.207612	-0.371748	-0.518744
8	1	0	-0.044720	-3.153474	-1.612638
9	1	0	-2.680580	-2.401569	-1.875319
10	1	0	1.401602	-1.239277	1.282352
11	1	0	1.817016	-2.469343	0.067823
12	1	0	2.672690	-0.776403	-1.421907
13	1	0	1.517779	0.428561	-0.810904
14	35	0	0.724227	1.526666	2.089694
15	1	0	-0.697083	0.174272	0.926356
16	6	0	-3.273231	-0.150595	-0.194166
17	6	0	-4.437471	-0.377912	-0.787316
18	1	0	-3.119439	0.646025	0.522364
19	1	0	-5.281768	0.255073	-0.552337
20	1	0	-4.599184	-1.171322	-1.505695
21	8	0	3.233936	0.114733	0.303772
22	1	0	2.800640	0.682751	0.973822

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.358207	0.000000			
3	N	2.205235	1.390749	0.000000		
4	C	2.211695	2.224518	1.347357	0.000000	
5	N	1.384235	2.210928	2.172379	1.333171	0.000000
6	C	2.571912	3.653263	3.592489	2.473237	1.478682
7	C	3.494009	4.474787	4.331060	3.229008	2.515911
8	H	1.076370	2.213751	3.264764	3.229247	2.158200
9	H	2.211884	1.074589	2.170761	3.245496	3.267212
10	H	3.331240	4.235122	3.896632	2.633458	2.075153
11	H	2.698795	3.974660	4.235076	3.302209	2.083900
12	H	3.645369	4.730409	4.868429	3.954510	3.037143
13	H	3.516780	4.209306	3.866124	2.855639	2.544379
14	Br	5.221926	5.522871	4.485309	3.308417	3.882644
15	H	3.270159	3.306503	2.215876	1.107197	2.146390
16	C	3.597409	2.535952	1.422303	2.430064	3.533118
17	C	4.337170	3.047554	2.435394	3.658539	4.603632
18	H	4.261682	3.412817	2.086584	2.559818	3.853066
19	H	5.398247	4.124802	3.400035	4.510189	5.567636
20	H	4.192428	2.834403	2.748800	4.088044	4.777387
21	O	4.783439	5.763604	5.467821	4.229404	3.668626
22	H	5.026228	5.850489	5.326292	4.027711	3.760667

	6	7	8	9	10

6	C	0.000000				
7	C	1.551291	0.000000			
8	H	2.875574	3.742673	0.000000		
9	H	4.680511	5.463963	2.753565	0.000000	
10	H	1.088974	2.155506	3.759915	5.290181	0.000000
11	H	1.090453	2.212810	2.599624	4.899874	1.777839
12	H	2.189413	1.093502	3.615406	5.612864	3.023728
13	H	2.165299	1.096230	3.989380	5.173861	2.678974
14	Br	3.599299	3.550825	6.016831	6.537972	2.959912
15	H	2.759602	3.289940	4.236268	4.291690	2.555256
16	C	4.875154	5.494897	4.631698	2.871306	5.021891
17	C	6.024840	6.650511	5.261289	2.892336	6.254618
18	H	5.001586	5.522430	5.333697	3.902475	4.956990
19	H	6.945464	7.515640	6.337910	3.946417	7.089894
20	H	6.250351	6.924295	4.968250	2.308933	6.617194
21	O	2.426266	1.402334	5.010329	6.786878	2.479599
22	H	2.678645	1.921303	5.431618	6.904665	2.397226

		11	12	13	14	15
11	H	0.000000				
12	H	2.411953	0.000000			
13	H	3.042950	1.777380	0.000000		
14	Br	4.609798	4.629468	3.201411	0.000000	
15	H	3.747863	4.215863	2.826368	2.280887	0.000000
16	C	5.599629	6.103520	4.865138	4.899887	2.828011
17	C	6.650109	7.149538	6.009656	6.208682	4.151154
18	H	5.854973	6.273137	4.829978	4.243326	2.500713
19	H	7.628878	8.068054	6.806673	6.683506	4.817924
20	H	6.732640	7.283072	6.360786	6.967401	4.790813
21	O	2.956482	2.021655	2.070311	3.388467	3.980461
22	H	3.424039	2.808028	2.212598	2.503768	3.534809

		16	17	18	19	20
16	C	0.000000				
17	C	1.326256	0.000000			
18	H	1.082438	2.121537	0.000000		
19	H	2.080162	1.081075	2.446118	0.000000	
20	H	2.126063	1.082460	3.099262	1.846461	0.000000
21	O	6.531582	7.764255	6.379296	8.559780	8.141615
22	H	6.241039	7.524418	5.937381	8.236345	8.021408

		21	22
21	O	0.000000	
22	H	0.979467	0.000000

Stoichiometry C7H11BrN2O

Framework group C1[X(C7H11BrN2O)]

Deg. of freedom 60

Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.864903	-1.998052	0.297348
2	6	0	-2.855127	-1.098443	0.063075
3	7	0	-2.253640	0.154736	0.019055
4	6	0	-0.930453	0.005217	0.224460
5	7	0	-0.678429	-1.292274	0.398662
6	6	0	0.685799	-1.832334	0.582283
7	6	0	1.465922	-1.924481	-0.755410
8	1	0	-1.904248	-3.068556	0.402456
9	1	0	-3.911732	-1.243586	-0.068305
10	1	0	1.213963	-1.140335	1.236533
11	1	0	0.590972	-2.798049	1.079766
12	1	0	1.325002	-2.906553	-1.215216
13	1	0	1.076618	-1.160879	-1.438838
14	35	0	2.032898	1.471964	0.111225
15	1	0	-0.136732	0.777154	0.222536
16	6	0	-2.856523	1.423287	-0.205123
17	6	0	-4.151974	1.618197	-0.411938
18	1	0	-2.131728	2.227120	-0.191174
19	1	0	-4.514800	2.623410	-0.575121
20	1	0	-4.882880	0.819941	-0.428721
21	8	0	2.839932	-1.755615	-0.531536
22	1	0	2.972700	-0.801065	-0.356712

Rotational constants (GHZ): 0.9796352 0.4470822 0.3186092
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 358 symmetry adapted cartesian basis functions of A symmetry.
There are 345 symmetry adapted basis functions of A symmetry.
345 basis functions, 553 primitive gaussians, 358 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 851.4371875211 Hartrees.
NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 4.64D-06 NBF= 345
NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345
Initial guess from the checkpoint file: "."
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 0.000305 -0.000048 -0.000446 Ang= 0.06 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.34328503 A.U. after 11 cycles
NFock= 11 Conv=0.51D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000067189	0.000147677	-0.000232074
2	6	0.000125165	-0.000068654	-0.000056039
3	7	-0.000294589	0.000221557	-0.000003140
4	6	0.000067989	0.000294135	0.000657074
5	7	0.000026654	0.000208812	0.000237511
6	6	0.000091174	-0.000301768	-0.000176170
7	6	0.000183687	-0.000102994	0.000186846
8	1	0.000017533	-0.000068794	0.000118481
9	1	-0.000040444	0.000065798	0.000013205
10	1	-0.000010749	0.000175772	0.000024417
11	1	-0.000030310	0.000026270	-0.000097029
12	1	0.000050070	0.000011920	0.000058245
13	1	-0.000167871	0.000082464	0.000009289

14	35	0.000014910	0.000007129	-0.000083244
15	1	-0.000050910	-0.000424620	-0.000538360
16	6	0.000265525	-0.000319505	-0.000003740
17	6	-0.000198566	-0.000031520	-0.000003633
18	1	-0.000074629	0.000120693	-0.000022828
19	1	0.000019789	0.000075432	0.000026357
20	1	-0.000003719	-0.000051043	-0.000016269
21	8	-0.000089331	0.000003589	-0.000112839
22	1	0.000031435	-0.000072349	0.000013941

Cartesian Forces: Max 0.000657074 RMS 0.000171104

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000671015 RMS 0.000104006
Search for a local minimum.
Step number 68 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 62 63 64 65 66
67 68
DE= -1.84D-05 DEPred=-1.09D-05 R= 1.68D+00
TightC=F SS= 1.41D+00 RLast= 9.84D-02 DXNew= 1.6377D+00 2.9529D-01
Trust test= 1.68D+00 RLast= 9.84D-02 DXMaxT set to 9.74D-01
ITU= 1 1 1 1 1 1 0 1 1 1 1 0 1 1 0 1 1 0 -1 1
ITU= 1 1 -1 1 0 -1 1 0 -1 0 -1 0 0 1 -1 0 1 1 1 1
ITU= 1 1 0 -1 1 1 1 1 1 0 -1 1 1 1 1 1 1 1 1 1
ITU= 1 1 1 0 0 -1 0 0
Eigenvalues --- 0.00132 0.00205 0.00255 0.00492 0.01026
Eigenvalues --- 0.01331 0.01494 0.01863 0.02144 0.02365
Eigenvalues --- 0.02527 0.03026 0.03179 0.03850 0.04109
Eigenvalues --- 0.04378 0.04839 0.05377 0.05744 0.08608
Eigenvalues --- 0.09090 0.09758 0.13178 0.14140 0.14671
Eigenvalues --- 0.15139 0.15525 0.16012 0.16103 0.16749
Eigenvalues --- 0.17743 0.20241 0.21497 0.23306 0.23355
Eigenvalues --- 0.24693 0.25211 0.27475 0.29472 0.32752
Eigenvalues --- 0.33767 0.33870 0.33959 0.34174 0.34422
Eigenvalues --- 0.34566 0.34851 0.35983 0.36319 0.36460
Eigenvalues --- 0.42669 0.43513 0.44886 0.45804 0.49134
Eigenvalues --- 0.53688 0.54903 0.57494 0.61190 0.76286
En-DIIS/RFO-DIIS IScMMF= 0 using points: 68 67 66 65 64

RFO step: Lambda=-2.30236536D-06.

DidBck=F Rises=F RFO-DIIS coefs: 1.75081 -0.95036 -0.25311 0.39094 0.06172

Iteration 1 RMS(Cart)= 0.01615719 RMS(Int)= 0.00008025

Iteration 2 RMS(Cart)= 0.00011405 RMS(Int)= 0.00000292

Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00000292

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56664	-0.00002	-0.00002	0.00001	-0.00001	2.56663
R2	2.61583	-0.00001	-0.00007	0.00007	0.00000	2.61583
R3	2.03405	0.00001	0.00003	0.00001	0.00004	2.03409
R4	2.62813	0.00003	-0.00023	0.00021	-0.00002	2.62812
R5	2.03068	0.00000	0.00001	0.00002	0.00003	2.03071
R6	2.54614	0.00022	0.00055	-0.00006	0.00049	2.54663
R7	2.68776	-0.00012	-0.00033	-0.00011	-0.00044	2.68732
R8	2.51933	0.00008	0.00008	0.00009	0.00018	2.51950
R9	2.09230	-0.00067	-0.00058	-0.00063	-0.00121	2.09109
R10	2.79430	0.00002	0.00035	-0.00021	0.00014	2.79445
R11	2.93151	-0.00009	-0.00076	0.00028	-0.00048	2.93104
R12	2.05786	0.00006	0.00006	-0.00010	-0.00004	2.05782
R13	2.06066	-0.00002	0.00003	0.00003	0.00006	2.06072
R14	2.06642	-0.00003	0.00008	-0.00008	0.00000	2.06642
R15	2.07157	0.00018	0.00039	-0.00002	0.00037	2.07194
R16	2.65003	-0.00012	-0.00053	0.00023	-0.00030	2.64973
R17	6.04979	-0.00007	-0.00889	0.00087	-0.00802	6.04177
R18	2.50626	0.00016	0.00015	0.00000	0.00015	2.50641
R19	2.04551	0.00006	-0.00013	0.00029	0.00016	2.04567
R20	2.04294	0.00003	0.00000	0.00006	0.00006	2.04300
R21	2.04555	0.00005	0.00002	0.00012	0.00013	2.04569
R22	1.85092	-0.00004	0.00010	0.00003	0.00013	1.85105
A1	1.87530	0.00005	0.00002	-0.00001	0.00001	1.87531
A2	2.27698	0.00003	-0.00013	0.00016	0.00004	2.27702
A3	2.13090	-0.00008	0.00011	-0.00016	-0.00005	2.13085
A4	1.86187	0.00005	0.00018	0.00002	0.00019	1.86206
A5	2.27640	0.00005	-0.00012	0.00020	0.00008	2.27648
A6	2.14491	-0.00010	-0.00005	-0.00022	-0.00027	2.14464
A7	1.89643	-0.00008	-0.00014	-0.00005	-0.00019	1.89624
A8	2.24636	-0.00010	-0.00056	0.00008	-0.00047	2.24589
A9	2.14038	0.00018	0.00069	-0.00003	0.00066	2.14104
A10	1.88975	0.00000	-0.00008	0.00006	-0.00002	1.88973
A11	2.24770	0.00006	-0.00019	-0.00033	-0.00053	2.24717
A12	2.14510	-0.00006	0.00000	0.00013	0.00013	2.14522
A13	1.90141	-0.00002	0.00002	-0.00002	0.00000	1.90142
A14	2.23148	-0.00032	0.00025	-0.00108	-0.00083	2.23065

A15	2.14849	0.00034	-0.00055	0.00099	0.00044	2.14893
A16	1.95905	0.00015	-0.00064	-0.00003	-0.00067	1.95839
A17	1.86501	-0.00004	-0.00043	-0.00008	-0.00051	1.86450
A18	1.87536	-0.00005	0.00045	-0.00004	0.00042	1.87577
A19	1.88800	-0.00009	-0.00018	0.00003	-0.00015	1.88785
A20	1.96549	-0.00007	0.00060	-0.00003	0.00057	1.96606
A21	1.90800	0.00010	0.00016	0.00015	0.00031	1.90831
A22	1.92958	0.00001	-0.00015	-0.00017	-0.00032	1.92926
A23	1.89402	-0.00003	-0.00059	0.00029	-0.00031	1.89372
A24	1.92614	0.00000	0.00070	-0.00039	0.00032	1.92646
A25	1.89407	-0.00001	-0.00024	0.00018	-0.00006	1.89401
A26	1.87711	-0.00005	-0.00070	0.00031	-0.00039	1.87671
A27	1.94293	0.00007	0.00097	-0.00021	0.00076	1.94369
A28	1.73648	0.00017	0.00110	0.00031	0.00142	1.73790
A29	2.17692	0.00012	-0.00016	0.00026	0.00011	2.17703
A30	1.95679	0.00005	0.00086	-0.00033	0.00053	1.95732
A31	2.14947	-0.00017	-0.00071	0.00007	-0.00064	2.14883
A32	2.08060	-0.00009	0.00003	-0.00041	-0.00039	2.08022
A33	2.15746	0.00003	0.00004	0.00019	0.00024	2.15769
A34	2.04512	0.00005	-0.00007	0.00022	0.00015	2.04527
A35	1.85320	0.00004	-0.00055	0.00070	0.00015	1.85335
D1	0.00394	0.00000	-0.00007	0.00015	0.00008	0.00402
D2	-3.13261	0.00002	-0.00068	-0.00012	-0.00079	-3.13341
D3	-3.14145	-0.00007	0.00300	-0.00175	0.00125	-3.14020
D4	0.00518	-0.00005	0.00240	-0.00202	0.00038	0.00556
D5	-0.00555	-0.00002	-0.00009	-0.00041	-0.00051	-0.00606
D6	-3.08353	-0.00004	0.00454	0.00140	0.00593	-3.07760
D7	3.13945	0.00005	-0.00286	0.00129	-0.00156	3.13789
D8	0.06148	0.00002	0.00178	0.00310	0.00487	0.06635
D9	-0.00103	0.00002	0.00021	0.00016	0.00037	-0.00066
D10	3.13546	0.00003	0.00084	0.00010	0.00094	3.13640
D11	3.13599	0.00000	0.00076	0.00041	0.00116	3.13716
D12	-0.01070	0.00001	0.00139	0.00034	0.00173	-0.00897
D13	-0.00242	-0.00003	-0.00027	-0.00042	-0.00069	-0.00311
D14	3.10104	-0.00006	-0.00733	-0.00449	-0.01183	3.08922
D15	-3.13928	-0.00004	-0.00086	-0.00036	-0.00122	-3.14050
D16	-0.03582	-0.00007	-0.00792	-0.00443	-0.01235	-0.04817
D17	0.00535	0.00005	0.02279	0.00724	0.03003	0.03538
D18	-3.13368	0.00007	0.02315	0.00698	0.03014	-3.10355
D19	3.14120	0.00006	0.02350	0.00717	0.03067	-3.11132
D20	0.00217	0.00008	0.02386	0.00691	0.03077	0.03294
D21	0.00491	0.00003	0.00023	0.00052	0.00074	0.00565
D22	3.08654	0.00003	-0.00409	-0.00128	-0.00538	3.08116
D23	-3.10128	0.00005	0.00679	0.00431	0.01110	-3.09018

D24	-0.01965	0.00005	0.00248	0.00251	0.00498	-0.01467
D25	1.71542	-0.00002	-0.01403	-0.00782	-0.02185	1.69357
D26	-2.50080	-0.00007	-0.01488	-0.00785	-0.02273	-2.52353
D27	-0.45467	0.00000	-0.01469	-0.00773	-0.02242	-0.47709
D28	-1.35433	-0.00003	-0.00883	-0.00573	-0.01456	-1.36889
D29	0.71264	-0.00008	-0.00968	-0.00576	-0.01544	0.69720
D30	2.75877	-0.00001	-0.00949	-0.00564	-0.01513	2.74363
D31	-1.59846	-0.00003	-0.00270	-0.00052	-0.00321	-1.60167
D32	0.47690	-0.00005	-0.00344	-0.00022	-0.00366	0.47324
D33	2.61022	0.00002	-0.00218	-0.00055	-0.00273	2.60749
D34	2.63138	-0.00001	-0.00168	-0.00042	-0.00210	2.62928
D35	-1.57644	-0.00003	-0.00243	-0.00013	-0.00255	-1.57899
D36	0.55688	0.00004	-0.00117	-0.00045	-0.00162	0.55527
D37	0.52077	-0.00003	-0.00213	-0.00061	-0.00274	0.51803
D38	2.59613	-0.00005	-0.00288	-0.00032	-0.00320	2.59294
D39	-1.55373	0.00002	-0.00162	-0.00064	-0.00226	-1.55599
D40	1.16575	0.00004	0.00403	-0.00055	0.00348	1.16923
D41	-3.01984	0.00004	0.00336	-0.00048	0.00288	-3.01696
D42	-0.95731	0.00001	0.00293	-0.00012	0.00281	-0.95451
D43	-1.30031	0.00003	0.00274	-0.00390	-0.00117	-1.30147
D44	2.87669	0.00004	0.00294	-0.00366	-0.00072	2.87596
D45	0.80397	0.00004	0.00310	-0.00394	-0.00084	0.80313
D46	-3.13950	0.00005	0.00235	0.00004	0.00239	-3.13711
D47	0.00138	0.00003	0.00241	0.00040	0.00281	0.00419
D48	-0.00074	0.00002	0.00195	0.00033	0.00228	0.00154
D49	3.14013	0.00000	0.00201	0.00069	0.00270	-3.14035

Item	Value	Threshold	Converged?
Maximum Force	0.000671	0.000450	NO
RMS Force	0.000104	0.000300	YES
Maximum Displacement	0.050586	0.001800	NO
RMS Displacement	0.016157	0.001200	NO

Predicted change in Energy=-5.104380D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.592570	-2.350480	-1.145635
2	6	0	-1.891031	-1.975779	-1.280963
3	7	0	-2.088601	-0.901777	-0.419779
4	6	0	-0.930021	-0.641702	0.217503
5	7	0	-0.014536	-1.512924	-0.207293

6	6	0	1.398759	-1.475844	0.226235
7	6	0	2.210896	-0.382068	-0.515255
8	1	0	-0.037716	-3.134977	-1.630738
9	1	0	-2.671312	-2.377455	-1.901117
10	1	0	1.396503	-1.235582	1.288348
11	1	0	1.811551	-2.474952	0.082892
12	1	0	2.679457	-0.794582	-1.413047
13	1	0	1.523570	0.417100	-0.817017
14	35	0	0.723714	1.546940	2.064921
15	1	0	-0.702018	0.166811	0.937773
16	6	0	-3.274047	-0.149069	-0.195199
17	6	0	-4.442911	-0.389447	-0.774113
18	1	0	-3.117841	0.657640	0.509553
19	1	0	-5.287195	0.244088	-0.540421
20	1	0	-4.608576	-1.194224	-1.478926
21	8	0	3.234539	0.108342	0.308004
22	1	0	2.799734	0.683062	0.971427

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.358203	0.000000			
3	N	2.205384	1.390739	0.000000		
4	C	2.211773	2.224568	1.347618	0.000000	
5	N	1.384236	2.210936	2.172648	1.333264	0.000000
6	C	2.571460	3.652985	3.592850	2.473679	1.478758
7	C	3.483022	4.466769	4.331846	3.235693	2.515198
8	H	1.076394	2.213788	3.264925	3.229338	2.158192
9	H	2.211933	1.074604	2.170608	3.245533	3.267249
10	H	3.335218	4.237585	3.895520	2.629090	2.074823
11	H	2.702696	3.977233	4.235416	3.300780	2.084298
12	H	3.632972	4.722502	4.871596	3.963634	3.037672
13	H	3.499363	4.195309	3.865879	2.865555	2.542150
14	Br	5.218252	5.517371	4.480967	3.307257	3.882104
15	H	3.269452	3.305636	2.215274	1.106556	2.146000
16	C	3.597201	2.535446	1.422071	2.430528	3.533363
17	C	4.336912	3.047202	2.435325	3.658870	4.603693
18	H	4.262092	3.412610	2.086809	2.561276	3.854311
19	H	5.397923	4.124336	3.399788	4.510436	5.567674
20	H	4.192412	2.834621	2.749108	4.088389	4.777429
21	O	4.775524	5.756721	5.466793	4.232531	3.667495
22	H	5.019169	5.843456	5.323814	4.029203	3.759236

		6	7	8	9	10
6	C	0.000000				

7	C	1.551039	0.000000			
8	H	2.874810	3.725462	0.000000		
9	H	4.680172	5.453268	2.753684	0.000000	
10	H	1.088951	2.155158	3.766397	5.293740	0.000000
11	H	1.090487	2.213012	2.606137	4.903250	1.778041
12	H	2.188961	1.093502	3.592752	5.601288	3.022910
13	H	2.164992	1.096424	3.964468	5.155759	2.679564
14	Br	3.601899	3.548252	6.013154	6.531197	2.966165
15	H	2.760048	3.301155	4.235605	4.290769	2.548215
16	C	4.875762	5.499211	4.631442	2.870392	5.019507
17	C	6.025451	6.658845	5.260940	2.891518	6.250475
18	H	5.003169	5.525094	5.334038	3.901605	4.956824
19	H	6.946071	7.524232	6.337500	3.945482	7.085593
20	H	6.250997	6.934945	4.968132	2.308955	6.612147
21	O	2.426194	1.402177	4.998549	6.777792	2.479029
22	H	2.679351	1.921317	5.422160	6.895696	2.398060

		11	12	13	14	15
11	H	0.000000				
12	H	2.411377	0.000000			
13	H	3.042488	1.777498	0.000000		
14	Br	4.613832	4.626436	3.197166	0.000000	
15	H	3.745366	4.229066	2.845202	2.282090	0.000000
16	C	5.599140	6.110977	4.870763	4.895578	2.828204
17	C	6.648465	7.162436	6.020902	6.205137	4.151416
18	H	5.856115	6.278057	4.833254	4.238817	2.502096
19	H	7.627181	8.081327	6.818575	6.679540	4.818181
20	H	6.730348	7.299279	6.374772	6.964636	4.791038
21	O	2.957867	2.021238	2.070849	3.385345	3.987042
22	H	3.426231	2.807778	2.213111	2.500374	3.539762

		16	17	18	19	20
16	C	0.000000				
17	C	1.326336	0.000000			
18	H	1.082523	2.121320	0.000000		
19	H	2.080028	1.081108	2.445315	0.000000	
20	H	2.126329	1.082531	3.099313	1.846634	0.000000
21	O	6.533082	7.769299	6.379269	8.564940	8.148880
22	H	6.240535	7.526825	5.935627	8.238738	8.025678

		21	22
21	O	0.000000	
22	H	0.979535	0.000000

Stoichiometry C7H11BrN2O

Framework group C1[X(C7H11BrN2O)]

Deg. of freedom 60

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.858603	-2.002610	0.273173
2	6	0	-2.848881	-1.103939	0.035569
3	7	0	-2.252210	0.152159	0.016733
4	6	0	-0.931330	0.005123	0.239738
5	7	0	-0.676713	-1.293557	0.401585
6	6	0	0.687306	-1.832000	0.591997
7	6	0	1.472145	-1.925722	-0.742532
8	1	0	-1.894917	-3.074644	0.362882
9	1	0	-3.902697	-1.251499	-0.114332
10	1	0	1.211916	-1.137414	1.246327
11	1	0	0.591778	-2.796603	1.091573
12	1	0	1.336288	-2.909975	-1.199189
13	1	0	1.081656	-1.166006	-1.429916
14	35	0	2.028139	1.475107	0.103237
15	1	0	-0.140174	0.778714	0.249479
16	6	0	-2.857783	1.420598	-0.199211
17	6	0	-4.155796	1.615738	-0.389602
18	1	0	-2.133223	2.224864	-0.194241
19	1	0	-4.519882	2.620990	-0.549924
20	1	0	-4.887494	0.817953	-0.395086
21	8	0	2.844736	-1.751580	-0.515003
22	1	0	2.974097	-0.795825	-0.343871

Rotational constants (GHZ): 0.9798940 0.4478885 0.3186785
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 358 symmetry adapted cartesian basis functions of A symmetry.
There are 345 symmetry adapted basis functions of A symmetry.
345 basis functions, 553 primitive gaussians, 358 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 851.6200934857 Hartrees.
NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 345 RedAO= T EigKep= 4.65D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345
Initial guess from the checkpoint file: "."
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 0.000049 0.000084 -0.000823 Ang= 0.09 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.34329573 A.U. after 11 cycles
NFock= 11 Conv=0.47D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000026657	0.000106006	-0.000197493
2	6	0.000084587	-0.000175326	0.000019944
3	7	0.000010602	0.000155974	0.000025380
4	6	-0.000018145	0.000116781	0.000318069
5	7	-0.000024226	0.000242018	0.000215176
6	6	-0.000112650	-0.000225855	-0.000065234
7	6	0.000195950	-0.000031348	-0.000047048
8	1	0.000001231	-0.000068362	0.000126521
9	1	-0.000012855	0.000087777	-0.000019472
10	1	0.000021171	0.000084860	0.000002440
11	1	-0.000042937	0.000036650	-0.000063337
12	1	0.000043029	0.000010573	0.000026357
13	1	-0.000038282	0.000040402	0.000090034
14	35	0.000002186	0.000005984	-0.000024116

15	1	-0.000056904	-0.000272443	-0.000334438
16	6	0.000122120	-0.000164421	0.000016586
17	6	-0.000149102	-0.000015352	-0.000020639
18	1	-0.000034556	0.000041446	-0.000016264
19	1	0.000016282	0.000038309	0.000017650
20	1	0.000010490	-0.000011315	0.000011431
21	8	-0.000050492	0.000045157	-0.000048596
22	1	0.000005845	-0.000047516	-0.000032949

Cartesian Forces: Max 0.000334438 RMS 0.000108229

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000429184 RMS 0.000072562
Search for a local minimum.
Step number 69 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 62 63 64 65 66
67 68 69
DE= -1.07D-05 DEPred=-5.10D-06 R= 2.09D+00
TightC=F SS= 1.41D+00 RLast= 8.13D-02 DXNew= 1.6377D+00 2.4396D-01
Trust test= 2.09D+00 RLast= 8.13D-02 DXMaxT set to 9.74D-01
ITU= 1 1 1 1 1 1 1 0 1 1 1 1 0 1 1 0 1 1 0 -1
ITU= 1 1 1 -1 1 0 -1 1 0 -1 0 -1 0 0 1 -1 0 1 1 1
ITU= 1 1 1 0 -1 1 1 1 1 1 0 -1 1 1 1 1 1 1 1 1
ITU= 1 1 1 1 0 0 -1 0 0
Eigenvalues --- 0.00133 0.00174 0.00246 0.00496 0.01006
Eigenvalues --- 0.01331 0.01470 0.01870 0.02154 0.02309
Eigenvalues --- 0.02512 0.03023 0.03178 0.03761 0.04074
Eigenvalues --- 0.04352 0.04983 0.05462 0.05711 0.08601
Eigenvalues --- 0.09053 0.09758 0.13156 0.14103 0.14598
Eigenvalues --- 0.15110 0.15564 0.15987 0.16095 0.16554
Eigenvalues --- 0.17700 0.20225 0.21194 0.23127 0.23357
Eigenvalues --- 0.24230 0.25641 0.27265 0.29796 0.32792
Eigenvalues --- 0.33772 0.33874 0.33958 0.34216 0.34349
Eigenvalues --- 0.34615 0.34848 0.36297 0.36324 0.36479
Eigenvalues --- 0.39770 0.43111 0.43841 0.45705 0.49057
Eigenvalues --- 0.53774 0.55314 0.57951 0.61029 0.77612
En-DIIS/RFO-DIIS IScMMF= 0 using points: 69 68 67 66 65
RFO step: Lambda=-1.11565536D-06.

DidBck=F Rises=F RFO-DIIS coefs: 1.64358 -0.79629 -0.05276 0.28369 -0.07822

Iteration 1 RMS(Cart)= 0.00847819 RMS(Int)= 0.00003293

Iteration 2 RMS(Cart)= 0.00004746 RMS(Int)= 0.00000537

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000537

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56663	-0.00007	-0.00005	-0.00010	-0.00015	2.56649
R2	2.61583	0.00001	0.00000	0.00005	0.00005	2.61587
R3	2.03409	-0.00001	0.00001	-0.00003	-0.00002	2.03407
R4	2.62812	0.00004	0.00002	0.00007	0.00009	2.62821
R5	2.03071	-0.00001	0.00000	-0.00002	-0.00001	2.03069
R6	2.54663	0.00000	0.00027	-0.00018	0.00010	2.54672
R7	2.68732	-0.00003	-0.00026	-0.00006	-0.00032	2.68701
R8	2.51950	-0.00004	0.00012	-0.00024	-0.00012	2.51938
R9	2.09109	-0.00043	-0.00109	-0.00040	-0.00149	2.08960
R10	2.79445	-0.00002	0.00006	-0.00017	-0.00011	2.79434
R11	2.93104	0.00010	0.00003	0.00029	0.00032	2.93136
R12	2.05782	0.00002	0.00006	-0.00006	0.00000	2.05782
R13	2.06072	-0.00004	-0.00002	-0.00007	-0.00009	2.06064
R14	2.06642	-0.00001	-0.00007	0.00003	-0.00004	2.06638
R15	2.07194	0.00003	0.00015	-0.00008	0.00007	2.07202
R16	2.64973	-0.00008	-0.00036	0.00006	-0.00030	2.64943
R17	6.04177	-0.00002	-0.00781	-0.00047	-0.00828	6.03349
R18	2.50641	0.00010	0.00016	0.00001	0.00018	2.50659
R19	2.04567	0.00001	0.00019	-0.00014	0.00005	2.04572
R20	2.04300	0.00001	0.00006	-0.00002	0.00004	2.04304
R21	2.04569	0.00000	0.00011	-0.00012	0.00000	2.04568
R22	1.85105	-0.00005	-0.00001	-0.00007	-0.00008	1.85097
A1	1.87531	0.00002	0.00004	0.00002	0.00006	1.87537
A2	2.27702	0.00004	0.00022	0.00008	0.00031	2.27732
A3	2.13085	-0.00006	-0.00027	-0.00010	-0.00037	2.13049
A4	1.86206	-0.00001	0.00008	-0.00012	-0.00004	1.86202
A5	2.27648	0.00006	0.00035	0.00017	0.00052	2.27699
A6	2.14464	-0.00006	-0.00043	-0.00005	-0.00047	2.14417
A7	1.89624	-0.00001	-0.00007	0.00007	-0.00001	1.89623
A8	2.24589	-0.00004	-0.00045	0.00011	-0.00034	2.24555
A9	2.14104	0.00005	0.00053	-0.00017	0.00036	2.14140
A10	1.88973	0.00000	-0.00005	0.00002	-0.00002	1.88970
A11	2.24717	0.00001	-0.00016	-0.00009	-0.00022	2.24695
A12	2.14522	-0.00001	0.00003	0.00001	0.00006	2.14529
A13	1.90142	0.00000	0.00000	0.00001	0.00002	1.90143
A14	2.23065	-0.00030	-0.00113	-0.00047	-0.00158	2.22907
A15	2.14893	0.00031	0.00103	0.00044	0.00149	2.15042

A16	1.95839	0.00019	0.00011	0.00003	0.00014	1.95853
A17	1.86450	-0.00002	-0.00005	0.00019	0.00013	1.86463
A18	1.87577	-0.00009	-0.00031	-0.00009	-0.00039	1.87538
A19	1.88785	-0.00009	-0.00046	-0.00011	-0.00057	1.88729
A20	1.96606	-0.00005	0.00019	-0.00006	0.00013	1.96619
A21	1.90831	0.00007	0.00052	0.00006	0.00059	1.90890
A22	1.92926	0.00003	-0.00005	0.00042	0.00037	1.92963
A23	1.89372	-0.00005	-0.00101	0.00009	-0.00092	1.89280
A24	1.92646	0.00004	0.00052	-0.00025	0.00027	1.92673
A25	1.89401	0.00004	0.00027	0.00048	0.00075	1.89476
A26	1.87671	-0.00003	-0.00026	0.00011	-0.00015	1.87656
A27	1.94369	-0.00002	0.00054	-0.00083	-0.00029	1.94339
A28	1.73790	0.00005	0.00147	0.00070	0.00217	1.74007
A29	2.17703	0.00011	0.00026	0.00020	0.00046	2.17749
A30	1.95732	-0.00001	0.00033	-0.00005	0.00029	1.95760
A31	2.14883	-0.00010	-0.00059	-0.00016	-0.00075	2.14809
A32	2.08022	-0.00005	-0.00039	-0.00005	-0.00044	2.07978
A33	2.15769	0.00001	0.00013	-0.00001	0.00012	2.15781
A34	2.04527	0.00004	0.00026	0.00006	0.00032	2.04559
A35	1.85335	-0.00003	0.00013	-0.00044	-0.00031	1.85304
D1	0.00402	0.00000	0.00013	0.00006	0.00019	0.00421
D2	-3.13341	-0.00001	-0.00088	-0.00115	-0.00202	-3.13543
D3	-3.14020	-0.00006	-0.00092	-0.00040	-0.00132	-3.14152
D4	0.00556	-0.00007	-0.00192	-0.00161	-0.00354	0.00203
D5	-0.00606	0.00000	-0.00058	0.00047	-0.00010	-0.00616
D6	-3.07760	-0.00003	0.00031	0.00068	0.00098	-3.07662
D7	3.13789	0.00005	0.00036	0.00089	0.00126	3.13914
D8	0.06635	0.00002	0.00125	0.00110	0.00234	0.06869
D9	-0.00066	0.00000	0.00035	-0.00057	-0.00022	-0.00088
D10	3.13640	0.00002	0.00117	0.00092	0.00208	3.13848
D11	3.13716	0.00001	0.00127	0.00052	0.00179	3.13895
D12	-0.00897	0.00003	0.00209	0.00201	0.00409	-0.00488
D13	-0.00311	-0.00001	-0.00071	0.00087	0.00016	-0.00295
D14	3.08922	-0.00003	-0.00322	-0.00056	-0.00379	3.08543
D15	-3.14050	-0.00002	-0.00147	-0.00051	-0.00198	3.14071
D16	-0.04817	-0.00004	-0.00397	-0.00194	-0.00592	-0.05409
D17	0.03538	0.00001	0.01776	-0.00118	0.01658	0.05196
D18	-3.10355	0.00002	0.01738	-0.00081	0.01657	-3.08697
D19	-3.11132	0.00003	0.01868	0.00049	0.01917	-3.09214
D20	0.03294	0.00004	0.01830	0.00087	0.01917	0.05211
D21	0.00565	0.00001	0.00080	-0.00083	-0.00004	0.00562
D22	3.08116	0.00001	-0.00012	-0.00108	-0.00121	3.07995
D23	-3.09018	0.00002	0.00313	0.00050	0.00364	-3.08654
D24	-0.01467	0.00003	0.00221	0.00026	0.00246	-0.01220

D25	1.69357	0.00001	-0.00239	-0.00319	-0.00558	1.68799
D26	-2.52353	-0.00001	-0.00292	-0.00319	-0.00611	-2.52964
D27	-0.47709	0.00001	-0.00249	-0.00307	-0.00556	-0.48265
D28	-1.36889	-0.00001	-0.00135	-0.00293	-0.00427	-1.37316
D29	0.69720	-0.00003	-0.00187	-0.00293	-0.00480	0.69240
D30	2.74363	-0.00001	-0.00144	-0.00281	-0.00425	2.73938
D31	-1.60167	0.00001	-0.00122	0.00060	-0.00062	-1.60230
D32	0.47324	0.00004	-0.00154	0.00149	-0.00005	0.47319
D33	2.60749	0.00001	-0.00120	0.00036	-0.00084	2.60666
D34	2.62928	-0.00002	-0.00094	0.00043	-0.00051	2.62878
D35	-1.57899	0.00001	-0.00125	0.00132	0.00007	-1.57893
D36	0.55527	-0.00002	-0.00091	0.00019	-0.00072	0.55454
D37	0.51803	-0.00001	-0.00140	0.00046	-0.00094	0.51709
D38	2.59294	0.00002	-0.00172	0.00135	-0.00037	2.59257
D39	-1.55599	-0.00001	-0.00137	0.00022	-0.00115	-1.55715
D40	1.16923	0.00000	0.00180	-0.00160	0.00020	1.16943
D41	-3.01696	0.00002	0.00131	-0.00076	0.00055	-3.01641
D42	-0.95451	-0.00001	0.00147	-0.00082	0.00066	-0.95385
D43	-1.30147	0.00004	-0.00055	0.00119	0.00065	-1.30083
D44	2.87596	0.00001	-0.00063	0.00076	0.00013	2.87609
D45	0.80313	-0.00001	-0.00111	0.00059	-0.00052	0.80261
D46	-3.13711	0.00002	0.00107	0.00043	0.00150	-3.13561
D47	0.00419	0.00001	0.00148	0.00023	0.00171	0.00590
D48	0.00154	0.00001	0.00150	0.00002	0.00151	0.00305
D49	-3.14035	0.00000	0.00191	-0.00018	0.00172	-3.13863

Item	Value	Threshold	Converged?
Maximum Force	0.000429	0.000450	YES
RMS Force	0.000073	0.000300	YES
Maximum Displacement	0.035985	0.001800	NO
RMS Displacement	0.008473	0.001200	NO

Predicted change in Energy=-2.383482D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.590934	-2.344599	-1.150089
2	6	0	-1.888743	-1.968843	-1.287942
3	7	0	-2.088299	-0.897653	-0.423637
4	6	0	-0.931477	-0.640520	0.218123
5	7	0	-0.015257	-1.510707	-0.207009
6	6	0	1.397449	-1.476870	0.228499

7	6	0	2.213756	-0.385879	-0.512872
8	1	0	-0.035042	-3.128296	-1.635274
9	1	0	-2.667262	-2.366503	-1.912866
10	1	0	1.394460	-1.235015	1.290250
11	1	0	1.807458	-2.477276	0.086572
12	1	0	2.683244	-0.800301	-1.409277
13	1	0	1.528250	0.414354	-0.816090
14	35	0	0.724726	1.551659	2.057018
15	1	0	-0.704628	0.166799	0.938887
16	6	0	-3.274732	-0.146955	-0.198612
17	6	0	-4.447177	-0.397360	-0.766136
18	1	0	-3.116726	0.667983	0.496242
19	1	0	-5.291209	0.236988	-0.533648
20	1	0	-4.615917	-1.211061	-1.459884
21	8	0	3.236771	0.103512	0.311500
22	1	0	2.801639	0.679665	0.973399

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.358125	0.000000			
3	N	2.205331	1.390789	0.000000		
4	C	2.211754	2.224642	1.347669	0.000000	
5	N	1.384261	2.210939	2.172618	1.333200	0.000000
6	C	2.570432	3.652490	3.593218	2.474568	1.478699
7	C	3.479786	4.465087	4.333307	3.239087	2.515410
8	H	1.076384	2.213861	3.264919	3.229196	2.157991
9	H	2.212114	1.074596	2.170374	3.245471	3.267333
10	H	3.335898	4.238513	3.896258	2.629232	2.074872
11	H	2.701706	3.976141	4.234672	3.300416	2.083923
12	H	3.629362	4.720516	4.873252	3.967388	3.038425
13	H	3.494898	4.192625	3.867145	2.869253	2.541506
14	Br	5.215105	5.514790	4.479497	3.306084	3.879624
15	H	3.268618	3.304823	2.214514	1.105768	2.145306
16	C	3.596904	2.535130	1.421903	2.430662	3.533280
17	C	4.337023	3.047527	2.435550	3.658966	4.603703
18	H	4.262122	3.412346	2.086877	2.562195	3.854915
19	H	5.397887	4.124491	3.399727	4.510260	5.567478
20	H	4.193015	2.835715	2.749706	4.088560	4.777610
21	O	4.772925	5.755325	5.468010	4.235162	3.667457
22	H	5.016465	5.841912	5.324579	4.031065	3.758457

		6	7	8	9	10
6	C	0.000000				
7	C	1.551208	0.000000			

8	H	2.872784	3.719909	0.000000		
9	H	4.679612	5.450430	2.754264	0.000000	
10	H	1.088953	2.154885	3.766521	5.295073	0.000000
11	H	1.090442	2.213222	2.604494	4.902361	1.778375
12	H	2.189366	1.093483	3.586044	5.597723	3.022811
13	H	2.164487	1.096464	3.957943	5.151544	2.678617
14	Br	3.601114	3.546209	6.009346	6.528212	2.966821
15	H	2.761345	3.306058	4.234654	4.289760	2.548472
16	C	4.876512	5.502667	4.631197	2.869509	5.020153
17	C	6.026134	6.665755	5.261211	2.891472	6.249408
18	H	5.004983	5.526570	5.334030	3.900503	4.960106
19	H	6.946677	7.530796	6.337666	3.945315	7.084601
20	H	6.251549	6.944220	4.969001	2.310303	6.609723
21	O	2.426438	1.402018	4.993924	6.775425	2.478653
22	H	2.679042	1.920936	5.417795	6.893370	2.397196

		11	12	13	14	15
11	H	0.000000				
12	H	2.411806	0.000000			
13	H	3.042085	1.777996	0.000000		
14	Br	4.613814	4.624144	3.192783	0.000000	
15	H	3.745417	4.234009	2.850784	2.282785	0.000000
16	C	5.598248	6.114740	4.874934	4.895796	2.828034
17	C	6.646323	7.170696	6.030513	6.206243	4.151150
18	H	5.857309	6.279053	4.833461	4.239536	2.503066
19	H	7.625154	8.089165	6.827610	6.680673	4.817677
20	H	6.727152	7.310884	6.388053	6.965895	4.790697
21	O	2.958715	2.020976	2.070538	3.384424	3.991522
22	H	3.426533	2.807394	2.212280	2.499634	3.543746

		16	17	18	19	20
16	C	0.000000				
17	C	1.326428	0.000000			
18	H	1.082549	2.121002	0.000000		
19	H	2.079866	1.081129	2.444342	0.000000	
20	H	2.126477	1.082529	3.099162	1.846829	0.000000
21	O	6.536254	7.775296	6.381198	8.570796	8.156630
22	H	6.243332	7.532018	5.937581	8.243867	8.032176

		21	22
21	O	0.000000	
22	H	0.979491	0.000000

Stoichiometry C7H11BrN2O

Framework group C1[X(C7H11BrN2O)]

Deg. of freedom 60

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.854116	-2.004464	0.264836
2	6	0	-2.845590	-1.107803	0.025078
3	7	0	-2.252130	0.149951	0.012704
4	6	0	-0.931947	0.005744	0.241901
5	7	0	-0.674736	-1.292674	0.401203
6	6	0	0.689000	-1.830279	0.595504
7	6	0	1.477377	-1.925188	-0.737051
8	1	0	-1.887841	-3.076748	0.352418
9	1	0	-3.898053	-1.257345	-0.132132
10	1	0	1.212005	-1.134546	1.249904
11	1	0	0.592262	-2.794307	1.095858
12	1	0	1.343857	-2.910104	-1.192921
13	1	0	1.087619	-1.166128	-1.425637
14	35	0	2.025437	1.476827	0.100519
15	1	0	-0.143106	0.780531	0.254484
16	6	0	-2.860749	1.417246	-0.200258
17	6	0	-4.161021	1.611807	-0.375899
18	1	0	-2.136766	2.222057	-0.206666
19	1	0	-4.526395	2.616556	-0.536590
20	1	0	-4.892995	0.814294	-0.368561
21	8	0	2.849105	-1.749179	-0.506754
22	1	0	2.976635	-0.793102	-0.336300

Rotational constants (GHZ): 0.9807186 0.4480083 0.3186478

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 851.7152723544 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 4.67D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Initial guess from the checkpoint file: "."
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 0.000083 0.000046 -0.000652 Ang= 0.08 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=1804729152.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3032.34329879 A.U. after 10 cycles
NFock= 10 Conv=0.94D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000004674	0.000025074	-0.000108413
2	6	0.000022904	-0.000106212	0.000031159
3	7	0.000045438	0.000017496	0.000033105
4	6	-0.000042265	-0.000002406	0.000004399
5	7	0.000012144	0.000088540	0.000104967
6	6	-0.000081057	-0.000079027	-0.000013576
7	6	0.000023884	-0.000007274	-0.000087923
8	1	0.000000036	-0.000033158	0.000055589
9	1	-0.000001652	0.000048461	-0.000021533
10	1	0.000010230	0.000014623	-0.000003242
11	1	-0.000009297	0.000012424	-0.000015607
12	1	-0.000002599	-0.000002378	0.000006912
13	1	0.000016690	0.000021685	0.000014594
14	35	0.000016072	0.000037000	0.000020151
15	1	-0.000005648	-0.000047693	-0.000054532

16	6	-0.000013842	-0.000012600	0.000010214
17	6	-0.000031422	0.000002010	-0.000009531
18	1	0.000001794	0.000006513	0.000006466
19	1	0.000004241	0.000000412	0.000008305
20	1	0.000006133	-0.000009068	0.000003798
21	8	0.000010622	0.000006106	0.000028403
22	1	0.000012921	0.000019470	-0.000013705

Cartesian Forces: Max 0.000108413 RMS 0.000037031

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000152858 RMS 0.000035145
Search for a local minimum.
Step number 70 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 62 63 64 65 66
67 68 69 70
DE= -3.06D-06 DEPred=-2.38D-06 R= 1.28D+00
TightC=F SS= 1.41D+00 RLast= 4.09D-02 DXNew= 1.6377D+00 1.2260D-01
Trust test= 1.28D+00 RLast= 4.09D-02 DXMaxT set to 9.74D-01
ITU= 1 1 1 1 1 1 1 1 0 1 1 1 1 0 1 1 0 1 1 0
ITU= -1 1 1 1 -1 1 0 -1 1 0 -1 0 -1 0 0 1 -1 0 1 1
ITU= 1 1 1 1 0 -1 1 1 1 1 1 0 -1 1 1 1 1 1 1 1
ITU= 1 1 1 1 1 0 0 -1 0 0
Eigenvalues --- 0.00132 0.00181 0.00250 0.00474 0.00999
Eigenvalues --- 0.01360 0.01517 0.01874 0.02035 0.02157
Eigenvalues --- 0.02523 0.03024 0.03179 0.03792 0.04058
Eigenvalues --- 0.04391 0.05006 0.05360 0.05705 0.08609
Eigenvalues --- 0.08857 0.09690 0.13182 0.13880 0.14617
Eigenvalues --- 0.14978 0.15519 0.15932 0.16058 0.16570
Eigenvalues --- 0.17733 0.19374 0.20362 0.22844 0.23374
Eigenvalues --- 0.23620 0.25250 0.27368 0.29731 0.32868
Eigenvalues --- 0.33778 0.33834 0.33961 0.34176 0.34291
Eigenvalues --- 0.34677 0.34843 0.35653 0.36313 0.36398
Eigenvalues --- 0.38449 0.43002 0.43785 0.45867 0.48930
Eigenvalues --- 0.53776 0.55630 0.57782 0.61033 0.71464
En-DIIS/RFO-DIIS IScMMF= 0 using points: 70 69 68 67 66
RFO step: Lambda=-2.10064472D-07.
DidBck=F Rises=F RFO-DIIS coefs: 1.23316 -0.12422 -0.26042 0.29388 -

0.14240

Iteration 1 RMS(Cart)= 0.00282052 RMS(Int)= 0.00000321

Iteration 2 RMS(Cart)= 0.00000393 RMS(Int)= 0.00000178

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000178

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56649	-0.00003	-0.00002	-0.00004	-0.00006	2.56643
R2	2.61587	0.00004	0.00002	0.00007	0.00009	2.61596
R3	2.03407	0.00000	0.00000	0.00000	0.00000	2.03407
R4	2.62821	0.00003	0.00005	0.00004	0.00009	2.62830
R5	2.03069	0.00000	0.00000	0.00000	-0.00001	2.03069
R6	2.54672	-0.00002	0.00000	-0.00006	-0.00006	2.54667
R7	2.68701	0.00002	-0.00012	0.00016	0.00004	2.68704
R8	2.51938	-0.00002	-0.00003	-0.00004	-0.00007	2.51931
R9	2.08960	-0.00007	-0.00035	-0.00006	-0.00041	2.08919
R10	2.79434	-0.00002	-0.00008	-0.00011	-0.00019	2.79415
R11	2.93136	0.00009	0.00007	0.00017	0.00023	2.93159
R12	2.05782	0.00000	-0.00002	-0.00002	-0.00003	2.05779
R13	2.06064	-0.00001	-0.00001	-0.00001	-0.00002	2.06061
R14	2.06638	-0.00001	0.00000	-0.00004	-0.00005	2.06634
R15	2.07202	0.00001	0.00002	-0.00005	-0.00003	2.07198
R16	2.64943	0.00004	0.00004	0.00010	0.00014	2.64957
R17	6.03349	0.00003	-0.00222	0.00139	-0.00082	6.03266
R18	2.50659	0.00002	0.00003	-0.00001	0.00002	2.50661
R19	2.04572	0.00001	0.00001	0.00002	0.00004	2.04576
R20	2.04304	0.00000	0.00001	-0.00002	-0.00001	2.04303
R21	2.04568	0.00000	-0.00001	0.00003	0.00002	2.04570
R22	1.85097	0.00000	-0.00003	-0.00001	-0.00003	1.85093
A1	1.87537	0.00000	0.00000	-0.00003	-0.00002	1.87535
A2	2.27732	0.00002	0.00008	0.00010	0.00018	2.27750
A3	2.13049	-0.00002	-0.00008	-0.00008	-0.00016	2.13033
A4	1.86202	-0.00001	0.00000	-0.00003	-0.00002	1.86200
A5	2.27699	0.00003	0.00010	0.00018	0.00027	2.27727
A6	2.14417	-0.00002	-0.00010	-0.00015	-0.00025	2.14392
A7	1.89623	0.00001	-0.00003	0.00005	0.00003	1.89626
A8	2.24555	-0.00002	0.00002	-0.00013	-0.00011	2.24543
A9	2.14140	0.00001	0.00001	0.00008	0.00009	2.14149
A10	1.88970	0.00000	0.00003	-0.00004	-0.00001	1.88969
A11	2.24695	0.00001	-0.00011	0.00005	-0.00007	2.24688
A12	2.14529	-0.00001	0.00004	-0.00003	0.00000	2.14528
A13	1.90143	0.00000	-0.00001	0.00003	0.00003	1.90146
A14	2.22907	-0.00015	-0.00037	-0.00026	-0.00063	2.22844
A15	2.15042	0.00015	0.00034	0.00020	0.00054	2.15096
A16	1.95853	0.00011	-0.00005	0.00020	0.00015	1.95868

A17	1.86463	0.00000	-0.00003	0.00018	0.00015	1.86478
A18	1.87538	-0.00007	0.00001	-0.00013	-0.00012	1.87526
A19	1.88729	-0.00003	-0.00010	-0.00009	-0.00019	1.88709
A20	1.96619	-0.00004	0.00005	-0.00013	-0.00008	1.96611
A21	1.90890	0.00002	0.00011	-0.00002	0.00010	1.90899
A22	1.92963	-0.00005	0.00008	-0.00009	-0.00001	1.92962
A23	1.89280	0.00006	-0.00004	-0.00008	-0.00012	1.89268
A24	1.92673	0.00002	-0.00016	0.00012	-0.00004	1.92669
A25	1.89476	0.00001	0.00019	0.00002	0.00021	1.89497
A26	1.87656	0.00001	0.00013	-0.00011	0.00002	1.87658
A27	1.94339	-0.00006	-0.00019	0.00015	-0.00004	1.94335
A28	1.74007	0.00001	0.00107	-0.00039	0.00068	1.74075
A29	2.17749	0.00001	0.00015	-0.00015	0.00000	2.17749
A30	1.95760	0.00000	-0.00002	0.00003	0.00002	1.95762
A31	2.14809	0.00000	-0.00013	0.00012	-0.00001	2.14808
A32	2.07978	0.00000	-0.00015	0.00007	-0.00007	2.07971
A33	2.15781	-0.00001	0.00006	-0.00010	-0.00004	2.15777
A34	2.04559	0.00001	0.00009	0.00003	0.00012	2.04571
A35	1.85304	0.00002	0.00009	-0.00001	0.00009	1.85313
D1	0.00421	0.00000	0.00005	0.00008	0.00013	0.00434
D2	-3.13543	-0.00001	-0.00035	-0.00061	-0.00096	-3.13639
D3	-3.14152	-0.00003	-0.00045	-0.00062	-0.00106	3.14061
D4	0.00203	-0.00004	-0.00084	-0.00131	-0.00215	-0.00012
D5	-0.00616	0.00000	-0.00007	-0.00016	-0.00023	-0.00639
D6	-3.07662	-0.00002	0.00052	0.00017	0.00069	-3.07593
D7	3.13914	0.00002	0.00038	0.00046	0.00084	3.13998
D8	0.06869	0.00001	0.00096	0.00079	0.00176	0.07045
D9	-0.00088	0.00001	-0.00001	0.00003	0.00001	-0.00086
D10	3.13848	0.00001	0.00051	-0.00031	0.00020	3.13869
D11	3.13895	0.00002	0.00035	0.00065	0.00100	3.13995
D12	-0.00488	0.00002	0.00087	0.00032	0.00119	-0.00369
D13	-0.00295	-0.00001	-0.00003	-0.00013	-0.00016	-0.00311
D14	3.08543	0.00000	-0.00154	-0.00041	-0.00195	3.08348
D15	3.14071	-0.00001	-0.00051	0.00018	-0.00033	3.14038
D16	-0.05409	-0.00001	-0.00202	-0.00010	-0.00212	-0.05622
D17	0.05196	0.00000	0.00315	-0.00059	0.00256	0.05452
D18	-3.08697	0.00000	0.00326	-0.00067	0.00259	-3.08439
D19	-3.09214	0.00000	0.00374	-0.00097	0.00277	-3.08937
D20	0.05211	0.00000	0.00385	-0.00105	0.00280	0.05491
D21	0.00562	0.00001	0.00006	0.00018	0.00024	0.00585
D22	3.07995	0.00000	-0.00053	-0.00015	-0.00069	3.07927
D23	-3.08654	0.00000	0.00146	0.00044	0.00191	-3.08463
D24	-0.01220	0.00000	0.00087	0.00011	0.00098	-0.01122
D25	1.68799	-0.00003	-0.00241	-0.00216	-0.00457	1.68342

D26	-2.52964	0.00001	-0.00257	-0.00205	-0.00462	-2.53426
D27	-0.48265	0.00000	-0.00245	-0.00204	-0.00449	-0.48714
D28	-1.37316	-0.00003	-0.00173	-0.00178	-0.00350	-1.37666
D29	0.69240	0.00000	-0.00189	-0.00166	-0.00356	0.68884
D30	2.73938	-0.00001	-0.00177	-0.00165	-0.00342	2.73596
D31	-1.60230	0.00004	-0.00031	0.00001	-0.00030	-1.60260
D32	0.47319	0.00006	-0.00006	-0.00007	-0.00013	0.47306
D33	2.60666	0.00005	-0.00042	0.00013	-0.00029	2.60637
D34	2.62878	-0.00001	-0.00019	-0.00027	-0.00046	2.62832
D35	-1.57893	0.00001	0.00007	-0.00036	-0.00029	-1.57921
D36	0.55454	-0.00001	-0.00029	-0.00015	-0.00044	0.55410
D37	0.51709	0.00000	-0.00029	-0.00011	-0.00040	0.51669
D38	2.59257	0.00002	-0.00004	-0.00019	-0.00023	2.59234
D39	-1.55715	0.00001	-0.00040	0.00002	-0.00039	-1.55753
D40	1.16943	0.00008	0.00019	0.00003	0.00023	1.16966
D41	-3.01641	0.00006	0.00038	-0.00012	0.00026	-3.01615
D42	-0.95385	0.00004	0.00054	-0.00015	0.00039	-0.95346
D43	-1.30083	-0.00005	-0.00102	-0.00009	-0.00111	-1.30194
D44	2.87609	0.00000	-0.00111	0.00003	-0.00108	2.87501
D45	0.80261	0.00001	-0.00131	-0.00001	-0.00132	0.80129
D46	-3.13561	0.00000	0.00032	-0.00015	0.00017	-3.13544
D47	0.00590	0.00000	0.00035	-0.00007	0.00028	0.00618
D48	0.00305	0.00000	0.00020	-0.00007	0.00014	0.00319
D49	-3.13863	0.00000	0.00024	0.00001	0.00025	-3.13838

Item	Value	Threshold	Converged?
Maximum Force	0.000153	0.000450	YES
RMS Force	0.000035	0.000300	YES
Maximum Displacement	0.008998	0.001800	NO
RMS Displacement	0.002821	0.001200	NO

Predicted change in Energy=-3.473107D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.590080	-2.341988	-1.151853
2	6	0	-1.887838	-1.966333	-1.290157
3	7	0	-2.088618	-0.897238	-0.423469
4	6	0	-0.932571	-0.641252	0.220081
5	7	0	-0.015707	-1.510226	-0.206030
6	6	0	1.396781	-1.477134	0.229905
7	6	0	2.214673	-0.387991	-0.512691

8	1	0	-0.033502	-3.124850	-1.637597
9	1	0	-2.665529	-2.361989	-1.917373
10	1	0	1.393816	-1.233697	1.291276
11	1	0	1.805771	-2.478152	0.089455
12	1	0	2.684357	-0.804264	-1.408105
13	1	0	1.530058	0.412411	-0.817412
14	35	0	0.725538	1.556420	2.052269
15	1	0	-0.706373	0.165290	0.941587
16	6	0	-3.275666	-0.147666	-0.197810
17	6	0	-4.448120	-0.399048	-0.764912
18	1	0	-3.118133	0.667318	0.497126
19	1	0	-5.292556	0.234610	-0.532031
20	1	0	-4.616406	-1.212941	-1.458558
21	8	0	3.237642	0.101716	0.311678
22	1	0	2.802810	0.680127	0.971775

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.358094	0.000000			
3	N	2.205326	1.390835	0.000000		
4	C	2.211787	2.224678	1.347639	0.000000	
5	N	1.384309	2.210936	2.172555	1.333164	0.000000
6	C	2.569989	3.652208	3.593214	2.474808	1.478600
7	C	3.477538	4.463878	4.334237	3.241333	2.515561
8	H	1.076382	2.213919	3.264944	3.229171	2.157940
9	H	2.212219	1.074593	2.170270	3.245426	3.267377
10	H	3.336620	4.239080	3.896268	2.628788	2.074886
11	H	2.701756	3.975932	4.234224	3.299967	2.083741
12	H	3.626596	4.719034	4.874366	3.969852	3.038702
13	H	3.491926	4.190933	3.868487	2.872479	2.541596
14	Br	5.214866	5.514647	4.479865	3.306963	3.879907
15	H	3.268403	3.304596	2.214260	1.105553	2.145088
16	C	3.596890	2.535120	1.421922	2.430711	3.533266
17	C	4.336959	3.047508	2.435575	3.658956	4.603624
18	H	4.262171	3.412348	2.086919	2.562380	3.855019
19	H	5.397807	4.124441	3.399718	4.510242	5.567394
20	H	4.192865	2.835674	2.749689	4.088435	4.777409
21	O	4.771275	5.754411	5.468766	4.236870	3.667514
22	H	5.015444	5.841426	5.325492	4.032885	3.758844

		6	7	8	9	10
6	C	0.000000				
7	C	1.551332	0.000000			
8	H	2.871975	3.716194	0.000000		

9	H	4.679331	5.448502	2.754596	0.000000	
10	H	1.088935	2.154838	3.767226	5.295919	0.000000
11	H	1.090430	2.213269	2.604583	4.902385	1.778412
12	H	2.189448	1.093459	3.581137	5.595279	3.022675
13	H	2.164490	1.096446	3.953433	5.148802	2.678582
14	Br	3.601948	3.546446	6.008788	6.527735	2.968242
15	H	2.761758	3.309616	4.234379	4.289416	2.547596
16	C	4.876698	5.504609	4.631223	2.869214	5.020050
17	C	6.026176	6.667574	5.261219	2.891182	6.249221
18	H	5.005450	5.529216	5.334091	3.900174	4.960062
19	H	6.946787	7.533027	6.337657	3.944968	7.084346
20	H	6.251330	6.945420	4.968950	2.310139	6.609447
21	O	2.426566	1.402092	4.991070	6.773917	2.478434
22	H	2.679751	1.921047	5.415841	6.892343	2.397930

		11	12	13	14	15
11	H	0.000000				
12	H	2.411742	0.000000			
13	H	3.042003	1.778095	0.000000		
14	Br	4.614902	4.624283	3.192347	0.000000	
15	H	3.744969	4.237705	2.856006	2.284563	0.000000
16	C	5.597740	6.117010	4.877763	4.896570	2.827973
17	C	6.645583	7.172874	6.033227	6.207020	4.151058
18	H	5.857048	6.282066	4.837217	4.240610	2.503230
19	H	7.624407	8.091842	6.830894	6.681560	4.817617
20	H	6.726178	7.312367	6.389981	6.966465	4.790467
21	O	2.958945	2.021034	2.070560	3.384744	3.994507
22	H	3.427434	2.807361	2.211959	2.500084	3.546877

		16	17	18	19	20
16	C	0.000000				
17	C	1.326441	0.000000			
18	H	1.082568	2.121024	0.000000		
19	H	2.079828	1.081124	2.444283	0.000000	
20	H	2.126472	1.082538	3.099177	1.846899	0.000000
21	O	6.537962	7.776937	6.383586	8.572852	8.157704
22	H	6.245081	7.533703	5.939951	8.245901	8.033368

		21	22
21	O	0.000000	
22	H	0.979472	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.852965	-2.004996	0.260149
2	6	0	-2.844681	-1.108666	0.020330
3	7	0	-2.252389	0.149729	0.013000
4	6	0	-0.932686	0.006189	0.245187
5	7	0	-0.674650	-1.292365	0.401715
6	6	0	0.688797	-1.829976	0.597274
7	6	0	1.478302	-1.925971	-0.734679
8	1	0	-1.885809	-3.077483	0.345542
9	1	0	-3.896475	-1.258589	-0.140921
10	1	0	1.211596	-1.133951	1.251498
11	1	0	0.591471	-2.793672	1.098128
12	1	0	1.345248	-2.911283	-1.189772
13	1	0	1.089042	-1.167412	-1.424070
14	35	0	2.025338	1.477467	0.098770
15	1	0	-0.144594	0.781386	0.260300
16	6	0	-2.861868	1.416994	-0.197802
17	6	0	-4.162268	1.610960	-0.373250
18	1	0	-2.138439	2.222337	-0.202742
19	1	0	-4.528230	2.615741	-0.532363
20	1	0	-4.893689	0.812916	-0.367141
21	8	0	2.849892	-1.749608	-0.503378
22	1	0	2.977410	-0.793241	-0.334657

Rotational constants (GHZ): 0.9806341 0.4479837 0.3185659
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 358 symmetry adapted cartesian basis functions of A symmetry.
There are 345 symmetry adapted basis functions of A symmetry.
345 basis functions, 553 primitive gaussians, 358 cartesian basis functions
55 alpha electrons 55 beta electrons
nuclear repulsion energy 851.6635159892 Hartrees.
NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 345 RedAO= T EigKep= 4.67D-06 NBF= 345
NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345
Initial guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000062 0.000011 -0.000108 Ang= 0.01 deg.

Keep R1 ints in memory in canonical form, NReq=1804729152.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3032.34329884 A.U. after 9 cycles

NFock= 9 Conv=0.96D-08 -V/T= 2.0017

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000005115	0.000000890	-0.000033611
2	6	0.000003382	-0.000044059	0.000033505
3	7	0.000009454	0.000021477	-0.000000012
4	6	-0.000006641	-0.000021531	-0.000000582
5	7	0.000023722	0.000032926	0.000034751
6	6	-0.000021371	-0.000014840	-0.000003083
7	6	-0.000003488	-0.000002991	-0.000023479
8	1	-0.000000036	-0.000010808	0.000019744
9	1	0.000003132	0.000015254	-0.000008230
10	1	-0.000001855	-0.000000386	0.000000645
11	1	0.000003873	0.000003310	0.000001763
12	1	0.000002186	-0.000003888	-0.000003579
13	1	0.000020524	0.000023055	0.000003031
14	35	-0.000002141	-0.000002211	-0.000005140
15	1	0.000004252	0.000008338	-0.000011164
16	6	-0.000007956	0.000000917	0.000007103
17	6	-0.000006246	-0.000000468	-0.000000890
18	1	0.000000568	-0.000003284	-0.000000901
19	1	-0.000003085	-0.000002585	0.000002387
20	1	-0.000000064	-0.000000902	0.000006565
21	8	-0.000006202	-0.000005485	-0.000014480
22	1	-0.000006892	0.000007272	-0.000004344

Cartesian Forces: Max 0.000044059 RMS 0.000013555

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000026819 RMS 0.000007796
Search for a local minimum.
Step number 71 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 62 63 64 65 66
67 68 69 70 71
DE= -5.17D-08 DEPred=-3.47D-07 R= 1.49D-01
Trust test= 1.49D-01 RLast= 1.28D-02 DXMaxT set to 9.74D-01
ITU= 0 1 1 1 1 1 1 1 1 0 1 1 1 1 0 1 1 0 1 1
ITU= 0 -1 1 1 1 -1 1 0 -1 1 0 -1 0 -1 0 0 1 -1 0 1
ITU= 1 1 1 1 1 0 -1 1 1 1 1 1 0 -1 1 1 1 1 1 1
ITU= 1 1 1 1 1 1 0 0 -1 0 0
Eigenvalues --- 0.00138 0.00173 0.00252 0.00532 0.00983
Eigenvalues --- 0.01361 0.01503 0.01706 0.01879 0.02156
Eigenvalues --- 0.02538 0.03023 0.03179 0.03862 0.04048
Eigenvalues --- 0.04379 0.04789 0.05352 0.05692 0.08585
Eigenvalues --- 0.08782 0.09778 0.13160 0.13866 0.14648
Eigenvalues --- 0.14877 0.15432 0.15988 0.16078 0.16725
Eigenvalues --- 0.17839 0.19060 0.20486 0.22788 0.23362
Eigenvalues --- 0.23558 0.25171 0.27283 0.29370 0.32708
Eigenvalues --- 0.33774 0.33807 0.33972 0.34079 0.34297
Eigenvalues --- 0.34458 0.34846 0.35550 0.36313 0.36399
Eigenvalues --- 0.38518 0.42924 0.44042 0.45706 0.48974
Eigenvalues --- 0.53728 0.54769 0.57695 0.61069 0.70069
En-DIIS/RFO-DIIS IScMMF= 0 using points: 71 70 69 68 67
RFO step: Lambda=-2.07116134D-08.
DidBck=F Rises=F RFO-DIIS coefs: 1.00981 0.11711 -0.23852 0.10958 0.00201
Iteration 1 RMS(Cart)= 0.00107557 RMS(Int)= 0.00000093
Iteration 2 RMS(Cart)= 0.00000060 RMS(Int)= 0.00000079

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56643	-0.00001	-0.00002	0.00000	-0.00002	2.56641
R2	2.61596	0.00001	0.00001	0.00003	0.00004	2.61600
R3	2.03407	0.00000	-0.00001	0.00000	0.00000	2.03407
R4	2.62830	0.00001	0.00002	0.00003	0.00004	2.62834
R5	2.03069	0.00000	-0.00001	0.00000	-0.00001	2.03068
R6	2.54667	0.00000	-0.00004	0.00004	0.00000	2.54667
R7	2.68704	0.00001	0.00001	0.00002	0.00003	2.68707
R8	2.51931	-0.00001	-0.00004	0.00001	-0.00002	2.51929
R9	2.08919	0.00000	-0.00006	0.00006	0.00000	2.08919

R10	2.79415	-0.00002	-0.00003	-0.00007	-0.00010	2.79405
R11	2.93159	0.00002	0.00010	-0.00003	0.00006	2.93166
R12	2.05779	0.00000	0.00001	0.00001	0.00001	2.05780
R13	2.06061	0.00000	-0.00002	0.00001	-0.00001	2.06061
R14	2.06634	0.00000	-0.00001	0.00000	-0.00001	2.06633
R15	2.07198	0.00000	-0.00003	0.00002	-0.00001	2.07198
R16	2.64957	-0.00002	0.00000	0.00001	0.00001	2.64958
R17	6.03266	0.00000	-0.00018	-0.00018	-0.00037	6.03229
R18	2.50661	0.00001	0.00001	0.00001	0.00002	2.50663
R19	2.04576	0.00000	-0.00001	0.00001	0.00000	2.04576
R20	2.04303	0.00000	0.00000	0.00001	0.00001	2.04304
R21	2.04570	0.00000	-0.00002	0.00001	0.00000	2.04570
R22	1.85093	0.00001	-0.00003	0.00001	-0.00002	1.85092
A1	1.87535	0.00000	0.00001	-0.00002	-0.00001	1.87534
A2	2.27750	0.00001	0.00004	0.00004	0.00008	2.27758
A3	2.13033	-0.00001	-0.00004	-0.00003	-0.00007	2.13026
A4	1.86200	0.00000	-0.00003	0.00004	0.00002	1.86202
A5	2.27727	0.00000	0.00006	0.00000	0.00006	2.27733
A6	2.14392	-0.00001	-0.00003	-0.00004	-0.00008	2.14384
A7	1.89626	-0.00001	0.00002	-0.00005	-0.00003	1.89623
A8	2.24543	0.00000	0.00001	-0.00001	0.00000	2.24543
A9	2.14149	0.00001	-0.00003	0.00006	0.00003	2.14152
A10	1.88969	0.00000	0.00000	0.00002	0.00002	1.88971
A11	2.24688	0.00000	0.00003	0.00005	0.00009	2.24697
A12	2.14528	0.00000	-0.00001	-0.00008	-0.00009	2.14520
A13	1.90146	0.00000	0.00000	0.00000	0.00000	1.90146
A14	2.22844	-0.00002	-0.00012	-0.00001	-0.00013	2.22831
A15	2.15096	0.00002	0.00015	0.00002	0.00017	2.15113
A16	1.95868	0.00002	0.00010	0.00001	0.00011	1.95878
A17	1.86478	-0.00001	0.00008	-0.00008	-0.00001	1.86477
A18	1.87526	0.00000	-0.00010	0.00010	0.00000	1.87526
A19	1.88709	0.00000	-0.00006	0.00002	-0.00004	1.88706
A20	1.96611	0.00000	-0.00005	-0.00005	-0.00010	1.96601
A21	1.90899	0.00000	0.00004	0.00001	0.00005	1.90904
A22	1.92962	0.00001	0.00008	-0.00005	0.00003	1.92965
A23	1.89268	0.00002	-0.00009	0.00024	0.00015	1.89283
A24	1.92669	-0.00002	0.00000	-0.00014	-0.00014	1.92654
A25	1.89497	0.00000	0.00011	0.00000	0.00011	1.89508
A26	1.87658	0.00000	0.00003	-0.00001	0.00002	1.87659
A27	1.94335	-0.00001	-0.00012	-0.00004	-0.00016	1.94319
A28	1.74075	-0.00002	0.00013	0.00001	0.00014	1.74089
A29	2.17749	0.00000	0.00005	-0.00001	0.00004	2.17753
A30	1.95762	0.00000	-0.00002	0.00001	-0.00002	1.95760
A31	2.14808	0.00000	-0.00002	0.00000	-0.00003	2.14805

A32	2.07971	0.00000	-0.00001	0.00001	0.00000	2.07970
A33	2.15777	0.00000	-0.00001	0.00000	-0.00002	2.15775
A34	2.04571	0.00000	0.00003	-0.00001	0.00002	2.04573
A35	1.85313	-0.00001	-0.00005	0.00001	-0.00004	1.85309
D1	0.00434	0.00000	0.00002	0.00008	0.00009	0.00443
D2	-3.13639	-0.00001	-0.00018	-0.00024	-0.00042	-3.13681
D3	3.14061	0.00000	-0.00033	-0.00006	-0.00038	3.14022
D4	-0.00012	-0.00001	-0.00053	-0.00037	-0.00090	-0.00102
D5	-0.00639	0.00000	0.00004	-0.00008	-0.00004	-0.00643
D6	-3.07593	0.00000	-0.00055	-0.00006	-0.00062	-3.07654
D7	3.13998	0.00000	0.00035	0.00004	0.00039	3.14037
D8	0.07045	0.00000	-0.00024	0.00005	-0.00019	0.07026
D9	-0.00086	0.00000	-0.00007	-0.00005	-0.00012	-0.00098
D10	3.13869	0.00000	0.00017	0.00003	0.00019	3.13888
D11	3.13995	0.00001	0.00011	0.00024	0.00035	3.14029
D12	-0.00369	0.00001	0.00034	0.00031	0.00066	-0.00303
D13	-0.00311	0.00000	0.00009	0.00000	0.00009	-0.00302
D14	3.08348	0.00000	0.00085	-0.00021	0.00064	3.08412
D15	3.14038	0.00000	-0.00012	-0.00007	-0.00020	3.14018
D16	-0.05622	-0.00001	0.00063	-0.00028	0.00035	-0.05586
D17	0.05452	0.00000	-0.00126	-0.00002	-0.00128	0.05324
D18	-3.08439	0.00000	-0.00127	-0.00004	-0.00131	-3.08570
D19	-3.08937	0.00000	-0.00099	0.00006	-0.00093	-3.09031
D20	0.05491	0.00000	-0.00101	0.00005	-0.00096	0.05394
D21	0.00585	0.00000	-0.00008	0.00005	-0.00003	0.00582
D22	3.07927	0.00000	0.00046	0.00003	0.00050	3.07976
D23	-3.08463	0.00001	-0.00079	0.00024	-0.00055	-3.08518
D24	-0.01122	0.00001	-0.00024	0.00022	-0.00002	-0.01124
D25	1.68342	0.00001	0.00177	0.00000	0.00177	1.68519
D26	-2.53426	0.00001	0.00180	-0.00002	0.00178	-2.53248
D27	-0.48714	0.00000	0.00183	0.00000	0.00183	-0.48531
D28	-1.37666	0.00001	0.00110	0.00002	0.00113	-1.37554
D29	0.68884	0.00001	0.00113	0.00000	0.00114	0.68998
D30	2.73596	0.00000	0.00117	0.00002	0.00119	2.73715
D31	-1.60260	-0.00001	0.00028	0.00021	0.00049	-1.60211
D32	0.47306	0.00001	0.00041	0.00032	0.00073	0.47379
D33	2.60637	-0.00001	0.00020	0.00034	0.00053	2.60690
D34	2.62832	-0.00001	0.00017	0.00029	0.00046	2.62878
D35	-1.57921	0.00001	0.00029	0.00041	0.00070	-1.57851
D36	0.55410	0.00000	0.00008	0.00042	0.00051	0.55461
D37	0.51669	0.00000	0.00019	0.00030	0.00048	0.51717
D38	2.59234	0.00001	0.00031	0.00042	0.00073	2.59307
D39	-1.55753	0.00000	0.00010	0.00043	0.00053	-1.55700
D40	1.16966	-0.00003	-0.00036	-0.00035	-0.00071	1.16895

D41	-3.01615	-0.00001	-0.00025	-0.00027	-0.00052	-3.01667
D42	-0.95346	-0.00001	-0.00022	-0.00030	-0.00053	-0.95399
D43	-1.30194	0.00000	0.00019	-0.00014	0.00005	-1.30188
D44	2.87501	0.00000	0.00008	0.00001	0.00009	2.87510
D45	0.80129	0.00000	0.00000	0.00004	0.00004	0.80133
D46	-3.13544	0.00000	-0.00008	-0.00004	-0.00012	-3.13556
D47	0.00618	0.00000	-0.00010	0.00000	-0.00010	0.00608
D48	0.00319	0.00000	-0.00006	-0.00003	-0.00009	0.00310
D49	-3.13838	0.00000	-0.00008	0.00002	-0.00007	-3.13845

Item	Value	Threshold	Converged?
Maximum Force	0.000027	0.000450	YES
RMS Force	0.000008	0.000300	YES
Maximum Displacement	0.003829	0.001800	NO
RMS Displacement	0.001075	0.001200	YES

Predicted change in Energy=-5.968132D-08

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.590351	-2.342598	-1.151156
2	6	0	-1.888186	-1.967183	-1.289309
3	7	0	-2.088691	-0.897145	-0.423688
4	6	0	-0.932419	-0.640489	0.219188
5	7	0	-0.015669	-1.509833	-0.206377
6	6	0	1.396830	-1.476810	0.229346
7	6	0	2.214660	-0.387265	-0.512801
8	1	0	-0.033941	-3.126125	-1.636015
9	1	0	-2.666050	-2.363259	-1.916041
10	1	0	1.393994	-1.233873	1.290838
11	1	0	1.805906	-2.477708	0.088310
12	1	0	2.683891	-0.802940	-1.408727
13	1	0	1.530261	0.413708	-0.816487
14	35	0	0.725834	1.554474	2.054295
15	1	0	-0.706029	0.166459	0.940179
16	6	0	-3.275774	-0.147552	-0.198191
17	6	0	-4.448198	-0.398915	-0.765385
18	1	0	-3.118304	0.667441	0.496750
19	1	0	-5.292661	0.234716	-0.532507
20	1	0	-4.616418	-1.212778	-1.459080
21	8	0	3.238066	0.101441	0.311627
22	1	0	2.803598	0.679357	0.972383

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.358086	0.000000			
3	N	2.205349	1.390857	0.000000		
4	C	2.211792	2.224673	1.347638	0.000000	
5	N	1.384328	2.210935	2.172564	1.333152	0.000000
6	C	2.569877	3.652138	3.593234	2.474861	1.478546
7	C	3.478349	4.464577	4.334369	3.240993	2.515636
8	H	1.076381	2.213950	3.264979	3.229152	2.157916
9	H	2.212239	1.074589	2.170242	3.245399	3.267386
10	H	3.336200	4.238821	3.896419	2.629208	2.074839
11	H	2.701218	3.975523	4.234172	3.300140	2.083689
12	H	3.627334	4.719492	4.874087	3.969155	3.038580
13	H	3.493740	4.192610	3.869037	2.872063	2.542075
14	Br	5.214827	5.514967	4.480222	3.306854	3.879489
15	H	3.268398	3.304624	2.214304	1.105552	2.145027
16	C	3.596924	2.535152	1.421937	2.430741	3.533293
17	C	4.337016	3.047561	2.435624	3.659023	4.603688
18	H	4.262214	3.412395	2.086921	2.562385	3.855029
19	H	5.397869	4.124507	3.399760	4.510292	5.567446
20	H	4.192913	2.835701	2.749739	4.088514	4.777489
21	O	4.771775	5.755055	5.469205	4.236973	3.667604
22	H	5.016026	5.842282	5.326244	4.033252	3.759028

		6	7	8	9	10
6	C	0.000000				
7	C	1.551366	0.000000			
8	H	2.871745	3.717414	0.000000		
9	H	4.679260	5.449309	2.754701	0.000000	
10	H	1.088941	2.154844	3.766442	5.295616	0.000000
11	H	1.090427	2.213225	2.603609	4.901930	1.778446
12	H	2.189500	1.093456	3.582661	5.595877	3.022779
13	H	2.164632	1.096442	3.955853	5.150689	2.678416
14	Br	3.601299	3.546397	6.008631	6.528176	2.967184
15	H	2.761817	3.308805	4.234334	4.289423	2.548330
16	C	4.876776	5.504663	4.631276	2.869169	5.020361
17	C	6.026252	6.667655	5.261306	2.891143	6.249513
18	H	5.005572	5.529205	5.334147	3.900159	4.960484
19	H	6.946872	7.533068	6.337753	3.944962	7.084680
20	H	6.251372	6.945542	4.969034	2.310055	6.609655
21	O	2.426477	1.402096	4.991645	6.774646	2.478410
22	H	2.679581	1.921016	5.416370	6.893298	2.397675

		11	12	13	14	15

11	H	0.000000				
12	H	2.411810	0.000000			
13	H	3.042191	1.778157	0.000000		
14	Br	4.614124	4.624273	3.192153	0.000000	
15	H	3.745279	4.236585	2.854471	2.284310	0.000000
16	C	5.597783	6.116579	4.878040	4.897290	2.828087
17	C	6.645600	7.172435	6.033651	6.207813	4.151196
18	H	5.857186	6.281586	4.837161	4.241482	2.503334
19	H	7.624455	8.091345	6.831175	6.682484	4.817743
20	H	6.726122	7.311978	6.390622	6.967148	4.790603
21	O	2.958540	2.021047	2.070447	3.385188	3.994394
22	H	3.426957	2.807351	2.211790	2.500693	3.547053

		16	17	18	19	20
16	C	0.000000				
17	C	1.326451	0.000000			
18	H	1.082568	2.121018	0.000000		
19	H	2.079839	1.081128	2.444268	0.000000	
20	H	2.126470	1.082536	3.099168	1.846911	0.000000
21	O	6.538502	7.777465	6.384204	8.573425	8.158155
22	H	6.246021	7.534657	5.940984	8.246927	8.034229

		21	22
21	O	0.000000	
22	H	0.979463	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.852977	-2.004770	0.261946
2	6	0	-2.844936	-1.108684	0.022270
3	7	0	-2.252596	0.149697	0.012664
4	6	0	-0.932640	0.006366	0.243529
5	7	0	-0.674460	-1.291997	0.401298
6	6	0	0.688990	-1.829559	0.596565
7	6	0	1.478350	-1.925642	-0.735506
8	1	0	-1.885737	-3.077123	0.349012
9	1	0	-3.896876	-1.258715	-0.137907
10	1	0	1.211914	-1.133502	1.250666

11	1	0	0.591782	-2.793267	1.097412
12	1	0	1.344868	-2.910804	-1.190791
13	1	0	1.089622	-1.166684	-1.424751
14	35	0	2.025502	1.477383	0.099347
15	1	0	-0.144502	0.781540	0.257320
16	6	0	-2.862333	1.416758	-0.198718
17	6	0	-4.162812	1.610481	-0.373924
18	1	0	-2.139017	2.222199	-0.204304
19	1	0	-4.528939	2.615146	-0.533412
20	1	0	-4.894120	0.812340	-0.367232
21	8	0	2.850009	-1.749930	-0.504093
22	1	0	2.977890	-0.793667	-0.335111

Rotational constants (GHZ): 0.9807504 0.4478907 0.3185454

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 358 symmetry adapted cartesian basis functions of A symmetry.

There are 345 symmetry adapted basis functions of A symmetry.

345 basis functions, 553 primitive gaussians, 358 cartesian basis functions

55 alpha electrons 55 beta electrons

nuclear repulsion energy 851.6537666465 Hartrees.

NAtoms= 22 NActive= 22 NUniq= 22 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 345 RedAO= T EigKep= 4.67D-06 NBF= 345

NBsUse= 345 1.00D-06 EigRej= -1.00D+00 NBFU= 345

Initial guess from the checkpoint file: "."

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000016 -0.000007 -0.000011 Ang= 0.00 deg.

Keep R1 ints in memory in canonical form, NReq=1804729152.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3032.34329903 A.U. after 8 cycles

NFock= 8 Conv=0.78D-08 -V/T= 2.0017

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

1	6	-0.000009753	-0.000000289	-0.000004293
2	6	-0.000005820	-0.000011533	0.000012285
3	7	0.000005747	-0.000001772	-0.000003160
4	6	-0.000002191	-0.000004774	-0.000006534
5	7	0.000001393	-0.000000357	-0.000001998
6	6	0.000002118	0.000012001	-0.000000570
7	6	-0.000011587	-0.000009162	0.000004436
8	1	-0.000001967	-0.000004271	0.000006518
9	1	0.000001553	-0.000000550	-0.000000224
10	1	0.000003007	0.000001903	0.000000465
11	1	0.000001652	0.000002366	0.000001917
12	1	-0.000001415	-0.000001805	-0.000005900
13	1	0.000004324	0.000005410	-0.000007135
14	35	0.000005415	0.000007867	-0.000004876
15	1	0.000002182	0.000006929	0.000008230
16	6	-0.000003913	0.000002096	0.000002012
17	6	0.000006720	-0.000001727	0.000004747
18	1	0.000001282	-0.000003248	-0.000001677
19	1	-0.000000518	-0.000003883	0.000000661
20	1	-0.000002642	-0.000001211	0.000005972
21	8	0.000005609	0.000003099	-0.000005370
22	1	-0.000001195	0.000002909	-0.000005505

Cartesian Forces: Max 0.000012285 RMS 0.000005055

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000014829 RMS 0.000004046
Search for a local minimum.
Step number 72 out of a maximum of 116
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 62 63 64 65 66
67 68 69 70 71
72
DE= -1.90D-07 DEPred=-5.97D-08 R= 3.18D+00
Trust test= 3.18D+00 RLast= 5.17D-03 DXMaxT set to 9.74D-01
ITU= 0 0 1 1 1 1 1 1 1 1 0 1 1 1 1 0 1 1 0 1
ITU= 1 0 -1 1 1 1 -1 1 0 -1 1 0 -1 0 -1 0 0 1 -1 0
ITU= 1 1 1 1 1 1 0 -1 1 1 1 1 1 0 -1 1 1 1 1 1

ITU= 1 1 1 1 1 1 1 0 0 -1 0 0

Eigenvalues --- 0.00140 0.00173 0.00245 0.00517 0.00969

Eigenvalues --- 0.01352 0.01476 0.01591 0.01928 0.02157

Eigenvalues --- 0.02533 0.03023 0.03182 0.03839 0.04045

Eigenvalues --- 0.04394 0.04788 0.05395 0.05759 0.08594

Eigenvalues --- 0.08935 0.09821 0.13255 0.14126 0.14609

Eigenvalues --- 0.14993 0.15461 0.15994 0.16111 0.16656

Eigenvalues --- 0.18009 0.19693 0.20707 0.23144 0.23447

Eigenvalues --- 0.23669 0.25215 0.27129 0.29398 0.32755

Eigenvalues --- 0.33784 0.33863 0.33976 0.34169 0.34339

Eigenvalues --- 0.34367 0.34845 0.35752 0.36313 0.36407

Eigenvalues --- 0.38525 0.42990 0.44148 0.45590 0.48928

Eigenvalues --- 0.53736 0.54384 0.57767 0.61218 0.70288

En-DIIS/RFO-DIIS IScMMF= 0 using points: 72 71 70 69 68

RFO step: Lambda=-2.94919821D-09.

DidBck=F Rises=F RFO-DIIS coefs: 1.00759 0.05800 -0.07551 0.00035 0.00957

Iteration 1 RMS(Cart)= 0.00018400 RMS(Int)= 0.00000008

Iteration 2 RMS(Cart)= 0.00000003 RMS(Int)= 0.00000008

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56641	-0.00001	0.00000	-0.00001	-0.00001	2.56640
R2	2.61600	0.00001	0.00001	0.00001	0.00002	2.61602
R3	2.03407	0.00000	0.00000	0.00000	0.00000	2.03406
R4	2.62834	0.00000	0.00001	0.00000	0.00000	2.62834
R5	2.03068	0.00000	0.00000	0.00000	0.00000	2.03068
R6	2.54667	0.00000	-0.00001	0.00000	0.00000	2.54666
R7	2.68707	0.00000	0.00001	-0.00002	-0.00001	2.68706
R8	2.51929	0.00000	-0.00001	-0.00001	-0.00001	2.51928
R9	2.08919	0.00001	0.00000	0.00001	0.00001	2.08920
R10	2.79405	0.00001	-0.00001	0.00001	0.00000	2.79405
R11	2.93166	0.00000	0.00002	-0.00004	-0.00002	2.93163
R12	2.05780	0.00000	0.00000	0.00000	0.00000	2.05780
R13	2.06061	0.00000	0.00000	0.00000	0.00000	2.06061
R14	2.06633	0.00000	0.00000	0.00001	0.00001	2.06634
R15	2.07198	0.00000	-0.00001	0.00000	0.00000	2.07197
R16	2.64958	0.00000	0.00002	0.00001	0.00002	2.64960
R17	6.03229	0.00000	0.00010	-0.00050	-0.00040	6.03190
R18	2.50663	-0.00001	0.00000	-0.00001	-0.00001	2.50662
R19	2.04576	0.00000	0.00000	-0.00001	-0.00001	2.04574
R20	2.04304	0.00000	0.00000	0.00000	-0.00001	2.04303
R21	2.04570	0.00000	0.00000	-0.00001	-0.00001	2.04569
R22	1.85092	0.00000	0.00000	0.00000	0.00000	1.85091
A1	1.87534	0.00000	0.00000	0.00001	0.00001	1.87534

A2	2.27758	0.00000	0.00001	-0.00001	0.00000	2.27758
A3	2.13026	0.00000	-0.00001	0.00000	-0.00001	2.13025
A4	1.86202	0.00000	0.00000	-0.00001	-0.00001	1.86201
A5	2.27733	0.00000	0.00001	-0.00001	0.00000	2.27733
A6	2.14384	0.00000	-0.00001	0.00002	0.00001	2.14385
A7	1.89623	0.00001	0.00000	0.00001	0.00001	1.89625
A8	2.24543	0.00000	0.00000	-0.00001	-0.00001	2.24543
A9	2.14152	0.00000	0.00000	0.00000	-0.00001	2.14151
A10	1.88971	0.00000	0.00000	0.00000	0.00000	1.88971
A11	2.24697	0.00000	0.00000	0.00001	0.00002	2.24698
A12	2.14520	0.00000	0.00000	-0.00001	-0.00001	2.14519
A13	1.90146	0.00000	0.00000	0.00000	0.00000	1.90146
A14	2.22831	0.00000	-0.00002	0.00003	0.00001	2.22832
A15	2.15113	0.00000	0.00002	-0.00002	-0.00001	2.15112
A16	1.95878	0.00001	0.00002	0.00000	0.00001	1.95880
A17	1.86477	0.00000	0.00001	0.00001	0.00002	1.86479
A18	1.87526	-0.00001	-0.00001	0.00001	0.00001	1.87526
A19	1.88706	0.00000	-0.00001	0.00001	0.00000	1.88706
A20	1.96601	-0.00001	-0.00001	-0.00002	-0.00003	1.96598
A21	1.90904	0.00000	0.00000	0.00000	0.00000	1.90904
A22	1.92965	-0.00001	0.00000	0.00000	0.00000	1.92966
A23	1.89283	0.00001	0.00001	0.00003	0.00004	1.89287
A24	1.92654	0.00000	-0.00001	-0.00001	-0.00002	1.92652
A25	1.89508	0.00000	0.00001	-0.00001	0.00000	1.89508
A26	1.87659	0.00000	0.00001	0.00000	0.00001	1.87660
A27	1.94319	-0.00001	-0.00001	-0.00002	-0.00003	1.94316
A28	1.74089	0.00000	0.00001	0.00008	0.00009	1.74098
A29	2.17753	0.00000	-0.00001	0.00000	0.00000	2.17752
A30	1.95760	0.00000	-0.00001	0.00000	-0.00001	1.95759
A31	2.14805	0.00000	0.00001	0.00000	0.00001	2.14807
A32	2.07970	0.00000	0.00000	0.00001	0.00001	2.07972
A33	2.15775	0.00000	-0.00001	0.00001	0.00000	2.15776
A34	2.04573	0.00000	0.00000	-0.00002	-0.00002	2.04571
A35	1.85309	0.00000	0.00001	-0.00003	-0.00002	1.85306
D1	0.00443	0.00000	0.00001	0.00002	0.00002	0.00446
D2	-3.13681	0.00000	-0.00004	-0.00013	-0.00017	-3.13697
D3	3.14022	0.00000	-0.00007	0.00003	-0.00004	3.14018
D4	-0.00102	0.00000	-0.00012	-0.00011	-0.00023	-0.00125
D5	-0.00643	0.00000	-0.00001	0.00001	0.00001	-0.00643
D6	-3.07654	0.00000	-0.00003	0.00001	-0.00002	-3.07656
D7	3.14037	0.00000	0.00006	0.00000	0.00006	3.14043
D8	0.07026	0.00000	0.00004	-0.00001	0.00004	0.07030
D9	-0.00098	0.00000	0.00000	-0.00004	-0.00004	-0.00102
D10	3.13888	0.00000	-0.00002	0.00005	0.00004	3.13891

D11	3.14029	0.00000	0.00004	0.00009	0.00013	3.14042
D12	-0.00303	0.00000	0.00003	0.00018	0.00021	-0.00283
D13	-0.00302	0.00000	0.00000	0.00005	0.00004	-0.00297
D14	3.08412	0.00000	0.00003	0.00006	0.00008	3.08420
D15	3.14018	0.00000	0.00001	-0.00003	-0.00003	3.14016
D16	-0.05586	0.00000	0.00004	-0.00003	0.00001	-0.05585
D17	0.05324	0.00000	-0.00029	-0.00004	-0.00034	0.05290
D18	-3.08570	0.00000	-0.00029	-0.00004	-0.00034	-3.08603
D19	-3.09031	0.00000	-0.00031	0.00006	-0.00025	-3.09056
D20	0.05394	0.00000	-0.00031	0.00006	-0.00025	0.05369
D21	0.00582	0.00000	0.00001	-0.00004	-0.00003	0.00579
D22	3.07976	0.00000	0.00002	-0.00003	-0.00001	3.07976
D23	-3.08518	0.00000	-0.00002	-0.00005	-0.00007	-3.08525
D24	-0.01124	0.00000	-0.00001	-0.00004	-0.00004	-0.01128
D25	1.68519	0.00000	-0.00002	-0.00009	-0.00012	1.68507
D26	-2.53248	0.00000	-0.00001	-0.00008	-0.00009	-2.53258
D27	-0.48531	0.00000	-0.00001	-0.00008	-0.00009	-0.48540
D28	-1.37554	-0.00001	-0.00004	-0.00011	-0.00015	-1.37568
D29	0.68998	0.00000	-0.00003	-0.00009	-0.00012	0.68986
D30	2.73715	0.00000	-0.00003	-0.00009	-0.00012	2.73703
D31	-1.60211	0.00001	0.00002	0.00023	0.00025	-1.60186
D32	0.47379	0.00001	0.00003	0.00024	0.00028	0.47406
D33	2.60690	0.00001	0.00002	0.00023	0.00025	2.60715
D34	2.62878	0.00000	0.00000	0.00022	0.00021	2.62899
D35	-1.57851	0.00000	0.00001	0.00023	0.00024	-1.57827
D36	0.55461	0.00000	0.00000	0.00022	0.00022	0.55482
D37	0.51717	0.00000	0.00001	0.00023	0.00024	0.51741
D38	2.59307	0.00000	0.00002	0.00025	0.00027	2.59334
D39	-1.55700	0.00000	0.00001	0.00023	0.00024	-1.55676
D40	1.16895	0.00001	-0.00003	-0.00012	-0.00014	1.16881
D41	-3.01667	0.00001	-0.00002	-0.00010	-0.00012	-3.01678
D42	-0.95399	0.00001	-0.00001	-0.00011	-0.00012	-0.95411
D43	-1.30188	-0.00001	-0.00007	0.00006	0.00000	-1.30189
D44	2.87510	0.00000	-0.00006	0.00006	0.00000	2.87510
D45	0.80133	0.00001	-0.00007	0.00008	0.00001	0.80134
D46	-3.13556	0.00000	-0.00003	0.00001	-0.00001	-3.13557
D47	0.00608	0.00000	-0.00003	0.00001	-0.00002	0.00607
D48	0.00310	0.00000	-0.00003	0.00001	-0.00002	0.00308
D49	-3.13845	0.00000	-0.00003	0.00001	-0.00002	-3.13847

Item	Value	Threshold	Converged?
Maximum Force	0.000015	0.000450	YES
RMS Force	0.000004	0.000300	YES
Maximum Displacement	0.000738	0.001800	YES
RMS Displacement	0.000184	0.001200	YES

Predicted change in Energy=-4.990683D-09

Optimization completed.

-- Stationary point found.

Optimized Parameters (Angstroms and Degrees)				
Name	Definition	Value	Derivative Info.	
R1	R(1,2)	1.3581	-DE/DX =	0.0
R2	R(1,5)	1.3843	-DE/DX =	0.0
R3	R(1,8)	1.0764	-DE/DX =	0.0
R4	R(2,3)	1.3909	-DE/DX =	0.0
R5	R(2,9)	1.0746	-DE/DX =	0.0
R6	R(3,4)	1.3476	-DE/DX =	0.0
R7	R(3,16)	1.4219	-DE/DX =	0.0
R8	R(4,5)	1.3332	-DE/DX =	0.0
R9	R(4,15)	1.1056	-DE/DX =	0.0
R10	R(5,6)	1.4785	-DE/DX =	0.0
R11	R(6,7)	1.5514	-DE/DX =	0.0
R12	R(6,10)	1.0889	-DE/DX =	0.0
R13	R(6,11)	1.0904	-DE/DX =	0.0
R14	R(7,12)	1.0935	-DE/DX =	0.0
R15	R(7,13)	1.0964	-DE/DX =	0.0
R16	R(7,21)	1.4021	-DE/DX =	0.0
R17	R(13,14)	3.1922	-DE/DX =	0.0
R18	R(16,17)	1.3265	-DE/DX =	0.0
R19	R(16,18)	1.0826	-DE/DX =	0.0
R20	R(17,19)	1.0811	-DE/DX =	0.0
R21	R(17,20)	1.0825	-DE/DX =	0.0
R22	R(21,22)	0.9795	-DE/DX =	0.0
A1	A(2,1,5)	107.4488	-DE/DX =	0.0
A2	A(2,1,8)	130.4957	-DE/DX =	0.0
A3	A(5,1,8)	122.0547	-DE/DX =	0.0
A4	A(1,2,3)	106.6856	-DE/DX =	0.0
A5	A(1,2,9)	130.4813	-DE/DX =	0.0
A6	A(3,2,9)	122.8331	-DE/DX =	0.0
A7	A(2,3,4)	108.6462	-DE/DX =	0.0
A8	A(2,3,16)	128.6538	-DE/DX =	0.0
A9	A(4,3,16)	122.6999	-DE/DX =	0.0
A10	A(3,4,5)	108.2726	-DE/DX =	0.0
A11	A(3,4,15)	128.7417	-DE/DX =	0.0
A12	A(5,4,15)	122.9108	-DE/DX =	0.0
A13	A(1,5,4)	108.9455	-DE/DX =	0.0

! A14	A(1,5,6)	127.6728	-DE/DX =	0.0	!
! A15	A(4,5,6)	123.2506	-DE/DX =	0.0	!
! A16	A(5,6,7)	112.2301	-DE/DX =	0.0	!
! A17	A(5,6,10)	106.8437	-DE/DX =	0.0	!
! A18	A(5,6,11)	107.4442	-DE/DX =	0.0	!
! A19	A(7,6,10)	108.1204	-DE/DX =	0.0	!
! A20	A(7,6,11)	112.6442	-DE/DX =	0.0	!
! A21	A(10,6,11)	109.3802	-DE/DX =	0.0	!
! A22	A(6,7,12)	110.5609	-DE/DX =	0.0	!
! A23	A(6,7,13)	108.4511	-DE/DX =	0.0	!
! A24	A(6,7,21)	110.3828	-DE/DX =	0.0	!
! A25	A(12,7,13)	108.5799	-DE/DX =	0.0	!
! A26	A(12,7,21)	107.521	-DE/DX =	0.0	!
! A27	A(13,7,21)	111.3365	-DE/DX =	0.0	!
! A28	A(7,13,14)	99.7455	-DE/DX =	0.0	!
! A29	A(3,16,17)	124.7632	-DE/DX =	0.0	!
! A30	A(3,16,18)	112.1624	-DE/DX =	0.0	!
! A31	A(17,16,18)	123.0742	-DE/DX =	0.0	!
! A32	A(16,17,19)	119.1583	-DE/DX =	0.0	!
! A33	A(16,17,20)	123.6301	-DE/DX =	0.0	!
! A34	A(19,17,20)	117.2116	-DE/DX =	0.0	!
! A35	A(7,21,22)	106.174	-DE/DX =	0.0	!
! D1	D(5,1,2,3)	0.2541	-DE/DX =	0.0	!
! D2	D(5,1,2,9)	-179.7257	-DE/DX =	0.0	!
! D3	D(8,1,2,3)	179.9214	-DE/DX =	0.0	!
! D4	D(8,1,2,9)	-0.0584	-DE/DX =	0.0	!
! D5	D(2,1,5,4)	-0.3687	-DE/DX =	0.0	!
! D6	D(2,1,5,6)	-176.273	-DE/DX =	0.0	!
! D7	D(8,1,5,4)	179.9298	-DE/DX =	0.0	!
! D8	D(8,1,5,6)	4.0256	-DE/DX =	0.0	!
! D9	D(1,2,3,4)	-0.0561	-DE/DX =	0.0	!
! D10	D(1,2,3,16)	179.8445	-DE/DX =	0.0	!
! D11	D(9,2,3,4)	179.9256	-DE/DX =	0.0	!
! D12	D(9,2,3,16)	-0.1738	-DE/DX =	0.0	!
! D13	D(2,3,4,5)	-0.173	-DE/DX =	0.0	!
! D14	D(2,3,4,15)	176.707	-DE/DX =	0.0	!
! D15	D(16,3,4,5)	179.9192	-DE/DX =	0.0	!
! D16	D(16,3,4,15)	-3.2008	-DE/DX =	0.0	!
! D17	D(2,3,16,17)	3.0504	-DE/DX =	0.0	!
! D18	D(2,3,16,18)	-176.7973	-DE/DX =	0.0	!
! D19	D(4,3,16,17)	-177.0615	-DE/DX =	0.0	!
! D20	D(4,3,16,18)	3.0908	-DE/DX =	0.0	!
! D21	D(3,4,5,1)	0.3336	-DE/DX =	0.0	!
! D22	D(3,4,5,6)	176.4575	-DE/DX =	0.0	!

! D23	D(15,4,5,1)	-176.7679	-DE/DX =	0.0	!
! D24	D(15,4,5,6)	-0.644	-DE/DX =	0.0	!
! D25	D(1,5,6,7)	96.5542	-DE/DX =	0.0	!
! D26	D(1,5,6,10)	-145.1005	-DE/DX =	0.0	!
! D27	D(1,5,6,11)	-27.8065	-DE/DX =	0.0	!
! D28	D(4,5,6,7)	-78.8125	-DE/DX =	0.0	!
! D29	D(4,5,6,10)	39.5329	-DE/DX =	0.0	!
! D30	D(4,5,6,11)	156.8269	-DE/DX =	0.0	!
! D31	D(5,6,7,12)	-91.7942	-DE/DX =	0.0	!
! D32	D(5,6,7,13)	27.1459	-DE/DX =	0.0	!
! D33	D(5,6,7,21)	149.3646	-DE/DX =	0.0	!
! D34	D(10,6,7,12)	150.6178	-DE/DX =	0.0	!
! D35	D(10,6,7,13)	-90.4421	-DE/DX =	0.0	!
! D36	D(10,6,7,21)	31.7765	-DE/DX =	0.0	!
! D37	D(11,6,7,12)	29.6317	-DE/DX =	0.0	!
! D38	D(11,6,7,13)	148.5718	-DE/DX =	0.0	!
! D39	D(11,6,7,21)	-89.2095	-DE/DX =	0.0	!
! D40	D(6,7,13,14)	66.9758	-DE/DX =	0.0	!
! D41	D(12,7,13,14)	-172.8423	-DE/DX =	0.0	!
! D42	D(21,7,13,14)	-54.6596	-DE/DX =	0.0	!
! D43	D(6,7,21,22)	-74.5924	-DE/DX =	0.0	!
! D44	D(12,7,21,22)	164.7311	-DE/DX =	0.0	!
! D45	D(13,7,21,22)	45.9129	-DE/DX =	0.0	!
! D46	D(3,16,17,19)	-179.6544	-DE/DX =	0.0	!
! D47	D(3,16,17,20)	0.3485	-DE/DX =	0.0	!
! D48	D(18,16,17,19)	0.1774	-DE/DX =	0.0	!
! D49	D(18,16,17,20)	-179.8198	-DE/DX =	0.0	!

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.590351	-2.342598	-1.151156
2	6	0	-1.888186	-1.967183	-1.289309
3	7	0	-2.088691	-0.897145	-0.423688
4	6	0	-0.932419	-0.640489	0.219188
5	7	0	-0.015669	-1.509833	-0.206377
6	6	0	1.396830	-1.476810	0.229346
7	6	0	2.214660	-0.387265	-0.512801
8	1	0	-0.033941	-3.126125	-1.636015
9	1	0	-2.666050	-2.363259	-1.916041

10	1	0	1.393994	-1.233873	1.290838
11	1	0	1.805906	-2.477708	0.088310
12	1	0	2.683891	-0.802940	-1.408727
13	1	0	1.530261	0.413708	-0.816487
14	35	0	0.725834	1.554474	2.054295
15	1	0	-0.706029	0.166459	0.940179
16	6	0	-3.275774	-0.147552	-0.198191
17	6	0	-4.448198	-0.398915	-0.765385
18	1	0	-3.118304	0.667441	0.496750
19	1	0	-5.292661	0.234716	-0.532507
20	1	0	-4.616418	-1.212778	-1.459080
21	8	0	3.238066	0.101441	0.311627
22	1	0	2.803598	0.679357	0.972383

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.358086	0.000000			
3	N	2.205349	1.390857	0.000000		
4	C	2.211792	2.224673	1.347638	0.000000	
5	N	1.384328	2.210935	2.172564	1.333152	0.000000
6	C	2.569877	3.652138	3.593234	2.474861	1.478546
7	C	3.478349	4.464577	4.334369	3.240993	2.515636
8	H	1.076381	2.213950	3.264979	3.229152	2.157916
9	H	2.212239	1.074589	2.170242	3.245399	3.267386
10	H	3.336200	4.238821	3.896419	2.629208	2.074839
11	H	2.701218	3.975523	4.234172	3.300140	2.083689
12	H	3.627334	4.719492	4.874087	3.969155	3.038580
13	H	3.493740	4.192610	3.869037	2.872063	2.542075
14	Br	5.214827	5.514967	4.480222	3.306854	3.879489
15	H	3.268398	3.304624	2.214304	1.105552	2.145027
16	C	3.596924	2.535152	1.421937	2.430741	3.533293
17	C	4.337016	3.047561	2.435624	3.659023	4.603688
18	H	4.262214	3.412395	2.086921	2.562385	3.855029
19	H	5.397869	4.124507	3.399760	4.510292	5.567446
20	H	4.192913	2.835701	2.749739	4.088514	4.777489
21	O	4.771775	5.755055	5.469205	4.236973	3.667604
22	H	5.016026	5.842282	5.326244	4.033252	3.759028

		6	7	8	9	10
6	C	0.000000				
7	C	1.551366	0.000000			
8	H	2.871745	3.717414	0.000000		
9	H	4.679260	5.449309	2.754701	0.000000	
10	H	1.088941	2.154844	3.766442	5.295616	0.000000

11	H	1.090427	2.213225	2.603609	4.901930	1.778446
12	H	2.189500	1.093456	3.582661	5.595877	3.022779
13	H	2.164632	1.096442	3.955853	5.150689	2.678416
14	Br	3.601299	3.546397	6.008631	6.528176	2.967184
15	H	2.761817	3.308805	4.234334	4.289423	2.548330
16	C	4.876776	5.504663	4.631276	2.869169	5.020361
17	C	6.026252	6.667655	5.261306	2.891143	6.249513
18	H	5.005572	5.529205	5.334147	3.900159	4.960484
19	H	6.946872	7.533068	6.337753	3.944962	7.084680
20	H	6.251372	6.945542	4.969034	2.310055	6.609655
21	O	2.426477	1.402096	4.991645	6.774646	2.478410
22	H	2.679581	1.921016	5.416370	6.893298	2.397675

		11	12	13	14	15
11	H	0.000000				
12	H	2.411810	0.000000			
13	H	3.042191	1.778157	0.000000		
14	Br	4.614124	4.624273	3.192153	0.000000	
15	H	3.745279	4.236585	2.854471	2.284310	0.000000
16	C	5.597783	6.116579	4.878040	4.897290	2.828087
17	C	6.645600	7.172435	6.033651	6.207813	4.151196
18	H	5.857186	6.281586	4.837161	4.241482	2.503334
19	H	7.624455	8.091345	6.831175	6.682484	4.817743
20	H	6.726122	7.311978	6.390622	6.967148	4.790603
21	O	2.958540	2.021047	2.070447	3.385188	3.994394
22	H	3.426957	2.807351	2.211790	2.500693	3.547053

		16	17	18	19	20
16	C	0.000000				
17	C	1.326451	0.000000			
18	H	1.082568	2.121018	0.000000		
19	H	2.079839	1.081128	2.444268	0.000000	
20	H	2.126470	1.082536	3.099168	1.846911	0.000000
21	O	6.538502	7.777465	6.384204	8.573425	8.158155
22	H	6.246021	7.534657	5.940984	8.246927	8.034229

		21	22
21	O	0.000000	
22	H	0.979463	0.000000

Stoichiometry C7H11BrN2O
Framework group C1[X(C7H11BrN2O)]
Deg. of freedom 60
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.852977	-2.004770	0.261946
2	6	0	-2.844936	-1.108684	0.022270
3	7	0	-2.252596	0.149697	0.012664
4	6	0	-0.932640	0.006366	0.243529
5	7	0	-0.674460	-1.291997	0.401298
6	6	0	0.688990	-1.829559	0.596565
7	6	0	1.478350	-1.925642	-0.735506
8	1	0	-1.885737	-3.077123	0.349012
9	1	0	-3.896876	-1.258715	-0.137907
10	1	0	1.211914	-1.133502	1.250666
11	1	0	0.591782	-2.793267	1.097412
12	1	0	1.344868	-2.910804	-1.190791
13	1	0	1.089622	-1.166684	-1.424751
14	35	0	2.025502	1.477383	0.099347
15	1	0	-0.144502	0.781540	0.257320
16	6	0	-2.862333	1.416758	-0.198718
17	6	0	-4.162812	1.610481	-0.373924
18	1	0	-2.139017	2.222199	-0.204304
19	1	0	-4.528939	2.615146	-0.533412
20	1	0	-4.894120	0.812340	-0.367232
21	8	0	2.850009	-1.749930	-0.504093
22	1	0	2.977890	-0.793667	-0.335111

Rotational constants (GHZ): 0.9807504 0.4478907 0.3185454

****

Population analysis using the SCF density.

****

Orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A)
The electronic state is 1-A.
Alpha occ. eigenvalues -- -482.70344 -62.35689 -56.17473 -56.17453 -56.17451
Alpha occ. eigenvalues -- -19.11011 -14.46076 -14.44739 -10.30312 -10.27890
Alpha occ. eigenvalues -- -10.27819 -10.27687 -10.24359 -10.23038 -10.22789
Alpha occ. eigenvalues -- -8.56605 -6.38938 -6.38881 -6.38847 -2.50174
Alpha occ. eigenvalues -- -2.50171 -2.50137 -2.50093 -2.50092 -1.12313
Alpha occ. eigenvalues -- -1.02041 -1.00671 -0.86175 -0.83162 -0.78464
Alpha occ. eigenvalues -- -0.72065 -0.68880 -0.65898 -0.64273 -0.63841
Alpha occ. eigenvalues -- -0.59189 -0.54909 -0.54010 -0.52699 -0.51722
Alpha occ. eigenvalues -- -0.50204 -0.49937 -0.48672 -0.47004 -0.45009
Alpha occ. eigenvalues -- -0.44338 -0.40510 -0.39518 -0.34166 -0.31967
Alpha occ. eigenvalues -- -0.31057 -0.27540 -0.20763 -0.20491 -0.19986
Alpha virt. eigenvalues -- -0.09100 -0.05220 -0.03532 -0.02036 -0.01421
Alpha virt. eigenvalues -- -0.00985 0.00400 0.00793 0.00842 0.02278
Alpha virt. eigenvalues -- 0.03379 0.03644 0.04392 0.04680 0.05467
Alpha virt. eigenvalues -- 0.05953 0.06501 0.07162 0.07629 0.07894
Alpha virt. eigenvalues -- 0.08288 0.08468 0.09001 0.09186 0.10028
Alpha virt. eigenvalues -- 0.10375 0.10867 0.11154 0.11587 0.11959
Alpha virt. eigenvalues -- 0.12475 0.12623 0.13089 0.13420 0.13605
Alpha virt. eigenvalues -- 0.14194 0.14564 0.14842 0.15220 0.15700
Alpha virt. eigenvalues -- 0.16083 0.16268 0.16788 0.17299 0.18029
Alpha virt. eigenvalues -- 0.18578 0.19172 0.19738 0.20700 0.20756
Alpha virt. eigenvalues -- 0.21591 0.21827 0.22300 0.22956 0.23280

Alpha virt. eigenvalues --	0.24269	0.24413	0.24754	0.25256	0.26908
Alpha virt. eigenvalues --	0.27110	0.27866	0.28258	0.28679	0.29736
Alpha virt. eigenvalues --	0.30186	0.31292	0.32181	0.33073	0.33928
Alpha virt. eigenvalues --	0.34858	0.35216	0.35612	0.35804	0.38156
Alpha virt. eigenvalues --	0.39211	0.40300	0.41249	0.42702	0.45710
Alpha virt. eigenvalues --	0.46666	0.47702	0.49104	0.50266	0.51665
Alpha virt. eigenvalues --	0.51968	0.53026	0.53249	0.54363	0.54904
Alpha virt. eigenvalues --	0.55958	0.57493	0.58068	0.58990	0.60253
Alpha virt. eigenvalues --	0.61041	0.61756	0.62385	0.63576	0.63887
Alpha virt. eigenvalues --	0.65452	0.67064	0.68067	0.68365	0.69308
Alpha virt. eigenvalues --	0.69572	0.72003	0.73094	0.73201	0.74386
Alpha virt. eigenvalues --	0.75203	0.76112	0.76450	0.77044	0.78981
Alpha virt. eigenvalues --	0.79374	0.80365	0.80771	0.82384	0.84062
Alpha virt. eigenvalues --	0.85240	0.87544	0.88743	0.90058	0.91918
Alpha virt. eigenvalues --	0.93511	0.96003	0.98271	0.98891	1.00184
Alpha virt. eigenvalues --	1.02546	1.03282	1.03625	1.04982	1.07433
Alpha virt. eigenvalues --	1.09678	1.10699	1.11830	1.13486	1.14762
Alpha virt. eigenvalues --	1.16489	1.20122	1.24470	1.27431	1.28251
Alpha virt. eigenvalues --	1.32073	1.35984	1.38102	1.40326	1.43557
Alpha virt. eigenvalues --	1.45373	1.47553	1.48143	1.49226	1.50097
Alpha virt. eigenvalues --	1.52444	1.53983	1.54433	1.57413	1.58531
Alpha virt. eigenvalues --	1.59100	1.60376	1.60915	1.63131	1.65745
Alpha virt. eigenvalues --	1.68186	1.68577	1.69475	1.70096	1.71318
Alpha virt. eigenvalues --	1.72837	1.74721	1.75744	1.76834	1.80296
Alpha virt. eigenvalues --	1.80587	1.84014	1.85155	1.85482	1.89170
Alpha virt. eigenvalues --	1.93059	1.94312	1.96185	2.00102	2.02965
Alpha virt. eigenvalues --	2.04157	2.04779	2.07261	2.08765	2.09394
Alpha virt. eigenvalues --	2.10324	2.12093	2.14354	2.15672	2.16053
Alpha virt. eigenvalues --	2.18935	2.21478	2.25524	2.26977	2.28165
Alpha virt. eigenvalues --	2.34675	2.38722	2.41907	2.43739	2.44265
Alpha virt. eigenvalues --	2.45841	2.48559	2.50293	2.51250	2.55175
Alpha virt. eigenvalues --	2.55556	2.57379	2.58431	2.59925	2.60216
Alpha virt. eigenvalues --	2.62918	2.66273	2.70243	2.70772	2.71499
Alpha virt. eigenvalues --	2.72838	2.74243	2.74955	2.78158	2.78824
Alpha virt. eigenvalues --	2.79940	2.81590	2.83872	2.86225	2.88815
Alpha virt. eigenvalues --	2.92808	2.94018	2.95003	3.00257	3.07407
Alpha virt. eigenvalues --	3.10195	3.13701	3.14703	3.24918	3.26417
Alpha virt. eigenvalues --	3.34433	3.36426	3.48329	3.53525	3.58802
Alpha virt. eigenvalues --	3.62563	3.63708	3.70872	3.74755	3.75638
Alpha virt. eigenvalues --	3.81061	3.82791	3.84163	3.86766	3.88868
Alpha virt. eigenvalues --	4.04590	4.05654	4.07703	4.18389	4.26048
Alpha virt. eigenvalues --	4.28825	4.31159	4.34263	4.40830	4.68000
Alpha virt. eigenvalues --	4.90310	5.01493	5.08850	5.21787	5.42004
Alpha virt. eigenvalues --	5.65783	6.77203	7.67771	7.71848	7.73522

Alpha virt. eigenvalues -- 23.68647 23.73544 23.81872 23.86775 23.87493
Alpha virt. eigenvalues -- 24.12680 24.21589 35.42994 35.55942 48.05394
Alpha virt. eigenvalues -- 49.93631 289.88506 289.92678 289.939621020.84375
Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	9.001856	-3.090748	0.792057	-1.147260	-0.669792	0.573366
2	C	-3.090748	8.588925	-0.564681	0.988740	0.903402	-0.597729
3	N	0.792057	-0.564681	6.899395	-0.171518	-0.462845	0.145747
4	C	-1.147260	0.988740	-0.171518	7.232453	0.815326	-0.425745
5	N	-0.669792	0.903402	-0.462845	0.815326	7.016248	-0.124695
6	C	0.573366	-0.597729	0.145747	-0.425745	-0.124695	6.159868
7	C	-0.154926	0.176042	-0.074333	0.006855	0.058244	-0.087755
8	H	0.556402	-0.168238	0.042471	-0.002945	-0.091510	0.010863
9	H	-0.129448	0.531118	-0.081759	-0.000015	0.029167	0.000371
10	H	0.095707	-0.098641	0.030461	-0.022639	-0.079430	0.494107
11	H	-0.123533	0.123952	0.002113	0.026442	-0.020459	0.265022
12	H	0.095183	-0.111469	0.016461	-0.044752	-0.047625	0.103179
13	H	-0.166390	0.154509	-0.043098	0.093357	0.069180	-0.150875
14	Br	-0.018266	0.003702	0.002446	-0.205136	-0.023741	0.070408
15	H	0.127192	-0.239601	0.095881	-0.574012	-0.204641	0.066613
16	C	0.606604	-0.580996	0.290393	-0.500787	-0.149555	0.015365
17	C	-0.181072	0.066291	-0.023358	-0.180137	-0.070536	-0.037205
18	H	-0.025671	0.042403	-0.088474	0.123329	0.025733	-0.007070
19	H	-0.003339	0.004123	0.022249	-0.003832	-0.000568	0.000723
20	H	-0.003026	0.007890	-0.035751	0.007444	0.002182	-0.001734
21	O	-0.022738	0.021648	-0.005104	0.010007	0.017361	-0.163419
22	H	-0.006479	0.004749	-0.000929	0.013254	-0.000930	0.021194

		7	8	9	10	11	12
1	C	-0.154926	0.556402	-0.129448	0.095707	-0.123533	0.095183
2	C	0.176042	-0.168238	0.531118	-0.098641	0.123952	-0.111469
3	N	-0.074333	0.042471	-0.081759	0.030461	0.002113	0.016461
4	C	0.006855	-0.002945	-0.000015	-0.022639	0.026442	-0.044752
5	N	0.058244	-0.091510	0.029167	-0.079430	-0.020459	-0.047625
6	C	-0.087755	0.010863	0.000371	0.494107	0.265022	0.103179
7	C	5.656262	-0.000645	-0.000387	-0.057987	-0.128785	0.350653
8	H	-0.000645	0.490710	-0.010988	0.007945	-0.029989	0.005703
9	H	-0.000387	-0.010988	0.500643	-0.000256	0.004351	-0.001170
10	H	-0.057987	0.007945	-0.000256	0.487326	-0.077823	0.023462
11	H	-0.128785	-0.029989	0.004351	-0.077823	0.772583	-0.031998
12	H	0.350653	0.005703	-0.001170	0.023462	-0.031998	0.656810
13	H	0.342474	-0.007650	0.001508	-0.041553	0.045976	-0.104605
14	Br	0.020008	-0.001565	-0.000865	-0.025304	0.023095	0.006328
15	H	-0.041270	-0.003469	-0.004035	-0.009940	0.014883	0.020580
16	C	-0.024295	0.013755	0.008223	0.018184	-0.006570	0.003601

17	C	-0.002142	-0.002460	-0.014125	-0.004112	0.000937	0.000684
18	H	0.003797	0.000451	0.001600	0.001007	-0.002570	-0.000670
19	H	-0.000265	-0.000263	-0.000424	-0.000137	0.000273	-0.000013
20	H	0.000407	0.000855	0.004217	0.000089	-0.000674	0.000025
21	O	0.281328	-0.001909	0.000006	-0.054282	0.039234	-0.104606
22	H	-0.038288	-0.000256	0.000167	0.016160	0.007868	0.009875

		13	14	15	16	17	18
1	C	-0.166390	-0.018266	0.127192	0.606604	-0.181072	-0.025671
2	C	0.154509	0.003702	-0.239601	-0.580996	0.066291	0.042403
3	N	-0.043098	0.002446	0.095881	0.290393	-0.023358	-0.088474
4	C	0.093357	-0.205136	-0.574012	-0.500787	-0.180137	0.123329
5	N	0.069180	-0.023741	-0.204641	-0.149555	-0.070536	0.025733
6	C	-0.150875	0.070408	0.066613	0.015365	-0.037205	-0.007070
7	C	0.342474	0.020008	-0.041270	-0.024295	-0.002142	0.003797
8	H	-0.007650	-0.001565	-0.003469	0.013755	-0.002460	0.000451
9	H	0.001508	-0.000865	-0.004035	0.008223	-0.014125	0.001600
10	H	-0.041553	-0.025304	-0.009940	0.018184	-0.004112	0.001007
11	H	0.045976	0.023095	0.014883	-0.006570	0.000937	-0.002570
12	H	-0.104605	0.006328	0.020580	0.003601	0.000684	-0.000670
13	H	0.695274	-0.017474	-0.060877	-0.020042	-0.000606	0.001163
14	Br	-0.017474	35.521855	0.269529	0.020508	0.031102	-0.006875
15	H	-0.060877	0.269529	1.377869	0.058817	0.151323	-0.068199
16	C	-0.020042	0.020508	0.058817	6.194639	-0.363285	0.420386
17	C	-0.000606	0.031102	0.151323	-0.363285	6.385109	-0.102313
18	H	0.001163	-0.006875	-0.068199	0.420386	-0.102313	0.469315
19	H	0.000159	-0.000249	0.003645	-0.088629	0.443742	-0.009619
20	H	-0.000180	0.000408	0.002881	0.064286	0.308239	0.004557
21	O	0.008371	-0.080035	0.002681	-0.000065	0.000488	0.000081
22	H	-0.010733	0.054406	-0.032746	-0.002482	-0.000701	0.000404

		19	20	21	22
1	C	-0.003339	-0.003026	-0.022738	-0.006479
2	C	0.004123	0.007890	0.021648	0.004749
3	N	0.022249	-0.035751	-0.005104	-0.000929
4	C	-0.003832	0.007444	0.010007	0.013254
5	N	-0.000568	0.002182	0.017361	-0.000930
6	C	0.000723	-0.001734	-0.163419	0.021194
7	C	-0.000265	0.000407	0.281328	-0.038288
8	H	-0.000263	0.000855	-0.001909	-0.000256
9	H	-0.000424	0.004217	0.000006	0.000167
10	H	-0.000137	0.000089	-0.054282	0.016160
11	H	0.000273	-0.000674	0.039234	0.007868
12	H	-0.000013	0.000025	-0.104606	0.009875
13	H	0.000159	-0.000180	0.008371	-0.010733
14	Br	-0.000249	0.000408	-0.080035	0.054406

15	H	0.003645	0.002881	0.002681	-0.032746
16	C	-0.088629	0.064286	-0.000065	-0.002482
17	C	0.443742	0.308239	0.000488	-0.000701
18	H	-0.009619	0.004557	0.000081	0.000404
19	H	0.462928	-0.021880	-0.000002	0.000001
20	H	-0.021880	0.533576	0.000009	-0.000028
21	O	-0.000002	0.000009	8.011925	0.244299
22	H	0.000001	-0.000028	0.244299	0.480646

Mulliken charges:

		1
1	C	-0.105679
2	C	-0.165389
3	N	0.212175
4	C	-0.038430
5	N	0.009484
6	C	-0.330599
7	C	-0.284993
8	H	0.192733
9	H	0.162099
10	H	0.297656
11	H	0.095672
12	H	0.154365
13	H	0.212112
14	Br	-0.644286
15	H	0.046899
16	C	0.021944
17	C	-0.405862
18	H	0.217234
19	H	0.191378
20	H	0.126210
21	O	-0.205274
22	H	0.240551

Sum of Mulliken charges = 0.00000

Mulliken charges with hydrogens summed into heavy atoms:

		1
1	C	0.087053
2	C	-0.003289
3	N	0.212175
4	C	0.008469
5	N	0.009484
6	C	0.062729
7	C	0.081484
14	Br	-0.644286
16	C	0.239178

17 C -0.088274

21 O 0.035277

Electronic spatial extent (au): <R**2>= 3206.9553

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= -13.0430 Y= -5.1781 Z= 0.3424 Tot= 14.0374

Quadrupole moment (field-independent basis, Debye-Ang):

XX= -79.8169 YY= -77.6950 ZZ= -83.8935

XY= -5.2877 XZ= 2.3249 YZ= -3.3506

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

XX= 0.6515 YY= 2.7735 ZZ= -3.4251

XY= -5.2877 XZ= 2.3249 YZ= -3.3506

Octapole moment (field-independent basis, Debye-Ang**2):

XXX= -79.0609 YYY= 4.0755 ZZZ= 2.8410 XYY= -36.4695

XXY= 17.3660 XXZ= -4.3327 XZZ= 24.6484 YZZ= 5.9461

YYZ= 2.6467 XYZ= -0.8545

Hexadecapole moment (field-independent basis, Debye-Ang**3):

XXXX= -2395.0034 YYYY= -1129.5204 ZZZZ= -187.5030 XXXY= 64.4104

XXXZ= 58.0491 YYYX= 45.3594 YYYZ= -17.3619 ZZZX= -2.7305

ZZZY= 5.8415 XXYY= -650.6553 XXZZ= -512.4103 YYZZ= -241.8027

XXYZ= -28.4103 YYXZ= 11.7179 ZZXY= 19.9296

N-N= 8.516537666465D+02 E-N=-8.924479410266D+03 KE= 3.027345417297D+03

1\1\GINC-CN004\FOpt\RB3LYP\6-311++G(d,p)\C7H11Br1N2O1\SYWANG\17-Jul-2024\0\\# opt b3lyp/6-311++g(d,p)\\oh\\0,1\C,-0.5903513936,-2.3425976974,-1.1511557446\C,-1.8881856651,-1.9671829416,-1.2893092811\N,-2.0886913986,-0.8971453559,-0.4236879911\C,-0.9324188073,-0.6404888238,0.2191875491\N,-0.0156689265,-1.5098327489,-0.2063765756\C,1.3968304869,-1.4768100587,0.2293461475\C,2.2146604268,-0.387265335,-0.5128010194\H,-0.0339409631,-3.1261247975,-1.6360150768\H,-2.6660501053,-2.3632589804,-1.9160413981\H,1.3939936111,-1.2338729219,1.2908383565\H,1.8059061832,-2.4777078875,0.0883102713\H,2.6838911354,-0.8029398666,-1.4087268585\H,1.5302611762,0.4137080316,-0.8164872025\Br,0.7258344509,1.5544737195,2.0542949251\H,-0.7060291385,0.1664586154,0.9401792119\C,-3.2757737978,-0.1475522001,-0.1981905918\C,-4.4481982793,-0.3989150612,-0.7653849344\H,-3.1183038447,0.6674411832,0.4967495449\H,-5.2926607776,0.2347157257,-0.5325065338\H,-4.6164180047,-1.2127782897,-1.4590800636\O,3.2380655227,0.1014406302,0.3116274166\H,2.8035980389,0.6793567806,0.9723834283\\Version=EM64L-G09RevD.01\State=1-A\HF=-3032.343299\RMSD=7.813e-09

\RMSF=5.055e-06\Dipole=-3.1505972,-3.3903698,-3.0132901\Quadrupole=4.0
793817,-0.7575616,-3.3218201,-3.8145587,1.1863284,-0.2254718\PG=C01 [X
(C7H11Br1N2O1)]\\@

THE ONLY TROUBLE WITH A SURE THING IS THE UNCERTAINTY.
-- FROM A TEABAG (BELONGING TO W.H.?)
Job cpu time: 0 days 15 hours 25 minutes 51.3 seconds.
File lengths (MBytes): RWF= 54 Int= 0 D2E= 0 Chk= 10 Scr= 1
Normal termination of Gaussian 09 at Wed Jul 17 23:44:55 2024.

Entering Gaussian System, Link 0=g09
Input=coohpo.gjf
Output=coohpo.log
Initial command:
/apps/gaussian/09_D01/g09/l1.exe "/scr/tmp/sywang/91540/Gau-12118.inp" -
scrdir="/scr/tmp/sywang/91540/"
Entering Link 1 = /apps/gaussian/09_D01/g09/l1.exe PID= 12119.

Cite this work as:
Gaussian 09, Revision D.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci,
G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian,
A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada,
M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima,
Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr.,
J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers,
K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand,
K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi,
M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross,
V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,
O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,
R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth,
P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels,
O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski,
and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

```
*****************************************
Gaussian 09:    EM64L-G09RevD.01 24-Apr-2013
                      22-Jul-2024
*****************************************
%chk=./coohpo.chk
%mem=40000MB
%nprocl=1
Will use up to        1 processors via Linda.
%nprocs=28
Will use up to      28 processors via shared memory.
-------------------------
# opt b3lyp/6-311++g(d,p)
-------------------------
1/14=-1,18=20,19=15,26=3,38=1/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=4,6=6,7=1111,11=2,16=1,25=1,30=1,71=1,74=-5/1,2,3;
4//1;
5/5=2,38=5/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(2);
2/9=110/2;
99//99;
2/9=110/2;
3/5=4,6=6,7=1111,11=2,16=1,25=1,30=1,71=1,74=-5/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;
------
coohpo
------
Symbolic Z-matrix:
Charge =    0 Multiplicity = 1
C                            -0.77922      1.02656      1.29428
C                            -1.67954      0.01913      1.40352
N                            -2.83723      0.43343      0.7507
C                            -2.62996      1.66277      0.25318
N                            -1.39665      2.0536       0.5918
C                            -0.78206      3.28912      0.10907
H                             0.24415      1.09159      1.61862
```

H	-1.59565	-0.95715	1.84533
H	-1.57343	4.00119	-0.11908
H	-0.16137	3.71831	0.89864
Br	-0.55106	-2.14655	-0.81344
H	-3.31028	2.19158	-0.40226
C	-4.01261	-0.33124	0.47334
C	-4.47289	-1.27168	1.28812
H	-4.45085	-0.0644	-0.48573
H	-5.34207	-1.84678	0.99773
H	-4.017	-1.50122	2.24427
C	3.39288	-0.64931	0.68001
C	4.42475	0.06634	1.44968
O	3.38483	0.80092	0.76676
H	3.65828	-1.02962	-0.30468
H	2.53806	-1.13038	1.15403
H	4.31436	0.10275	2.53281
C	5.824	0.26498	0.93197
H	6.22389	1.22605	1.26108
H	6.47842	-0.52275	1.31317
H	5.83802	0.23554	-0.15795
C	0.04762	3.12691	-1.17815
H	0.47107	4.07095	-1.45088
H	-0.58411	2.77781	-1.96805
C	1.17707	2.10844	-0.93595
O	1.24321	0.91497	-1.22718
O	2.24106	2.66108	-0.30041
H	2.93738	1.99875	-0.16036

Add virtual bond connecting atoms H34 and O20 Dist= 2.98D+00.
Add virtual bond connecting atoms Br11 and H8 Dist= 5.85D+00.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Initialization pass.

! Initial Parameters !
! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.	!
! R1	R(1,2)	1.3555	estimate D2E/DX2	!
! R2	R(1,5)	1.3891	estimate D2E/DX2	!
! R3	R(1,7)	1.0755	estimate D2E/DX2	!
! R4	R(2,3)	1.3921	estimate D2E/DX2	!

! R5	R(2,8)	1.0749	estimate D2E/DX2	!
! R6	R(3,4)	1.3423	estimate D2E/DX2	!
! R7	R(3,13)	1.4294	estimate D2E/DX2	!
! R8	R(4,5)	1.3373	estimate D2E/DX2	!
! R9	R(4,12)	1.0826	estimate D2E/DX2	!
! R10	R(5,6)	1.4619	estimate D2E/DX2	!
! R11	R(6,9)	1.0887	estimate D2E/DX2	!
! R12	R(6,10)	1.0922	estimate D2E/DX2	!
! R13	R(6,28)	1.54	estimate D2E/DX2	!
! R14	R(8,11)	3.0943	estimate D2E/DX2	!
! R15	R(13,14)	1.3267	estimate D2E/DX2	!
! R16	R(13,15)	1.0877	estimate D2E/DX2	!
! R17	R(14,16)	1.0819	estimate D2E/DX2	!
! R18	R(14,17)	1.0839	estimate D2E/DX2	!
! R19	R(18,19)	1.4729	estimate D2E/DX2	!
! R20	R(18,20)	1.4528	estimate D2E/DX2	!
! R21	R(18,21)	1.0884	estimate D2E/DX2	!
! R22	R(18,22)	1.0894	estimate D2E/DX2	!
! R23	R(19,20)	1.4448	estimate D2E/DX2	!
! R24	R(19,23)	1.0893	estimate D2E/DX2	!
! R25	R(19,24)	1.5051	estimate D2E/DX2	!
! R26	R(20,34)	1.5794	estimate D2E/DX2	!
! R27	R(24,25)	1.0917	estimate D2E/DX2	!
! R28	R(24,26)	1.0927	estimate D2E/DX2	!
! R29	R(24,27)	1.0904	estimate D2E/DX2	!
! R30	R(28,29)	1.07	estimate D2E/DX2	!
! R31	R(28,30)	1.07	estimate D2E/DX2	!
! R32	R(28,31)	1.54	estimate D2E/DX2	!
! R33	R(31,32)	1.2303	estimate D2E/DX2	!
! R34	R(31,33)	1.357	estimate D2E/DX2	!
! R35	R(33,34)	0.9712	estimate D2E/DX2	!
! A1	A(2,1,5)	107.1598	estimate D2E/DX2	!
! A2	A(2,1,7)	130.7398	estimate D2E/DX2	!
! A3	A(5,1,7)	122.0563	estimate D2E/DX2	!
! A4	A(1,2,3)	107.0596	estimate D2E/DX2	!
! A5	A(1,2,8)	131.0198	estimate D2E/DX2	!
! A6	A(3,2,8)	121.8671	estimate D2E/DX2	!
! A7	A(2,3,4)	108.5393	estimate D2E/DX2	!
! A8	A(2,3,13)	127.9956	estimate D2E/DX2	!
! A9	A(4,3,13)	123.0241	estimate D2E/DX2	!
! A10	A(3,4,5)	108.4336	estimate D2E/DX2	!
! A11	A(3,4,12)	125.0795	estimate D2E/DX2	!
! A12	A(5,4,12)	126.1614	estimate D2E/DX2	!
! A13	A(1,5,4)	108.7769	estimate D2E/DX2	!

! A14	A(1,5,6)	127.2284	estimate D2E/DX2	!
! A15	A(4,5,6)	123.4404	estimate D2E/DX2	!
! A16	A(5,6,9)	108.4433	estimate D2E/DX2	!
! A17	A(5,6,10)	109.4083	estimate D2E/DX2	!
! A18	A(5,6,28)	114.4233	estimate D2E/DX2	!
! A19	A(9,6,10)	107.9122	estimate D2E/DX2	!
! A20	A(9,6,28)	106.5787	estimate D2E/DX2	!
! A21	A(10,6,28)	109.8447	estimate D2E/DX2	!
! A22	A(2,8,11)	91.2774	estimate D2E/DX2	!
! A23	A(3,13,14)	123.0467	estimate D2E/DX2	!
! A24	A(3,13,15)	111.7876	estimate D2E/DX2	!
! A25	A(14,13,15)	125.1437	estimate D2E/DX2	!
! A26	A(13,14,16)	119.3852	estimate D2E/DX2	!
! A27	A(13,14,17)	123.0908	estimate D2E/DX2	!
! A28	A(16,14,17)	117.5239	estimate D2E/DX2	!
! A29	A(19,18,21)	118.145	estimate D2E/DX2	!
! A30	A(19,18,22)	122.4732	estimate D2E/DX2	!
! A31	A(20,18,21)	113.8385	estimate D2E/DX2	!
! A32	A(20,18,22)	114.2339	estimate D2E/DX2	!
! A33	A(21,18,22)	115.5103	estimate D2E/DX2	!
! A34	A(18,19,23)	117.6989	estimate D2E/DX2	!
! A35	A(18,19,24)	122.391	estimate D2E/DX2	!
! A36	A(20,19,23)	112.3366	estimate D2E/DX2	!
! A37	A(20,19,24)	116.0694	estimate D2E/DX2	!
! A38	A(23,19,24)	115.5821	estimate D2E/DX2	!
! A39	A(18,20,34)	136.3485	estimate D2E/DX2	!
! A40	A(19,20,34)	150.1083	estimate D2E/DX2	!
! A41	A(19,24,25)	110.6722	estimate D2E/DX2	!
! A42	A(19,24,26)	109.9757	estimate D2E/DX2	!
! A43	A(19,24,27)	110.6223	estimate D2E/DX2	!
! A44	A(25,24,26)	108.0632	estimate D2E/DX2	!
! A45	A(25,24,27)	108.6857	estimate D2E/DX2	!
! A46	A(26,24,27)	108.7551	estimate D2E/DX2	!
! A47	A(6,28,29)	109.4712	estimate D2E/DX2	!
! A48	A(6,28,30)	109.4712	estimate D2E/DX2	!
! A49	A(6,28,31)	109.4712	estimate D2E/DX2	!
! A50	A(29,28,30)	109.4712	estimate D2E/DX2	!
! A51	A(29,28,31)	109.4713	estimate D2E/DX2	!
! A52	A(30,28,31)	109.4712	estimate D2E/DX2	!
! A53	A(28,31,32)	130.0733	estimate D2E/DX2	!
! A54	A(28,31,33)	112.2947	estimate D2E/DX2	!
! A55	A(32,31,33)	117.632	estimate D2E/DX2	!
! A56	A(31,33,34)	110.6079	estimate D2E/DX2	!
! A57	A(20,34,33)	143.6104	estimate D2E/DX2	!

! D1	D(5,1,2,3)	0.7263	estimate D2E/DX2	!
! D2	D(5,1,2,8)	178.0396	estimate D2E/DX2	!
! D3	D(7,1,2,3)	-176.8406	estimate D2E/DX2	!
! D4	D(7,1,2,8)	0.4727	estimate D2E/DX2	!
! D5	D(2,1,5,4)	-1.5812	estimate D2E/DX2	!
! D6	D(2,1,5,6)	-173.2019	estimate D2E/DX2	!
! D7	D(7,1,5,4)	176.2437	estimate D2E/DX2	!
! D8	D(7,1,5,6)	4.623	estimate D2E/DX2	!
! D9	D(1,2,3,4)	0.3676	estimate D2E/DX2	!
! D10	D(1,2,3,13)	172.841	estimate D2E/DX2	!
! D11	D(8,2,3,4)	-177.2458	estimate D2E/DX2	!
! D12	D(8,2,3,13)	-4.7724	estimate D2E/DX2	!
! D13	D(1,2,8,11)	-88.2966	estimate D2E/DX2	!
! D14	D(3,2,8,11)	88.6788	estimate D2E/DX2	!
! D15	D(2,3,4,5)	-1.3616	estimate D2E/DX2	!
! D16	D(2,3,4,12)	172.4143	estimate D2E/DX2	!
! D17	D(13,3,4,5)	-174.2897	estimate D2E/DX2	!
! D18	D(13,3,4,12)	-0.5138	estimate D2E/DX2	!
! D19	D(2,3,13,14)	34.233	estimate D2E/DX2	!
! D20	D(2,3,13,15)	-144.1395	estimate D2E/DX2	!
! D21	D(4,3,13,14)	-154.2849	estimate D2E/DX2	!
! D22	D(4,3,13,15)	27.3425	estimate D2E/DX2	!
! D23	D(3,4,5,1)	1.8215	estimate D2E/DX2	!
! D24	D(3,4,5,6)	173.8286	estimate D2E/DX2	!
! D25	D(12,4,5,1)	-171.8693	estimate D2E/DX2	!
! D26	D(12,4,5,6)	0.1379	estimate D2E/DX2	!
! D27	D(1,5,6,9)	-162.7188	estimate D2E/DX2	!
! D28	D(1,5,6,10)	-45.2515	estimate D2E/DX2	!
! D29	D(1,5,6,28)	78.4791	estimate D2E/DX2	!
! D30	D(4,5,6,9)	26.7982	estimate D2E/DX2	!
! D31	D(4,5,6,10)	144.2655	estimate D2E/DX2	!
! D32	D(4,5,6,28)	-92.0039	estimate D2E/DX2	!
! D33	D(5,6,28,29)	-179.1381	estimate D2E/DX2	!
! D34	D(5,6,28,30)	60.8619	estimate D2E/DX2	!
! D35	D(5,6,28,31)	-59.1381	estimate D2E/DX2	!
! D36	D(9,6,28,29)	61.0124	estimate D2E/DX2	!
! D37	D(9,6,28,30)	-58.9875	estimate D2E/DX2	!
! D38	D(9,6,28,31)	-178.9875	estimate D2E/DX2	!
! D39	D(10,6,28,29)	-55.6417	estimate D2E/DX2	!
! D40	D(10,6,28,30)	-175.6417	estimate D2E/DX2	!
! D41	D(10,6,28,31)	64.3584	estimate D2E/DX2	!
! D42	D(3,13,14,16)	-177.1421	estimate D2E/DX2	!
! D43	D(3,13,14,17)	2.7111	estimate D2E/DX2	!
! D44	D(15,13,14,16)	1.0097	estimate D2E/DX2	!

! D45	D(15,13,14,17)	-179.137	estimate D2E/DX2	!
! D46	D(21,18,19,23)	-156.6265	estimate D2E/DX2	!
! D47	D(21,18,19,24)	-1.0377	estimate D2E/DX2	!
! D48	D(22,18,19,23)	0.2129	estimate D2E/DX2	!
! D49	D(22,18,19,24)	155.8016	estimate D2E/DX2	!
! D50	D(21,18,20,34)	39.1834	estimate D2E/DX2	!
! D51	D(22,18,20,34)	-96.4792	estimate D2E/DX2	!
! D52	D(23,19,20,34)	115.7285	estimate D2E/DX2	!
! D53	D(24,19,20,34)	-20.3853	estimate D2E/DX2	!
! D54	D(18,19,24,25)	145.7162	estimate D2E/DX2	!
! D55	D(18,19,24,26)	-94.9585	estimate D2E/DX2	!
! D56	D(18,19,24,27)	25.1949	estimate D2E/DX2	!
! D57	D(20,19,24,25)	76.473	estimate D2E/DX2	!
! D58	D(20,19,24,26)	-164.2016	estimate D2E/DX2	!
! D59	D(20,19,24,27)	-44.0482	estimate D2E/DX2	!
! D60	D(23,19,24,25)	-58.2184	estimate D2E/DX2	!
! D61	D(23,19,24,26)	61.1069	estimate D2E/DX2	!
! D62	D(23,19,24,27)	-178.7397	estimate D2E/DX2	!
! D63	D(18,20,34,33)	103.2228	estimate D2E/DX2	!
! D64	D(19,20,34,33)	-142.0276	estimate D2E/DX2	!
! D65	D(6,28,31,32)	99.1254	estimate D2E/DX2	!
! D66	D(6,28,31,33)	-80.8715	estimate D2E/DX2	!
! D67	D(29,28,31,32)	-140.8746	estimate D2E/DX2	!
! D68	D(29,28,31,33)	39.1285	estimate D2E/DX2	!
! D69	D(30,28,31,32)	-20.8746	estimate D2E/DX2	!
! D70	D(30,28,31,33)	159.1285	estimate D2E/DX2	!
! D71	D(28,31,33,34)	179.9996	estimate D2E/DX2	!
! D72	D(32,31,33,34)	0.0023	estimate D2E/DX2	!
! D73	D(31,33,34,20)	-80.134	estimate D2E/DX2	!

Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-06

Number of steps in this run= 175 maximum allowed number of steps= 204.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.779220	1.026560	1.294278
2	6	0	-1.679541	0.019132	1.403519
3	7	0	-2.837226	0.433426	0.750697
4	6	0	-2.629963	1.662768	0.253183
5	7	0	-1.396651	2.053605	0.591805

6	6	0	-0.782064	3.289120	0.109066
7	1	0	0.244150	1.091587	1.618623
8	1	0	-1.595647	-0.957147	1.845331
9	1	0	-1.573426	4.001190	-0.119085
10	1	0	-0.161366	3.718311	0.898640
11	35	0	-0.551058	-2.146547	-0.813439
12	1	0	-3.310281	2.191578	-0.402256
13	6	0	-4.012606	-0.331241	0.473336
14	6	0	-4.472893	-1.271676	1.288121
15	1	0	-4.450851	-0.064401	-0.485730
16	1	0	-5.342070	-1.846775	0.997734
17	1	0	-4.016995	-1.501220	2.244274
18	6	0	3.392878	-0.649305	0.680009
19	6	0	4.424751	0.066344	1.449679
20	8	0	3.384832	0.800919	0.766761
21	1	0	3.658283	-1.029624	-0.304675
22	1	0	2.538061	-1.130377	1.154034
23	1	0	4.314357	0.102746	2.532808
24	6	0	5.823997	0.264982	0.931971
25	1	0	6.223895	1.226053	1.261077
26	1	0	6.478416	-0.522747	1.313173
27	1	0	5.838022	0.235540	-0.157951
28	6	0	0.047618	3.126912	-1.178147
29	1	0	0.471067	4.070949	-1.450883
30	1	0	-0.584111	2.777812	-1.968051
31	6	0	1.177067	2.108438	-0.935953
32	8	0	1.243211	0.914968	-1.227183
33	8	0	2.241059	2.661085	-0.300411
34	1	0	2.937378	1.998751	-0.160365

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.355514	0.000000			
3	N	2.209678	1.392139	0.000000		
4	C	2.216729	2.219935	1.342296	0.000000	
5	N	1.389068	2.208616	2.173818	1.337340	0.000000
6	C	2.554196	3.629586	3.576363	2.465872	1.461934
7	H	1.075507	2.212920	3.268234	3.232832	2.161495
8	H	2.214792	1.074876	2.161813	3.235537	3.267347
9	H	3.387740	4.264547	3.883639	2.592889	2.080793
10	H	2.789946	4.030345	4.239409	3.276560	2.095549
11	Br	3.816168	3.298264	3.785412	4.468826	4.508993
12	H	3.262171	3.261848	2.155035	1.082623	2.160827

13	C	3.601715	2.535981	1.429392	2.436440	3.541856
14	C	4.350304	3.079338	2.423139	3.616414	4.583188
15	H	4.223682	3.355056	2.092933	2.616245	3.869776
16	H	5.400332	4.130423	3.396261	4.497418	5.562740
17	H	4.216082	2.912393	2.713942	3.987370	4.715256
18	C	4.537869	5.167176	6.323884	6.465484	5.500281
19	C	5.294099	6.104649	7.304768	7.331382	6.210787
20	O	4.203393	5.163769	6.232922	6.097893	4.945949
21	H	5.145482	5.701770	6.741363	6.863106	5.988517
22	H	3.959344	4.378559	5.612654	5.943204	5.092721
23	H	5.322774	6.099926	7.377697	7.473549	6.339476
24	C	6.656857	7.522358	8.664757	8.595580	7.446653
25	H	7.006035	7.996326	9.110031	8.921736	7.694510
26	H	7.421186	8.176433	9.381462	9.426698	8.317129
27	H	6.820746	7.681066	8.724949	8.597255	7.497199
28	C	3.347839	4.393901	4.392907	3.370736	2.524011
29	H	4.285724	5.402771	5.387330	4.280136	3.424999
30	H	3.707794	4.491966	4.238426	3.219117	2.781647
31	C	3.157760	4.242468	4.665298	4.013246	2.993505
32	O	3.234261	4.033062	4.560028	4.213332	3.402070
33	O	3.786396	5.025375	5.644136	5.002995	3.794472
34	H	4.107828	5.261232	6.051969	5.592781	4.399157

		6	7	8	9	10
6	C	0.000000				
7	H	2.856752	0.000000			
8	H	4.659111	2.762890	0.000000		
9	H	1.088738	3.845647	5.333341	0.000000	
10	H	1.092199	2.753634	4.981294	1.763434	0.000000
11	Br	5.518229	4.127080	3.094333	6.270728	6.122061
12	H	2.803201	4.234137	4.231558	2.524193	3.733485
13	C	4.865810	4.632072	2.848828	5.007047	5.604624
14	C	5.984418	5.286278	2.947534	6.179826	6.606129
15	H	5.005985	5.273295	3.792497	4.994300	5.884307
16	H	6.925374	6.342344	3.942783	7.046180	7.603926
17	H	6.162082	5.027071	2.513583	6.467844	6.627225
18	C	5.767782	3.718359	5.132068	6.850535	5.635292
19	C	6.268529	4.307794	6.119581	7.343171	5.888376
20	O	4.897624	3.267115	5.390666	5.967476	4.593918
21	H	6.208012	4.455886	5.677285	7.260462	6.211326
22	H	5.625580	3.227228	4.194693	6.697622	5.555350
23	H	6.480818	4.287205	6.043521	7.542969	5.981213
24	C	7.311813	5.682381	7.574889	8.353791	6.910221
25	H	7.393702	5.991934	8.139591	8.390735	6.863983
26	H	8.288231	6.447127	8.103233	9.346097	7.889557

27	H	7.295285	5.931310	7.790705	8.313314	7.017032
28	C	1.540000	3.464548	5.340531	2.124561	2.169440
29	H	2.148263	4.283685	6.357522	2.441005	2.458573
30	H	2.148263	4.048901	5.432771	2.427771	3.046501
31	C	2.514809	2.903477	4.982098	3.437294	2.783671
32	O	3.394686	3.021246	4.583041	4.322741	3.788230
33	O	3.114702	3.183342	5.693516	4.047104	2.885671
34	H	3.946124	3.352794	5.771349	4.935466	3.698729

		11	12	13	14	15
11	Br	0.000000				
12	H	5.157685	0.000000			
13	C	4.115027	2.761256	0.000000		
14	C	4.534616	4.025316	1.326709	0.000000	
15	H	4.432957	2.529289	1.087690	2.145821	0.000000
16	H	5.130692	4.732487	2.083101	1.081911	2.484310
17	H	4.666774	4.597860	2.122520	1.083864	3.115382
18	C	4.475126	7.360317	7.415193	7.913754	7.951424
19	C	5.897225	8.232679	8.502960	8.999137	9.085109
20	O	5.164864	6.937223	7.489324	8.143175	7.982194
21	H	4.384622	7.677666	7.741808	8.289247	8.168384
22	H	3.800817	6.903661	6.634246	7.013660	7.257412
23	H	6.318936	8.432848	8.588835	8.980759	9.271913
24	C	7.035855	9.430110	9.865323	10.417010	10.377420
25	H	7.847167	9.726224	10.384202	10.984564	10.893429
26	H	7.521483	10.301886	10.526327	10.976916	11.085802
27	H	6.850135	9.358270	9.887095	10.520351	10.298461
28	C	5.319849	3.571043	5.583156	6.772376	5.558789
29	H	6.333113	4.350891	6.571546	7.777437	6.500608
30	H	5.058016	3.198029	5.232701	6.490272	5.022661
31	C	4.594162	4.519739	5.905153	6.949369	6.049577
32	O	3.572598	4.800471	5.662898	6.616797	5.825053
33	O	5.583228	5.572090	6.975746	7.941486	7.228020
34	H	5.457031	6.255313	7.357494	8.228361	7.677785

		16	17	18	19	20
16	H	0.000000				
17	H	1.851781	0.000000			
18	C	8.822369	7.620952	0.000000		
19	C	9.962684	8.622744	1.472857	0.000000	
20	O	9.122633	7.891130	1.452839	1.444787	0.000000
21	H	9.130737	8.101200	1.088433	2.205986	2.138607
22	H	7.914172	6.655443	1.089422	2.253696	2.144039
23	H	9.970138	8.489251	2.201719	1.089349	2.114328
24	C	11.364193	10.083984	2.609549	1.505114	2.502808
25	H	11.970094	10.643332	3.445180	2.148816	2.912965

26	H	11.898589	10.581966	3.152373	2.140841	3.408947
27	H	11.430927	10.291180	2.732006	2.147193	2.681956
28	C	7.649886	7.046534	5.376181	5.952465	4.508869
29	H	8.649147	8.052698	5.946300	6.331014	4.909283
30	H	7.267796	6.916537	5.879949	6.642412	5.209588
31	C	7.866511	7.079672	3.889255	4.517615	3.079459
32	O	7.479532	6.749722	3.271911	4.243578	2.928372
33	O	8.916828	7.934951	3.639587	3.816282	2.430492
34	H	9.202093	8.148337	2.815299	2.922108	1.579423

		21	22	23	24	25
21	H	0.000000				
22	H	1.841977	0.000000			
23	H	3.124741	2.564534	0.000000		
24	C	2.809913	3.576830	2.206357	0.000000	
25	H	3.757928	4.376024	2.554496	1.091735	0.000000
26	H	3.290517	3.990104	2.561621	1.092748	1.767992
27	H	2.524565	3.804836	3.095056	1.090410	1.773036
28	C	5.574643	5.455812	6.412630	6.783051	6.907204
29	H	6.122743	6.173479	6.810822	6.986933	6.967294
30	H	5.938122	5.896551	7.169985	7.469155	7.693124
31	C	4.049986	4.087821	5.088977	5.336799	5.574587
32	O	3.234971	3.395625	4.922314	5.105686	5.576327
33	O	3.953464	4.071708	4.344053	4.483025	4.512266
34	H	3.116341	3.417388	3.569885	3.540016	3.663161

		26	27	28	29	30
26	H	0.000000				
27	H	1.774630	0.000000			
28	C	7.802682	6.552069	0.000000		
29	H	8.051726	6.722071	1.070000	0.000000	
30	H	8.458097	7.140266	1.070000	1.747303	0.000000
31	C	6.331351	5.083064	1.540000	2.148263	2.148263
32	O	5.993981	4.766253	2.514864	3.256756	2.712596
33	O	5.540364	4.340704	2.408027	2.538537	3.282717
34	H	4.590012	3.394503	3.264865	3.470178	4.034297

		31	32	33	34
31	C	0.000000			
32	O	1.230269	0.000000		
33	O	1.356986	2.214392	0.000000	
34	H	1.926724	2.276596	0.971165	0.000000

Stoichiometry C11H17BrN2O3

Framework group C1[X(C11H17BrN2O3)]

Deg. of freedom 96

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.766421	0.874750	1.177483
2	6	0	-1.810730	0.022399	1.320087
3	7	0	-2.901515	0.601896	0.677886
4	6	0	-2.514240	1.775428	0.153864
5	7	0	-1.228969	1.974099	0.465450
6	6	0	-0.438192	3.090283	-0.050360
7	1	0	0.260410	0.784255	1.484314
8	1	0	-1.872012	-0.947649	1.779009
9	1	0	-1.112845	3.913507	-0.279475
10	1	0	0.256443	3.429974	0.720996
11	35	0	-1.075423	-2.328972	-0.872837
12	1	0	-3.115768	2.393336	-0.500678
13	6	0	-4.186770	0.025985	0.433738
14	6	0	-4.772945	-0.817494	1.273440
15	1	0	-4.595756	0.342377	-0.523183
16	1	0	-5.726462	-1.254284	1.007821
17	1	0	-4.340760	-1.099862	2.226459
18	6	0	3.080908	-1.442621	0.529324
19	6	0	4.225940	-0.884646	1.268831
20	8	0	3.300877	-0.007754	0.588590
21	1	0	3.265365	-1.875777	-0.452021
22	1	0	2.170453	-1.776323	1.025868
23	1	0	4.142730	-0.813761	2.352682
24	6	0	5.629174	-0.915702	0.725382
25	1	0	6.180192	-0.023736	1.029785
26	1	0	6.159624	-1.789737	1.111107
27	1	0	5.618172	-0.964757	-0.363868
28	6	0	0.331944	2.779362	-1.347210
29	1	0	0.892376	3.641003	-1.644514
30	1	0	-0.361094	2.520485	-2.120244
31	6	0	1.292930	1.600912	-1.103572
32	8	0	1.166602	0.407186	-1.373056
33	8	0	2.441754	1.990700	-0.495558
34	1	0	3.028669	1.230015	-0.353964

Rotational constants (GHZ): 0.4142027 0.2141096 0.1652131

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 538 symmetry adapted cartesian basis functions of A symmetry.

```
 There are      519 symmetry adapted basis functions of A      symmetry.
    519 basis functions,      823 primitive gaussians,      538 cartesian basis functions
     78 alpha electrons              78 beta electrons
          nuclear repulsion energy           1583.4062796134 Hartrees.
 NAtoms=       34 NActive=       34 NUniq=       34 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      519 RedAO= T EigKep=    2.98D-06    NBF=      519
 NBsUse=      519 1.00D-06 EigRej= -1.00D+00 NBFU=      519
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn=                5 AccDes=
0.00D+00
 Harris functional with IExCor=    402 and IRadAn=             5 diagonalized for initial guess.
 HarFok:    IExCor=    402 AccDes= 0.00D+00 IRadAn=                5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=    3500011 ScaDFX=    1.000000    1.000000    1.000000    1.000000
 FoFCou: FMM=F IPFlag=                  0 FMFlag=           100000 FMFlg1=                  0
             NFxFlg=                    0 DoJE=T BraDBF=F KetDBF=T FulRan=T
             wScrn=      0.000000  ICntrl=             500  IOpCl=      0  I1Cent=        200000004  NGrid=
0
             NMat0=         1 NMatS0=            1 NMatT0=         0 NMatD0=         1 NMtDS0=         0
NMtDT0=        0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                       energy=1.00D-06.
 No special actions if energy rises.
 EnCoef did          6 forward-backward iterations
 EnCoef did      100 forward-backward iterations
 Restarting incremental Fock formation.
 SCF Done:    E(RB3LYP) =    -3338.86246820          A.U. after      23 cycles
                NFock= 23    Conv=0.18D-08          -V/T= 2.0019

 ******************************************************************************

                Population analysis using the SCF density.

 ******************************************************************************

 Orbital symmetries:
          Occupied    (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                      (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
                      (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
```

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A)
Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A)
The electronic state is 1-A.
Alpha occ. eigenvalues -- -482.65451 -62.30748 -56.12542 -56.12525 -56.12505
Alpha occ. eigenvalues -- -19.14967 -19.14394 -19.10464 -14.44797 -14.44448

Alpha occ. eigenvalues -- -10.30941 -10.30645 -10.27656 -10.25936 -10.25449
Alpha occ. eigenvalues -- -10.25343 -10.24099 -10.22495 -10.22085 -10.21160
Alpha occ. eigenvalues -- -10.17815 -8.51620 -6.33963 -6.33905 -6.33838
Alpha occ. eigenvalues -- -2.45200 -2.45193 -2.45140 -2.45094 -2.45085
Alpha occ. eigenvalues -- -1.11265 -1.09691 -1.08054 -1.00181 -0.99585
Alpha occ. eigenvalues -- -0.86057 -0.82193 -0.80935 -0.76170 -0.73548
Alpha occ. eigenvalues -- -0.70223 -0.68003 -0.65917 -0.64081 -0.62055
Alpha occ. eigenvalues -- -0.60431 -0.58836 -0.58514 -0.55292 -0.52698
Alpha occ. eigenvalues -- -0.52226 -0.51972 -0.50666 -0.50296 -0.49249
Alpha occ. eigenvalues -- -0.48744 -0.48108 -0.47105 -0.46366 -0.45067
Alpha occ. eigenvalues -- -0.43885 -0.42865 -0.42137 -0.41788 -0.41152
Alpha occ. eigenvalues -- -0.38967 -0.38332 -0.37915 -0.37244 -0.32260
Alpha occ. eigenvalues -- -0.30823 -0.30424 -0.29546 -0.29285 -0.26953
Alpha occ. eigenvalues -- -0.15321 -0.15220 -0.14764
Alpha virt. eigenvalues -- -0.08143 -0.04091 -0.03568 -0.01736 -0.01137
Alpha virt. eigenvalues -- -0.00865 -0.00432 0.00159 0.00490 0.00848
Alpha virt. eigenvalues -- 0.01186 0.01683 0.02304 0.02961 0.03404
Alpha virt. eigenvalues -- 0.03654 0.03885 0.04432 0.05043 0.05528
Alpha virt. eigenvalues -- 0.05968 0.06105 0.06629 0.06952 0.07015
Alpha virt. eigenvalues -- 0.07429 0.07620 0.08185 0.08338 0.08695
Alpha virt. eigenvalues -- 0.09183 0.09333 0.09887 0.10077 0.10482
Alpha virt. eigenvalues -- 0.10829 0.11257 0.11405 0.11568 0.11823
Alpha virt. eigenvalues -- 0.12299 0.12623 0.12718 0.12816 0.12989
Alpha virt. eigenvalues -- 0.13416 0.13570 0.13830 0.13920 0.14138
Alpha virt. eigenvalues -- 0.14331 0.14831 0.15027 0.15443 0.15821
Alpha virt. eigenvalues -- 0.16027 0.16434 0.16858 0.17063 0.17358
Alpha virt. eigenvalues -- 0.17520 0.17598 0.17984 0.18600 0.18772
Alpha virt. eigenvalues -- 0.19013 0.19410 0.19926 0.20039 0.20340
Alpha virt. eigenvalues -- 0.20715 0.21123 0.21470 0.21665 0.21994
Alpha virt. eigenvalues -- 0.22317 0.22497 0.22846 0.23385 0.23659
Alpha virt. eigenvalues -- 0.23859 0.24527 0.25561 0.25754 0.26212
Alpha virt. eigenvalues -- 0.26410 0.27087 0.27431 0.27772 0.28474
Alpha virt. eigenvalues -- 0.29079 0.29620 0.29734 0.30043 0.30512
Alpha virt. eigenvalues -- 0.30527 0.31410 0.31945 0.32412 0.33126
Alpha virt. eigenvalues -- 0.33795 0.34051 0.34568 0.34762 0.35087
Alpha virt. eigenvalues -- 0.35491 0.35855 0.36013 0.36965 0.37952
Alpha virt. eigenvalues -- 0.38504 0.39507 0.39931 0.40231 0.41098
Alpha virt. eigenvalues -- 0.41497 0.42048 0.42508 0.43564 0.45625
Alpha virt. eigenvalues -- 0.46458 0.46523 0.48625 0.48979 0.49468
Alpha virt. eigenvalues -- 0.50026 0.51038 0.52879 0.52927 0.54220
Alpha virt. eigenvalues -- 0.54310 0.54650 0.55022 0.56161 0.56993
Alpha virt. eigenvalues -- 0.57346 0.57693 0.58702 0.59731 0.60236
Alpha virt. eigenvalues -- 0.60452 0.61345 0.61906 0.62463 0.62842
Alpha virt. eigenvalues -- 0.63456 0.63940 0.64178 0.65168 0.65328

Alpha virt. eigenvalues --	0.66052	0.66438	0.67356	0.67502	0.68453
Alpha virt. eigenvalues --	0.68978	0.69578	0.69980	0.70710	0.70842
Alpha virt. eigenvalues --	0.71837	0.72004	0.73065	0.73748	0.74181
Alpha virt. eigenvalues --	0.74546	0.74946	0.75135	0.76578	0.77130
Alpha virt. eigenvalues --	0.77628	0.78094	0.79239	0.79660	0.80119
Alpha virt. eigenvalues --	0.81668	0.82743	0.83626	0.84274	0.84536
Alpha virt. eigenvalues --	0.86169	0.87817	0.88572	0.89697	0.90605
Alpha virt. eigenvalues --	0.92228	0.92493	0.92975	0.95466	0.96016
Alpha virt. eigenvalues --	0.97813	0.99729	1.00011	1.02018	1.03119
Alpha virt. eigenvalues --	1.03758	1.04532	1.06148	1.07033	1.08254
Alpha virt. eigenvalues --	1.09416	1.11083	1.11893	1.12644	1.13679
Alpha virt. eigenvalues --	1.14531	1.16809	1.18543	1.19793	1.21307
Alpha virt. eigenvalues --	1.21899	1.23108	1.23435	1.24311	1.27287
Alpha virt. eigenvalues --	1.27408	1.30555	1.31515	1.32847	1.34407
Alpha virt. eigenvalues --	1.35333	1.38056	1.40215	1.41244	1.41407
Alpha virt. eigenvalues --	1.42150	1.44742	1.45358	1.47260	1.48360
Alpha virt. eigenvalues --	1.49478	1.50624	1.52332	1.52546	1.53487
Alpha virt. eigenvalues --	1.55550	1.56236	1.56874	1.57380	1.57776
Alpha virt. eigenvalues --	1.58726	1.59476	1.59663	1.60567	1.61589
Alpha virt. eigenvalues --	1.62156	1.63382	1.63873	1.64321	1.65036
Alpha virt. eigenvalues --	1.65201	1.66885	1.68366	1.69351	1.70428
Alpha virt. eigenvalues --	1.70878	1.71202	1.72222	1.72538	1.72980
Alpha virt. eigenvalues --	1.75580	1.76898	1.76951	1.78289	1.79814
Alpha virt. eigenvalues --	1.80355	1.82529	1.82983	1.84749	1.85593
Alpha virt. eigenvalues --	1.86999	1.87683	1.89135	1.90221	1.90667
Alpha virt. eigenvalues --	1.93406	1.94583	1.95904	1.98568	2.00856
Alpha virt. eigenvalues --	2.02585	2.03165	2.06379	2.07169	2.07699
Alpha virt. eigenvalues --	2.09380	2.10012	2.10884	2.12353	2.13361
Alpha virt. eigenvalues --	2.15927	2.16634	2.18670	2.18915	2.19917
Alpha virt. eigenvalues --	2.21201	2.21815	2.22233	2.23842	2.26456
Alpha virt. eigenvalues --	2.28031	2.29843	2.31529	2.33550	2.34655
Alpha virt. eigenvalues --	2.38260	2.40736	2.42248	2.44495	2.47166
Alpha virt. eigenvalues --	2.47254	2.48841	2.49212	2.51626	2.52966
Alpha virt. eigenvalues --	2.53451	2.54057	2.54410	2.55730	2.56164
Alpha virt. eigenvalues --	2.58525	2.59325	2.59641	2.62470	2.63238
Alpha virt. eigenvalues --	2.65493	2.66375	2.67113	2.67711	2.68688
Alpha virt. eigenvalues --	2.71109	2.73236	2.73819	2.74592	2.75131
Alpha virt. eigenvalues --	2.76062	2.76462	2.77582	2.79362	2.79848
Alpha virt. eigenvalues --	2.81318	2.82087	2.82613	2.83507	2.84600
Alpha virt. eigenvalues --	2.85602	2.86395	2.88242	2.90165	2.91180
Alpha virt. eigenvalues --	2.93872	2.94026	2.95485	2.96803	2.98165
Alpha virt. eigenvalues --	3.02128	3.06426	3.08471	3.11701	3.12971
Alpha virt. eigenvalues --	3.13674	3.15524	3.19001	3.20149	3.23321
Alpha virt. eigenvalues --	3.24067	3.28083	3.31341	3.35821	3.39281

Alpha virt. eigenvalues -- 3.41844 3.48671 3.54654 3.55813 3.61986
Alpha virt. eigenvalues -- 3.62474 3.64536 3.68183 3.69977 3.72818
Alpha virt. eigenvalues -- 3.74331 3.76300 3.79388 3.80389 3.82545
Alpha virt. eigenvalues -- 3.84047 3.84911 3.86542 3.89759 3.92547
Alpha virt. eigenvalues -- 3.96204 4.03847 4.09794 4.10539 4.10846
Alpha virt. eigenvalues -- 4.15172 4.17935 4.32838 4.33299 4.34160
Alpha virt. eigenvalues -- 4.37193 4.40974 4.50748 4.68328 4.92213
Alpha virt. eigenvalues -- 5.00125 5.06618 5.08857 5.15258 5.22065
Alpha virt. eigenvalues -- 5.23888 5.41733 5.49446 5.56723 5.67987
Alpha virt. eigenvalues -- 5.91939 6.79415 7.73346 7.76663 7.78153
Alpha virt. eigenvalues -- 23.71172 23.74675 23.77483 23.84127 23.85384
Alpha virt. eigenvalues -- 23.86935 23.90342 23.92171 23.97170 24.16654
Alpha virt. eigenvalues -- 24.22924 35.43477 35.57508 48.08165 49.90049
Alpha virt. eigenvalues -- 49.94372 50.01216 289.94105 289.97236 289.98732
Alpha virt. eigenvalues -- 1020.86521

Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	16.062245	-9.934904	1.083289	0.147164	-1.218865	-0.652060
2	C	-9.934904	15.751297	-0.778893	-0.475453	1.239040	0.384296
3	N	1.083289	-0.778893	6.739883	0.412440	-0.505262	-0.094376
4	C	0.147164	-0.475453	0.412440	5.622111	0.486711	-0.310276
5	N	-1.218865	1.239040	-0.505262	0.486711	7.112904	0.206036
6	C	-0.652060	0.384296	-0.094376	-0.310276	0.206036	6.668440
7	H	0.842580	-0.381807	0.072656	-0.010733	-0.181462	-0.089633
8	H	-0.176119	0.573299	-0.083698	-0.006953	0.037735	0.010912
9	H	0.071185	-0.069546	0.008748	0.037132	-0.081484	0.386089
10	H	-0.038936	0.043443	-0.011835	-0.053488	-0.051585	0.557624
11	Br	-0.107956	0.289484	-0.022349	-0.037651	-0.030631	-0.004172
12	H	0.020360	0.007061	-0.049346	0.435846	-0.039352	-0.042136
13	C	0.982171	-1.175953	0.334514	-0.128377	-0.229740	-0.103357
14	C	-0.318792	0.431651	-0.208825	-0.074731	0.002342	-0.010617
15	H	-0.003091	0.011462	-0.093231	0.024200	-0.000209	0.009501
16	H	0.011278	-0.007962	0.020569	-0.002628	-0.001577	-0.000965
17	H	-0.037088	0.039046	-0.035313	-0.004530	0.000650	0.000912
18	C	0.011445	-0.058555	0.001418	-0.002858	0.002360	0.002001
19	C	0.022886	0.032663	-0.002416	0.001751	-0.000363	0.001501
20	O	0.001319	-0.005253	-0.000596	-0.000794	-0.002539	0.004033
21	H	-0.006088	0.006695	-0.000975	-0.000354	0.001796	0.001566
22	H	-0.027963	0.034804	0.000110	0.001033	-0.001458	-0.003422
23	H	-0.002676	0.004094	-0.000718	-0.000387	0.001195	0.000862
24	C	-0.010542	0.005959	0.000236	-0.000106	-0.000294	0.000258
25	H	-0.000711	0.000366	0.000016	-0.000024	-0.000052	0.000222
26	H	0.000121	-0.000114	0.000006	-0.000010	-0.000017	0.000032
27	H	0.001351	-0.000912	0.000000	-0.000024	-0.000109	0.000130

28	C	-0.323465	0.487441	-0.054585	-0.042959	-0.027174	-0.148915
29	H	-0.030122	0.025418	-0.004242	-0.009586	0.021662	-0.030225
30	H	0.003657	-0.007636	-0.002330	-0.021562	-0.001849	0.054829
31	C	-0.182142	-0.055347	0.015018	0.103719	0.050536	-0.469882
32	O	-0.021818	-0.032480	-0.007621	-0.003564	0.024411	0.069373
33	O	-0.025428	0.009601	-0.000033	0.005714	0.017295	-0.018809
34	H	0.024164	-0.023969	0.001342	0.008355	0.006303	-0.037975
		7	8	9	10	11	12
1	C	0.842580	-0.176119	0.071185	-0.038936	-0.107956	0.020360
2	C	-0.381807	0.573299	-0.069546	0.043443	0.289484	0.007061
3	N	0.072656	-0.083698	0.008748	-0.011835	-0.022349	-0.049346
4	C	-0.010733	-0.006953	0.037132	-0.053488	-0.037651	0.435846
5	N	-0.181462	0.037735	-0.081484	-0.051585	-0.030631	-0.039352
6	C	-0.089633	0.010912	0.386089	0.557624	-0.004172	-0.042136
7	H	0.559728	-0.012460	-0.001942	-0.007532	0.020882	-0.000305
8	H	-0.012460	0.448200	-0.001429	0.001468	0.022850	0.000060
9	H	-0.001942	-0.001429	0.600545	-0.047430	-0.001200	-0.005002
10	H	-0.007532	0.001468	-0.047430	0.515681	0.001970	0.000566
11	Br	0.020882	0.022850	-0.001200	0.001970	35.685481	-0.002743
12	H	-0.000305	0.000060	-0.005002	0.000566	-0.002743	0.478266
13	C	0.041977	-0.029700	0.004255	-0.006544	0.016930	-0.011540
14	C	-0.009775	0.012360	0.000227	-0.000270	-0.012558	0.007801
15	H	0.001861	0.002906	0.000304	-0.000022	0.005083	-0.003803
16	H	0.000322	0.000474	0.000046	-0.000097	-0.002271	0.000425
17	H	0.000268	-0.003811	-0.000096	0.000164	0.005622	-0.000233
18	C	0.061116	-0.004342	-0.000098	-0.002285	-0.005683	-0.000223
19	C	-0.063124	0.003510	0.000473	0.000049	0.010503	0.000166
20	O	0.011572	-0.000646	0.000017	0.001197	0.000861	-0.000038
21	H	-0.004827	0.000546	-0.000017	-0.000056	-0.004273	0.000000
22	H	-0.001923	-0.000580	0.000206	-0.000368	0.007675	0.000028
23	H	-0.005461	0.000851	-0.000088	-0.000218	0.000769	0.000011
24	C	0.004116	-0.000176	-0.000105	0.000788	-0.002301	-0.000002
25	H	0.000212	0.000010	0.000018	0.000057	0.000045	-0.000003
26	H	0.000103	-0.000007	0.000004	0.000017	-0.000076	-0.000001
27	H	0.000207	0.000012	0.000012	-0.000038	0.000223	-0.000002
28	C	0.007198	0.008932	-0.021559	-0.041904	0.019188	0.001090
29	H	-0.001364	0.000529	-0.015509	0.000792	-0.000051	0.001595
30	H	-0.003192	0.000125	-0.019144	0.019441	0.001436	-0.003888
31	C	-0.029733	-0.001875	-0.009488	-0.122259	-0.059242	0.010510
32	O	-0.010359	0.000125	-0.005028	0.009560	-0.019167	0.000068
33	O	-0.005338	-0.000758	-0.002995	0.000571	-0.001345	0.000862
34	H	0.004880	-0.001354	-0.001635	-0.003561	0.000074	0.000649
		13	14	15	16	17	18
1	C	0.982171	-0.318792	-0.003091	0.011278	-0.037088	0.011445

2	C	-1.175953	0.431651	0.011462	-0.007962	0.039046	-0.058555
3	N	0.334514	-0.208825	-0.093231	0.020569	-0.035313	0.001418
4	C	-0.128377	-0.074731	0.024200	-0.002628	-0.004530	-0.002858
5	N	-0.229740	0.002342	-0.000209	-0.001577	0.000650	0.002360
6	C	-0.103357	-0.010617	0.009501	-0.000965	0.000912	0.002001
7	H	0.041977	-0.009775	0.001861	0.000322	0.000268	0.061116
8	H	-0.029700	0.012360	0.002906	0.000474	-0.003811	-0.004342
9	H	0.004255	0.000227	0.000304	0.000046	-0.000096	-0.000098
10	H	-0.006544	-0.000270	-0.000022	-0.000097	0.000164	-0.002285
11	Br	0.016930	-0.012558	0.005083	-0.002271	0.005622	-0.005683
12	H	-0.011540	0.007801	-0.003803	0.000425	-0.000233	-0.000223
13	C	6.045076	-0.069821	0.426421	-0.039552	-0.001746	0.002066
14	C	-0.069821	5.774804	-0.055157	0.400080	0.384534	-0.000593
15	H	0.426421	-0.055157	0.508769	-0.007769	0.005232	0.000136
16	H	-0.039552	0.400080	-0.007769	0.486376	-0.023551	0.000019
17	H	-0.001746	0.384534	0.005232	-0.023551	0.527112	-0.000049
18	C	0.002066	-0.000593	0.000136	0.000019	-0.000049	7.139706
19	C	-0.002214	0.000808	-0.000135	-0.000007	-0.000027	-1.867957
20	O	-0.000151	0.000009	-0.000003	-0.000001	-0.000011	0.161455
21	H	-0.000724	0.000032	0.000001	0.000005	-0.000016	0.243208
22	H	-0.000754	0.000948	-0.000132	-0.000009	0.000149	0.424870
23	H	-0.000410	0.000118	-0.000010	0.000001	-0.000008	-0.037490
24	C	0.000111	-0.000027	0.000009	-0.000002	0.000016	0.245302
25	H	-0.000002	0.000001	0.000000	0.000000	0.000000	-0.002327
26	H	0.000005	-0.000002	0.000000	0.000000	0.000000	0.015742
27	H	0.000007	-0.000001	0.000000	0.000000	-0.000001	-0.026973
28	C	-0.032662	0.005469	-0.001261	0.000012	0.000213	-0.030450
29	H	-0.002028	0.000202	0.000060	-0.000017	0.000019	-0.002102
30	H	-0.001655	0.000674	-0.000056	-0.000029	0.000090	0.000590
31	C	0.030750	-0.001993	0.000498	0.000193	0.000024	-0.027906
32	O	-0.002924	0.000258	0.000073	-0.000057	0.000126	-0.011161
33	O	0.000689	0.000047	-0.000046	-0.000005	0.000012	0.011613
34	H	0.001457	-0.000093	-0.000036	-0.000001	-0.000007	0.055459

		19	20	21	22	23	24
1	C	0.022886	0.001319	-0.006088	-0.027963	-0.002676	-0.010542
2	C	0.032663	-0.005253	0.006695	0.034804	0.004094	0.005959
3	N	-0.002416	-0.000596	-0.000975	0.000110	-0.000718	0.000236
4	C	0.001751	-0.000794	-0.000354	0.001033	-0.000387	-0.000106
5	N	-0.000363	-0.002539	0.001796	-0.001458	0.001195	-0.000294
6	C	0.001501	0.004033	0.001566	-0.003422	0.000862	0.000258
7	H	-0.063124	0.011572	-0.004827	-0.001923	-0.005461	0.004116
8	H	0.003510	-0.000646	0.000546	-0.000580	0.000851	-0.000176
9	H	0.000473	0.000017	-0.000017	0.000206	-0.000088	-0.000105
10	H	0.000049	0.001197	-0.000056	-0.000368	-0.000218	0.000788

11	Br	0.010503	0.000861	-0.004273	0.007675	0.000769	-0.002301
12	H	0.000166	-0.000038	0.000000	0.000028	0.000011	-0.000002
13	C	-0.002214	-0.000151	-0.000724	-0.000754	-0.000410	0.000111
14	C	0.000808	0.000009	0.000032	0.000948	0.000118	-0.000027
15	H	-0.000135	-0.000003	0.000001	-0.000132	-0.000010	0.000009
16	H	-0.000007	-0.000001	0.000005	-0.000009	0.000001	-0.000002
17	H	-0.000027	-0.000011	-0.000016	0.000149	-0.000008	0.000016
18	C	-1.867957	0.161455	0.243208	0.424870	-0.037490	0.245302
19	C	7.816550	-0.095729	0.146244	-0.040867	0.384638	-0.256117
20	O	-0.095729	8.304582	-0.046773	-0.031715	-0.017079	-0.057983
21	H	0.146244	-0.046773	0.504806	-0.004275	0.006612	-0.032380
22	H	-0.040867	-0.031715	-0.004275	0.464117	-0.002270	0.001067
23	H	0.384638	-0.017079	0.006612	-0.002270	0.543316	-0.060267
24	C	-0.256117	-0.057983	-0.032380	0.001067	-0.060267	5.484780
25	H	-0.000621	-0.021865	-0.003197	0.000017	-0.001551	0.378364
26	H	-0.111073	0.017921	-0.002419	0.001309	-0.001359	0.445919
27	H	-0.024991	0.004866	0.002910	0.001037	0.006938	0.393996
28	C	-0.009744	-0.004812	-0.008163	0.008832	-0.006056	0.014119
29	H	0.002543	-0.000184	0.000378	-0.000594	0.000393	0.000103
30	H	-0.000984	0.000528	0.000140	0.000039	-0.000058	-0.000130
31	C	0.018321	0.033202	0.003660	-0.006557	0.001010	0.009314
32	O	0.013761	-0.005476	0.002739	-0.004768	-0.001714	-0.000389
33	O	-0.016751	-0.029237	0.001025	-0.001186	0.003573	0.000561
34	H	-0.064264	-0.001181	-0.002380	-0.001711	-0.000266	0.014315

		25	26	27	28	29	30
1	C	-0.000711	0.000121	0.001351	-0.323465	-0.030122	0.003657
2	C	0.000366	-0.000114	-0.000912	0.487441	0.025418	-0.007636
3	N	0.000016	0.000006	0.000000	-0.054585	-0.004242	-0.002330
4	C	-0.000024	-0.000010	-0.000024	-0.042959	-0.009586	-0.021562
5	N	-0.000052	-0.000017	-0.000109	-0.027174	0.021662	-0.001849
6	C	0.000222	0.000032	0.000130	-0.148915	-0.030225	0.054829
7	H	0.000212	0.000103	0.000207	0.007198	-0.001364	-0.003192
8	H	0.000010	-0.000007	0.000012	0.008932	0.000529	0.000125
9	H	0.000018	0.000004	0.000012	-0.021559	-0.015509	-0.019144
10	H	0.000057	0.000017	-0.000038	-0.041904	0.000792	0.019441
11	Br	0.000045	-0.000076	0.000223	0.019188	-0.000051	0.001436
12	H	-0.000003	-0.000001	-0.000002	0.001090	0.001595	-0.003888
13	C	-0.000002	0.000005	0.000007	-0.032662	-0.002028	-0.001655
14	C	0.000001	-0.000002	-0.000001	0.005469	0.000202	0.000674
15	H	0.000000	0.000000	0.000000	-0.001261	0.000060	-0.000056
16	H	0.000000	0.000000	0.000000	0.000012	-0.000017	-0.000029
17	H	0.000000	0.000000	-0.000001	0.000213	0.000019	0.000090
18	C	-0.002327	0.015742	-0.026973	-0.030450	-0.002102	0.000590
19	C	-0.000621	-0.111073	-0.024991	-0.009744	0.002543	-0.000984

20	O	-0.021865	0.017921	0.004866	-0.004812	-0.000184	0.000528
21	H	-0.003197	-0.002419	0.002910	-0.008163	0.000378	0.000140
22	H	0.000017	0.001309	0.001037	0.008832	-0.000594	0.000039
23	H	-0.001551	-0.001359	0.006938	-0.006056	0.000393	-0.000058
24	C	0.378364	0.445919	0.393996	0.014119	0.000103	-0.000130
25	H	0.570402	-0.041640	-0.030565	0.001045	-0.000104	0.000053
26	H	-0.041640	0.555642	-0.025817	0.000699	-0.000032	0.000010
27	H	-0.030565	-0.025817	0.552710	-0.002060	-0.000007	0.000016
28	C	0.001045	0.000699	-0.002060	7.865426	0.343208	0.412343
29	H	-0.000104	-0.000032	-0.000007	0.343208	0.509063	-0.029422
30	H	0.000053	0.000010	0.000016	0.412343	-0.029422	0.512900
31	C	0.002490	-0.000024	-0.000338	-1.431452	0.013463	-0.142971
32	O	0.000686	-0.000012	-0.000700	-0.104610	-0.005658	0.015662
33	O	-0.002958	0.000169	0.001477	-0.426801	0.002754	0.008505
34	H	-0.003103	-0.000192	-0.002085	-0.062789	0.002506	-0.002731

		31	32	33	34
1	C	-0.182142	-0.021818	-0.025428	0.024164
2	C	-0.055347	-0.032480	0.009601	-0.023969
3	N	0.015018	-0.007621	-0.000033	0.001342
4	C	0.103719	-0.003564	0.005714	0.008355
5	N	0.050536	0.024411	0.017295	0.006303
6	C	-0.469882	0.069373	-0.018809	-0.037975
7	H	-0.029733	-0.010359	-0.005338	0.004880
8	H	-0.001875	0.000125	-0.000758	-0.001354
9	H	-0.009488	-0.005028	-0.002995	-0.001635
10	H	-0.122259	0.009560	0.000571	-0.003561
11	Br	-0.059242	-0.019167	-0.001345	0.000074
12	H	0.010510	0.000068	0.000862	0.000649
13	C	0.030750	-0.002924	0.000689	0.001457
14	C	-0.001993	0.000258	0.000047	-0.000093
15	H	0.000498	0.000073	-0.000046	-0.000036
16	H	0.000193	-0.000057	-0.000005	-0.000001
17	H	0.000024	0.000126	0.000012	-0.000007
18	C	-0.027906	-0.011161	0.011613	0.055459
19	C	0.018321	0.013761	-0.016751	-0.064264
20	O	0.033202	-0.005476	-0.029237	-0.001181
21	H	0.003660	0.002739	0.001025	-0.002380
22	H	-0.006557	-0.004768	-0.001186	-0.001711
23	H	0.001010	-0.001714	0.003573	-0.000266
24	C	0.009314	-0.000389	0.000561	0.014315
25	H	0.002490	0.000686	-0.002958	-0.003103
26	H	-0.000024	-0.000012	0.000169	-0.000192
27	H	-0.000338	-0.000700	0.001477	-0.002085
28	C	-1.431452	-0.104610	-0.426801	-0.062789

29	H	0.013463	-0.005658	0.002754	0.002506
30	H	-0.142971	0.015662	0.008505	-0.002731
31	C	7.499497	0.476600	0.387723	0.001535
32	O	0.476600	7.902730	-0.196893	-0.004245
33	O	0.387723	-0.196893	8.069306	0.319612
34	H	0.001535	-0.004245	0.319612	0.345252

Mulliken charges:

		1
1	C	-0.166450
2	C	-0.368334
3	N	0.266397
4	C	-0.099127
5	N	0.163048
6	C	-0.341795
7	H	0.191295
8	H	0.199005
9	H	0.174532
10	H	0.235043
11	Br	-0.775408
12	H	0.193252
13	C	-0.046577
14	C	-0.259112
15	H	0.168446
16	H	0.166699
17	H	0.142297
18	C	-0.297454
19	C	0.101015
20	O	-0.219497
21	H	0.194554
22	H	0.184308
23	H	0.183701
24	C	-0.578513
25	H	0.154719
26	H	0.145094
27	H	0.148729
28	C	-0.393793
29	H	0.206557
30	H	0.206601
31	C	-0.116856
32	O	-0.077526
33	O	-0.112528
34	H	0.427675

Sum of Mulliken charges = 0.00000

Mulliken charges with hydrogens summed into heavy atoms:

		1
1	C	0.024844
2	C	-0.169330
3	N	0.266397
4	C	0.094125
5	N	0.163048
6	C	0.067780
11	Br	-0.775408
13	C	0.121869
14	C	0.049884
18	C	0.081408
19	C	0.284717
20	O	-0.219497
24	C	-0.129971
28	C	0.019366
31	C	-0.116856
32	O	-0.077526
33	O	0.315147

Electronic spatial extent (au): <R**2>= 6648.4524

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= -1.5135 Y= 11.6168 Z= 5.8070 Tot= 13.0753

Quadrupole moment (field-independent basis, Debye-Ang):

XX= -77.7868 YY= -121.1208 ZZ= -114.8198

XY= -21.9284 XZ= -1.4139 YZ= -17.1784

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

XX= 26.7890 YY= -16.5450 ZZ= -10.2440

XY= -21.9284 XZ= -1.4139 YZ= -17.1784

Octapole moment (field-independent basis, Debye-Ang**2):

XXX= -37.8783 YYY= 67.7049 ZZZ= -11.3989 XYY= 6.6186

XXY= -42.3143 XXZ= 16.8091 XZZ= 3.8868 YZZ= -5.6049

YYZ= -0.8926 XYZ= 23.1759

Hexadecapole moment (field-independent basis, Debye-Ang**3):

XXXX= -4660.6702 YYYY= -2251.8018 ZZZZ= -770.5609 XXXY= 2.8491

XXXZ= 87.8806 YYYX= -80.7753 YYYZ= -50.9934 ZZZX= 18.8685

ZZZY= -6.7852 XXYY= -1292.4752 XXZZ= -1014.3577 YYZZ= -499.8649

XXYZ= -84.0828 YYXZ= -8.3220 ZZXY= 28.8128

N-N= 1.583406279613D+03 E-N=-1.110741232087D+04 KE= 3.332617027656D+03

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.002159762	0.009582924	0.003314720
2	6	-0.006228727	-0.006215020	-0.002934853
3	7	0.001078549	-0.000887451	0.000450545
4	6	0.001980937	-0.003221616	-0.004996461
5	7	0.000218770	-0.002292551	-0.005067092
6	6	0.005793236	0.012902327	-0.004407380
7	1	-0.000041068	-0.000047284	-0.000174796
8	1	0.001193477	-0.000310287	-0.002727860
9	1	-0.004101255	0.000033253	0.005041511
10	1	-0.001801712	-0.002829491	0.001127066
11	35	-0.003853944	0.000608421	0.005452320
12	1	0.002351674	-0.000336246	0.005164260
13	6	0.002488779	0.001012585	0.002358285
14	6	-0.001571297	0.002141836	-0.002546649
15	1	-0.000611817	-0.003907135	0.003943987
16	1	0.000411808	-0.000041020	0.000120443
17	1	0.000915014	-0.000227726	-0.001789325
18	6	0.001242953	0.001533604	-0.002952002
19	6	-0.000579787	-0.001360299	0.000180901
20	8	0.007972411	-0.013658281	0.010656949
21	1	-0.002796372	0.000331905	0.001842511
22	1	0.003462327	0.000823889	-0.001413465
23	1	-0.000179458	-0.000264338	-0.000459393
24	6	-0.001563744	-0.001569597	0.001107427
25	1	0.000538456	0.001074189	0.000340487
26	1	0.000873146	-0.000508230	-0.000024843
27	1	0.000420653	-0.000251350	-0.001015473
28	6	0.008608478	-0.029815172	0.019099683
29	1	0.005812112	0.012754250	-0.001243559
30	1	-0.006273231	-0.006749060	-0.011177818
31	6	0.039814055	-0.038194235	-0.005946386
32	8	-0.025490659	0.041427617	-0.003084645
33	8	-0.028414639	0.040614767	-0.012208486
34	1	0.000490636	-0.012155176	0.003969389

Cartesian Forces: Max 0.041427617 RMS 0.010414584

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.040832356 RMS 0.006908953
Search for a local minimum.
Step number 1 out of a maximum of 175
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Second derivative matrix not updated -- first step.
ITU= 0

Eigenvalues ---	0.00230	0.00237	0.00237	0.00435	0.00640
Eigenvalues ---	0.00698	0.00873	0.01281	0.01303	0.01410
Eigenvalues ---	0.01519	0.01607	0.01813	0.01917	0.02114
Eigenvalues ---	0.02261	0.02267	0.02268	0.02293	0.02409
Eigenvalues ---	0.02506	0.03007	0.03058	0.03058	0.03761
Eigenvalues ---	0.03963	0.04356	0.05173	0.05410	0.05463
Eigenvalues ---	0.05804	0.05894	0.08669	0.09503	0.09628
Eigenvalues ---	0.11947	0.12376	0.12596	0.13026	0.13636
Eigenvalues ---	0.15432	0.15851	0.15970	0.15983	0.15996
Eigenvalues ---	0.16000	0.16000	0.16000	0.16000	0.16000
Eigenvalues ---	0.16000	0.16986	0.21983	0.22001	0.22037
Eigenvalues ---	0.22784	0.23494	0.24587	0.24683	0.25000
Eigenvalues ---	0.25000	0.25000	0.25000	0.28519	0.28519
Eigenvalues ---	0.29090	0.31847	0.32654	0.34497	0.34560
Eigenvalues ---	0.34613	0.34765	0.34879	0.34888	0.34959
Eigenvalues ---	0.34994	0.35081	0.35531	0.35679	0.35764
Eigenvalues ---	0.36543	0.36621	0.36723	0.37230	0.37230
Eigenvalues ---	0.37717	0.41077	0.42393	0.45693	0.49311
Eigenvalues ---	0.53140	0.53562	0.55299	0.56121	0.60290
Eigenvalues ---	0.90974				

RFO step: Lambda=-3.25428785D-02 EMin= 2.30000000D-03
Linear search not attempted -- first point.
Maximum step size (0.300) exceeded in Quadratic search.
-- Step size scaled by 0.904
Iteration 1 RMS(Cart)= 0.19417223 RMS(Int)= 0.01704665
Iteration 2 RMS(Cart)= 0.07162061 RMS(Int)= 0.00171268
Iteration 3 RMS(Cart)= 0.00294674 RMS(Int)= 0.00057213
Iteration 4 RMS(Cart)= 0.00000706 RMS(Int)= 0.00057213
Iteration 5 RMS(Cart)= 0.00000001 RMS(Int)= 0.00057213

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56155	0.00650	0.00000	0.01070	0.01065	2.57220
R2	2.62496	-0.00196	0.00000	-0.00345	-0.00334	2.62162

R3	2.03241	-0.00010	0.00000	-0.00022	-0.00022	2.03220
R4	2.63076	-0.00636	0.00000	-0.01119	-0.01132	2.61944
R5	2.03122	0.00064	0.00000	0.00146	0.00146	2.03268
R6	2.53657	0.00221	0.00000	0.00305	0.00302	2.53960
R7	2.70116	-0.00119	0.00000	-0.00242	-0.00242	2.69874
R8	2.52721	0.00067	0.00000	0.00061	0.00071	2.52792
R9	2.04586	-0.00477	0.00000	-0.01107	-0.01107	2.03479
R10	2.76266	0.00534	0.00000	0.01207	0.01207	2.77473
R11	2.05742	0.00195	0.00000	0.00460	0.00460	2.06202
R12	2.06396	-0.00132	0.00000	-0.00316	-0.00316	2.06080
R13	2.91018	0.00467	0.00000	0.01327	0.01327	2.92345
R14	5.84744	-0.00621	0.00000	-0.12381	-0.12381	5.72363
R15	2.50712	-0.00382	0.00000	-0.00544	-0.00544	2.50168
R16	2.05544	-0.00419	0.00000	-0.00987	-0.00987	2.04556
R17	2.04452	-0.00034	0.00000	-0.00078	-0.00078	2.04373
R18	2.04821	-0.00115	0.00000	-0.00267	-0.00267	2.04553
R19	2.78330	-0.00072	0.00000	-0.00255	-0.00253	2.78077
R20	2.74547	-0.00184	0.00000	-0.00493	-0.00491	2.74056
R21	2.05684	-0.00246	0.00000	-0.00582	-0.00582	2.05102
R22	2.05871	-0.00370	0.00000	-0.00877	-0.00877	2.04994
R23	2.73025	0.00119	0.00000	0.00422	0.00419	2.73444
R24	2.05857	-0.00045	0.00000	-0.00106	-0.00106	2.05751
R25	2.84425	-0.00005	0.00000	-0.00013	-0.00013	2.84412
R26	2.98468	0.01797	0.00000	0.12731	0.12731	3.11199
R27	2.06308	0.00125	0.00000	0.00299	0.00299	2.06607
R28	2.06499	0.00088	0.00000	0.00210	0.00210	2.06709
R29	2.06058	0.00103	0.00000	0.00244	0.00244	2.06301
R30	2.02201	0.01387	0.00000	0.03095	0.03095	2.05296
R31	2.02201	0.01416	0.00000	0.03160	0.03160	2.05360
R32	2.91018	-0.01635	0.00000	-0.04649	-0.04649	2.86369
R33	2.32487	-0.04083	0.00000	-0.03915	-0.03915	2.28572
R34	2.56433	-0.00853	0.00000	-0.01357	-0.01357	2.55076
R35	1.83524	0.02655	0.00000	0.04254	0.04254	1.87777
A1	1.87029	0.00225	0.00000	0.00775	0.00779	1.87808
A2	2.28184	-0.00099	0.00000	-0.00258	-0.00322	2.27862
A3	2.13028	-0.00113	0.00000	-0.00320	-0.00386	2.12643
A4	1.86854	-0.00132	0.00000	-0.00455	-0.00474	1.86380
A5	2.28673	0.00273	0.00000	0.01281	0.01228	2.29900
A6	2.12698	-0.00128	0.00000	-0.00610	-0.00662	2.12036
A7	1.89437	0.00006	0.00000	-0.00058	-0.00042	1.89395
A8	2.23394	-0.00466	0.00000	-0.01348	-0.01371	2.22024
A9	2.14718	0.00475	0.00000	0.01690	0.01670	2.16387
A10	1.89252	0.00275	0.00000	0.00794	0.00776	1.90028
A11	2.18305	-0.00011	0.00000	0.00437	0.00351	2.18656

A12	2.20193	-0.00223	0.00000	-0.00568	-0.00657	2.19536
A13	1.89852	-0.00381	0.00000	-0.01147	-0.01172	1.88680
A14	2.22055	-0.00001	0.00000	0.00340	0.00224	2.22279
A15	2.15444	0.00435	0.00000	0.01789	0.01680	2.17124
A16	1.89269	-0.00735	0.00000	-0.03183	-0.03300	1.85969
A17	1.90953	-0.00806	0.00000	-0.03944	-0.03995	1.86958
A18	1.99706	0.01638	0.00000	0.06174	0.06168	2.05874
A19	1.88342	0.00135	0.00000	-0.00723	-0.00812	1.87530
A20	1.86015	-0.00038	0.00000	0.01505	0.01528	1.87543
A21	1.91715	-0.00244	0.00000	-0.00063	-0.00003	1.91712
A22	1.59309	0.00892	0.00000	0.02852	0.02852	1.62161
A23	2.14757	0.00044	0.00000	0.00152	0.00151	2.14908
A24	1.95106	0.00355	0.00000	0.01685	0.01684	1.96790
A25	2.18417	-0.00400	0.00000	-0.01862	-0.01863	2.16554
A26	2.08366	0.00071	0.00000	0.00332	0.00326	2.08692
A27	2.14834	-0.00112	0.00000	-0.00527	-0.00534	2.14300
A28	2.05118	0.00041	0.00000	0.00191	0.00185	2.05303
A29	2.06202	0.00253	0.00000	0.01294	0.01304	2.07506
A30	2.13756	-0.00161	0.00000	-0.00661	-0.00671	2.13085
A31	1.98686	0.00098	0.00000	0.00083	0.00083	1.98768
A32	1.99376	-0.00097	0.00000	0.00045	0.00044	1.99420
A33	2.01604	-0.00102	0.00000	-0.00643	-0.00643	2.00960
A34	2.05423	0.00133	0.00000	0.00415	0.00419	2.05842
A35	2.13613	-0.00116	0.00000	-0.00599	-0.00601	2.13011
A36	1.96064	0.00006	0.00000	-0.00043	-0.00042	1.96022
A37	2.02579	0.00096	0.00000	0.00616	0.00616	2.03195
A38	2.01729	-0.00029	0.00000	-0.00031	-0.00033	2.01695
A39	2.37973	-0.00232	0.00000	-0.01854	-0.01835	2.36138
A40	2.61988	0.00235	0.00000	0.01109	0.01094	2.63083
A41	1.93159	-0.00003	0.00000	-0.00005	-0.00005	1.93154
A42	1.91944	0.00058	0.00000	0.00264	0.00264	1.92207
A43	1.93072	0.00040	0.00000	0.00184	0.00184	1.93256
A44	1.88606	-0.00026	0.00000	-0.00118	-0.00118	1.88488
A45	1.89692	-0.00016	0.00000	-0.00058	-0.00058	1.89634
A46	1.89814	-0.00056	0.00000	-0.00282	-0.00282	1.89531
A47	1.91063	-0.00966	0.00000	-0.05019	-0.04947	1.86116
A48	1.91063	0.00082	0.00000	0.02559	0.02532	1.93595
A49	1.91063	0.01765	0.00000	0.06547	0.06525	1.97588
A50	1.91063	0.00318	0.00000	0.00378	0.00370	1.91434
A51	1.91063	-0.00400	0.00000	-0.01960	-0.01881	1.89182
A52	1.91063	-0.00799	0.00000	-0.02505	-0.02676	1.88388
A53	2.27021	-0.02803	0.00000	-0.08963	-0.09024	2.17996
A54	1.95991	-0.00560	0.00000	-0.01791	-0.01869	1.94123
A55	2.05307	0.03363	0.00000	0.10754	0.10660	2.15967

A56	1.93047	-0.01635	0.00000	-0.07672	-0.07672	1.85375
A57	2.50648	0.01845	0.00000	0.05902	0.05902	2.56549
D1	0.01268	0.00121	0.00000	0.01690	0.01711	0.02978
D2	3.10738	0.00430	0.00000	0.07065	0.07099	-3.10481
D3	-3.08645	-0.00227	0.00000	-0.03738	-0.03719	-3.12364
D4	0.00825	0.00081	0.00000	0.01638	0.01670	0.02495
D5	-0.02760	-0.00189	0.00000	-0.02682	-0.02688	-0.05448
D6	-3.02294	-0.00619	0.00000	-0.10197	-0.10140	-3.12434
D7	3.07603	0.00122	0.00000	0.02169	0.02165	3.09769
D8	0.08069	-0.00308	0.00000	-0.05346	-0.05286	0.02783
D9	0.00642	-0.00006	0.00000	-0.00118	-0.00124	0.00518
D10	3.01664	0.00168	0.00000	0.02442	0.02406	3.04070
D11	-3.09352	-0.00294	0.00000	-0.04955	-0.04902	3.14065
D12	-0.08329	-0.00120	0.00000	-0.02395	-0.02372	-0.10701
D13	-1.54107	-0.00754	0.00000	-0.17207	-0.17207	-1.71314
D14	1.54774	-0.00404	0.00000	-0.11142	-0.11142	1.43631
D15	-0.02376	-0.00118	0.00000	-0.01580	-0.01589	-0.03965
D16	3.00920	0.00263	0.00000	0.04701	0.04729	3.05649
D17	-3.04193	-0.00198	0.00000	-0.03717	-0.03746	-3.07939
D18	-0.00897	0.00183	0.00000	0.02563	0.02572	0.01675
D19	0.59748	-0.00177	0.00000	-0.03230	-0.03233	0.56515
D20	-2.51571	-0.00116	0.00000	-0.02304	-0.02297	-2.53868
D21	-2.69278	-0.00026	0.00000	-0.00496	-0.00503	-2.69780
D22	0.47722	0.00036	0.00000	0.00431	0.00434	0.48155
D23	0.03179	0.00188	0.00000	0.02626	0.02630	0.05809
D24	3.03388	0.00557	0.00000	0.09660	0.09670	3.13058
D25	-2.99968	-0.00216	0.00000	-0.03821	-0.03808	-3.03777
D26	0.00241	0.00154	0.00000	0.03213	0.03232	0.03473
D27	-2.83998	0.00754	0.00000	0.10293	0.10238	-2.73759
D28	-0.78979	0.00047	0.00000	0.05405	0.05514	-0.73465
D29	1.36972	0.00285	0.00000	0.06729	0.06757	1.43729
D30	0.46772	0.00334	0.00000	0.02003	0.01894	0.48665
D31	2.51791	-0.00373	0.00000	-0.02884	-0.02830	2.48960
D32	-1.60577	-0.00134	0.00000	-0.01561	-0.01588	-1.62165
D33	-3.12655	0.00024	0.00000	0.01730	0.01764	-3.10891
D34	1.06224	0.00175	0.00000	0.02774	0.02848	1.09072
D35	-1.03215	0.00023	0.00000	0.00265	0.00207	-1.03008
D36	1.06487	-0.00018	0.00000	0.00946	0.00925	1.07412
D37	-1.02953	0.00134	0.00000	0.01989	0.02009	-1.00944
D38	-3.12392	-0.00019	0.00000	-0.00519	-0.00632	-3.13024
D39	-0.97113	-0.00031	0.00000	0.01000	0.01038	-0.96075
D40	-3.06553	0.00120	0.00000	0.02043	0.02122	-3.04431
D41	1.12327	-0.00032	0.00000	-0.00465	-0.00519	1.11808
D42	-3.09171	0.00049	0.00000	0.00788	0.00784	-3.08387

D43	0.04732	-0.00101	0.00000	-0.01347	-0.01351	0.03380
D44	0.01762	-0.00007	0.00000	-0.00200	-0.00195	0.01567
D45	-3.12653	-0.00157	0.00000	-0.02335	-0.02331	3.13335
D46	-2.73365	-0.00055	0.00000	-0.00756	-0.00757	-2.74122
D47	-0.01811	-0.00091	0.00000	-0.01325	-0.01327	-0.03138
D48	0.00372	-0.00103	0.00000	-0.00912	-0.00913	-0.00542
D49	2.71925	-0.00139	0.00000	-0.01481	-0.01483	2.70442
D50	0.68388	-0.00078	0.00000	-0.01159	-0.01149	0.67239
D51	-1.68388	0.00078	0.00000	-0.00303	-0.00294	-1.68681
D52	2.01984	0.00190	0.00000	0.02787	0.02793	2.04777
D53	-0.35579	0.00122	0.00000	0.02206	0.02210	-0.33369
D54	2.54323	-0.00033	0.00000	0.00035	0.00032	2.54355
D55	-1.65734	-0.00031	0.00000	0.00054	0.00051	-1.65683
D56	0.43973	-0.00037	0.00000	-0.00010	-0.00013	0.43961
D57	1.33471	0.00057	0.00000	0.00189	0.00192	1.33663
D58	-2.86586	0.00059	0.00000	0.00208	0.00211	-2.86375
D59	-0.76879	0.00052	0.00000	0.00145	0.00148	-0.76731
D60	-1.01610	-0.00031	0.00000	-0.00419	-0.00419	-1.02029
D61	1.06652	-0.00029	0.00000	-0.00400	-0.00400	1.06252
D62	-3.11960	-0.00035	0.00000	-0.00463	-0.00463	-3.12423
D63	1.80158	0.00029	0.00000	0.00191	0.00195	1.80352
D64	-2.47885	-0.00112	0.00000	-0.02344	-0.02348	-2.50233
D65	1.73006	0.00482	0.00000	0.06920	0.07008	1.80015
D66	-1.41147	0.00798	0.00000	0.14247	0.14110	-1.27037
D67	-2.45873	0.00135	0.00000	0.03582	0.03676	-2.42196
D68	0.68292	0.00451	0.00000	0.10910	0.10778	0.79071
D69	-0.36433	-0.00210	0.00000	0.01311	0.01466	-0.34967
D70	2.77732	0.00106	0.00000	0.08638	0.08569	2.86300
D71	3.14159	-0.00272	0.00000	-0.05380	-0.05718	3.08441
D72	0.00004	0.00001	0.00000	0.00949	0.01287	0.01291
D73	-1.39860	0.00415	0.00000	0.08035	0.08035	-1.31825

Item	Value	Threshold	Converged?
Maximum Force	0.040832	0.000450	NO
RMS Force	0.006909	0.000300	NO
Maximum Displacement	1.256549	0.001800	NO
RMS Displacement	0.258346	0.001200	NO

Predicted change in Energy=-2.024539D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.840774	1.070667	1.341698
2	6	0	-1.752002	0.074511	1.515097
3	7	0	-2.859695	0.407761	0.751316
4	6	0	-2.614304	1.573669	0.129625
5	7	0	-1.411478	2.020856	0.507408
6	6	0	-0.798583	3.263840	0.022306
7	1	0	0.149908	1.189649	1.742771
8	1	0	-1.725478	-0.825494	2.103574
9	1	0	-1.619301	3.934367	-0.237459
10	1	0	-0.266458	3.709025	0.863677
11	35	0	-0.937345	-2.536762	-0.267951
12	1	0	-3.263483	2.043755	-0.589409
13	6	0	-4.023722	-0.388029	0.524890
14	6	0	-4.510852	-1.229623	1.423196
15	1	0	-4.435763	-0.254359	-0.467121
16	1	0	-5.364697	-1.843763	1.171368
17	1	0	-4.077306	-1.351974	2.407456
18	6	0	3.534277	-0.650871	0.274990
19	6	0	4.386416	-0.101526	1.341501
20	8	0	3.386811	0.727013	0.702651
21	1	0	3.947479	-0.759538	-0.722729
22	1	0	2.675664	-1.278324	0.489097
23	1	0	4.129441	-0.338382	2.372677
24	6	0	5.823160	0.276525	1.100666
25	1	0	6.099632	1.145957	1.703156
26	1	0	6.481925	-0.551051	1.379363
27	1	0	5.988954	0.514129	0.048115
28	6	0	0.138094	3.179349	-1.206017
29	1	0	0.510297	4.184508	-1.383060
30	1	0	-0.401322	2.829190	-2.082018
31	6	0	1.324300	2.261260	-0.990470
32	8	0	1.425155	1.143382	-1.441231
33	8	0	2.225700	2.816002	-0.152784
34	1	0	2.938419	2.135995	-0.022360

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.361150	0.000000			
3	N	2.205456	1.386147	0.000000		
4	C	2.206251	2.215982	1.343896	0.000000	
5	N	1.387301	2.218030	2.181490	1.337718	0.000000
6	C	2.559802	3.648185	3.596780	2.482951	1.468323
7	H	1.075392	2.216446	3.263747	3.223443	2.157534

8	H	2.226787	1.075647	2.153130	3.231481	3.278422
9	H	3.361640	4.241174	3.866937	2.587988	2.063866
10	H	2.742130	3.980061	4.199506	3.257447	2.070728
11	Br	3.951435	3.265222	3.661222	4.457117	4.647350
12	H	3.247397	3.254450	2.153384	1.076765	2.152546
13	C	3.595292	2.520946	1.428114	2.447642	3.553429
14	C	4.332141	3.052944	2.420489	3.623350	4.583710
15	H	4.236917	3.352599	2.099281	2.648680	3.908019
16	H	5.384124	4.104813	3.394236	4.508739	5.568129
17	H	4.180929	2.870227	2.705928	3.986010	4.700299
18	C	4.821061	5.478027	6.498497	6.540241	5.626067
19	C	5.357010	6.143395	7.287923	7.299658	6.230232
20	O	4.289401	5.243398	6.254848	6.087575	4.973503
21	H	5.526199	6.179610	7.062082	7.016221	6.161350
22	H	4.313934	4.742053	5.792395	6.020535	5.252585
23	H	5.267958	5.957961	7.213430	7.359710	6.304524
24	C	6.715414	7.589179	8.690871	8.591642	7.465563
25	H	6.950220	7.926633	9.039938	8.865192	7.655850
26	H	7.500220	8.258771	9.411674	9.424312	8.347503
27	H	6.973398	7.890988	8.877184	8.668640	7.566212
28	C	3.448997	4.540589	4.527648	3.455119	2.584396
29	H	4.352667	5.514471	5.493289	4.343711	3.456657
30	H	3.873932	4.727772	4.464828	3.371199	2.894640
31	C	3.397656	4.530273	4.896436	4.152108	3.128244
32	O	3.589487	4.469529	4.869121	4.355453	3.551569
33	O	3.831832	5.110745	5.698970	5.004876	3.781160
34	H	4.156667	5.349162	6.099466	5.583193	4.383550

		6	7	8	9	10
6	C	0.000000				
7	H	2.856904	0.000000			
8	H	4.681182	2.776339	0.000000		
9	H	1.091175	3.819017	5.305468	0.000000	
10	H	1.090528	2.700634	4.922190	1.758825	0.000000
11	Br	5.809517	4.371643	3.028815	6.507035	6.382831
12	H	2.817541	4.221350	4.224950	2.530142	3.723807
13	C	4.897986	4.625094	2.822329	5.004551	5.569350
14	C	5.994551	5.260959	2.895607	6.147002	6.535915
15	H	5.083931	5.291235	3.778930	5.052785	5.904451
16	H	6.946751	6.319728	3.892273	7.028483	7.544546
17	H	6.143673	4.977047	2.429119	6.401779	6.520700
18	C	5.844868	4.122602	5.571286	6.917107	5.813848
19	C	6.320615	4.447038	6.201624	7.406091	6.033063
20	O	4.941244	3.431242	5.523438	6.019310	4.718549
21	H	6.266398	4.929458	6.338357	7.297757	6.343658

22	H	5.737555	3.747270	4.709739	6.793140	5.802590
23	H	6.541075	4.309100	5.881308	7.623466	6.162996
24	C	7.344004	5.782031	7.694297	8.400036	6.994403
25	H	7.409187	5.950016	8.079561	8.433454	6.913837
26	H	8.330713	6.576970	8.243862	9.400156	7.997177
27	H	7.323403	6.117405	8.095182	8.346563	7.071258
28	C	1.547023	3.557302	5.519517	2.143967	2.174362
29	H	2.129753	4.343947	6.500417	2.431081	2.424305
30	H	2.185158	4.197732	5.712204	2.471292	3.077242
31	C	2.556856	3.161985	5.329381	3.468587	2.839788
32	O	3.403424	3.430198	5.135037	4.302020	3.841443
33	O	3.062271	3.247624	5.827817	4.005239	2.835760
34	H	3.903743	3.433227	5.919624	4.904408	3.678413

		11	12	13	14	15
11	Br	0.000000				
12	H	5.147366	0.000000			
13	C	3.843355	2.780863	0.000000		
14	C	4.163957	4.039989	1.323831	0.000000	
15	H	4.181861	2.582735	1.082465	2.128397	0.000000
16	H	4.706732	4.756914	2.082140	1.081498	2.464501
17	H	4.291955	4.601574	2.115683	1.082450	3.097812
18	C	4.883316	7.363269	7.566696	8.147234	8.014330
19	C	6.071503	8.176282	8.454547	8.968872	9.006960
20	O	5.503873	6.901423	7.496061	8.168273	7.970203
21	H	5.217935	7.737841	8.076795	8.738954	8.402338
22	H	3.900080	6.890054	6.758379	7.247132	7.248121
23	H	6.121937	8.312873	8.360075	8.737877	9.024092
24	C	7.449304	9.409917	9.886063	10.448172	10.391598
25	H	8.183320	9.681416	10.306490	10.876770	10.847375
26	H	7.855078	10.275312	10.541599	11.013787	11.076707
27	H	7.575055	9.399669	10.064536	10.732075	10.465695
28	C	5.891559	3.638751	5.748299	6.925641	5.766845
29	H	6.965242	4.410683	6.716078	7.899356	6.708651
30	H	5.689604	3.322161	5.501658	6.756383	5.328497
31	C	5.353325	4.610413	6.157629	7.215334	6.307184
32	O	4.527852	4.849701	5.991754	7.005160	6.103519
33	O	6.218536	5.560407	7.055518	8.014482	7.341731
34	H	6.075896	6.228454	7.425738	8.301123	7.764674

		16	17	18	19	20
16	H	0.000000				
17	H	1.851255	0.000000			
18	C	9.023204	7.935688	0.000000		
19	C	9.906994	8.621745	1.471518	0.000000	
20	O	9.133317	7.933574	1.450243	1.447002	0.000000

21	H	9.564505	8.634015	1.085351	2.210586	2.134453
22	H	8.089043	7.020551	1.084783	2.244576	2.138390
23	H	9.687516	8.269177	2.202761	1.088788	2.115550
24	C	11.387219	10.118248	2.603995	1.505044	2.509412
25	H	11.859682	10.502656	3.442281	2.149911	2.921630
26	H	11.918758	10.639352	3.149322	2.143516	3.416300
27	H	11.650182	10.506114	2.726562	2.149420	2.691632
28	C	7.820763	7.166567	5.328980	5.941568	4.495679
29	H	8.796630	8.128145	5.939232	6.388867	4.957701
30	H	7.553548	7.151948	5.758060	6.575106	5.150096
31	C	8.140481	7.333397	3.868578	4.516348	3.078072
32	O	7.864528	7.163538	3.257784	4.249995	2.935590
33	O	9.004494	7.978392	3.730224	3.926010	2.538469
34	H	9.284675	8.203069	2.865325	2.993879	1.646793

		21	22	23	24	25
21	H	0.000000				
22	H	1.831713	0.000000			
23	H	3.129220	2.558287	0.000000		
24	C	2.813606	3.563468	2.205630	0.000000	
25	H	3.761329	4.367452	2.556007	1.093318	0.000000
26	H	3.299344	3.976068	2.562436	1.093857	1.769414
27	H	2.526667	3.792789	3.096474	1.091700	1.774998
28	C	5.500891	5.402178	6.411890	6.787278	6.938148
29	H	6.057544	6.167359	6.903644	7.047534	7.070939
30	H	5.799888	5.740222	7.099692	7.442429	7.708646
31	C	4.009734	4.067427	5.092908	5.343385	5.594937
32	O	3.240287	3.339850	4.904557	5.153167	5.633641
33	O	4.009219	4.168691	4.466802	4.578406	4.608787
34	H	3.145286	3.462398	3.643800	3.611170	3.735084

		26	27	28	29	30
26	H	0.000000				
27	H	1.774781	0.000000			
28	C	7.800273	6.550481	0.000000		
29	H	8.106592	6.748009	1.086381	0.000000	
30	H	8.413457	7.122682	1.086720	1.776649	0.000000
31	C	6.334531	5.088234	1.515398	2.124997	2.119385
32	O	6.033056	4.841732	2.420127	3.176287	2.566822
33	O	5.639146	4.416001	2.366309	2.515749	3.259350
34	H	4.662775	3.455601	3.214257	3.455964	3.984543

		31	32	33	34
31	C	0.000000			
32	O	1.209549	0.000000		
33	O	1.349806	2.258013	0.000000	
34	H	1.886347	2.299661	0.993674	0.000000

Stoichiometry C11H17BrN2O3
Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.689552	0.929674	1.199530
2	6	0	-1.815080	0.169782	1.291623
3	7	0	-2.799934	0.823652	0.567800
4	6	0	-2.273873	1.946092	0.048719
5	7	0	-1.004417	2.057520	0.455604
6	6	0	-0.105047	3.154584	0.076715
7	1	0	0.295061	0.772560	1.602420
8	1	0	-2.013046	-0.757827	1.798937
9	1	0	-0.737667	4.022169	-0.117580
10	1	0	0.506262	3.384676	0.949991
11	35	0	-1.624104	-2.396117	-0.718691
12	1	0	-2.781465	2.618513	-0.621820
13	6	0	-4.117296	0.352724	0.280929
14	6	0	-4.804314	-0.422127	1.105636
15	1	0	-4.471347	0.666641	-0.692640
16	1	0	-5.776704	-0.789543	0.807140
17	1	0	-4.426567	-0.729581	2.072320
18	6	0	3.160833	-1.691215	-0.044700
19	6	0	4.104582	-1.456596	1.059682
20	8	0	3.341455	-0.360514	0.502854
21	1	0	3.550026	-1.808925	-1.051010
22	1	0	2.174064	-2.110711	0.119813
23	1	0	3.783883	-1.713341	2.067995
24	6	0	5.593297	-1.414513	0.842627
25	1	0	6.061323	-0.692221	1.516859
26	1	0	6.030830	-2.396786	1.043197
27	1	0	5.825955	-1.133340	-0.186266
28	6	0	0.801386	2.954761	-1.160916
29	1	0	1.405820	3.852861	-1.252021
30	1	0	0.206231	2.821304	-2.060326
31	6	0	1.730198	1.764020	-1.034914
32	8	0	1.566886	0.697912	-1.582411
33	8	0	2.726285	2.011868	-0.158354

```
      34        1        0        3.253610        1.172200      -0.092962
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.3890756           0.2054060           0.1524787
 Standard basis: 6-311++G(d,p) (5D, 7F)
 There are     538 symmetry adapted cartesian basis functions of A      symmetry.
 There are     519 symmetry adapted basis functions of A      symmetry.
    519 basis functions,      823 primitive gaussians,      538 cartesian basis functions
     78 alpha electrons              78 beta electrons
          nuclear repulsion energy           1553.1641954351 Hartrees.
 NAtoms=       34 NActive=       34 NUniq=       34 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      519 RedAO= T EigKep=    3.49D-06    NBF=      519
 NBsUse=      519 1.00D-06 EigRej= -1.00D+00 NBFU=      519
 Initial guess from the checkpoint file:    "./coohpo.chk"
 B after Tr=          0.000000        0.000000        0.000000
             Rot=        0.998664      -0.014138      -0.000454        0.049697 Ang=    -5.92 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn=                5 AccDes=
0.00D+00
 Harris functional with IExCor=    402 and IRadAn=             5 diagonalized for initial guess.
 HarFok:    IExCor=    402 AccDes= 0.00D+00 IRadAn=                5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=    3500011 ScaDFX=    1.000000    1.000000    1.000000    1.000000
 FoFCou: FMM=F IPFlag=                  0 FMFlag=           100000 FMFlg1=                  0
             NFxFlg=                   0 DoJE=T BraDBF=F KetDBF=T FulRan=T
             wScrn=      0.000000 ICntrl=             500 IOpCl=      0 I1Cent=        200000004 NGrid=
0
             NMat0=        1 NMatS0=           1 NMatT0=        0 NMatD0=        1 NMtDS0=        0
NMtDT0=        0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                    energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3338.87859586          A.U. after      17 cycles
                  NFock= 17    Conv=0.27D-08         -V/T= 2.0019
 Calling FoFJK, ICntrl=             2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 ---------------------------------------------------------------------
 Center          Atomic                             Forces (Hartrees/Bohr)
 Number          Number                       X                      Y                      Z
```

1	6	-0.001501069	0.006207430	0.007315362
2	6	-0.001177563	-0.002350005	-0.001178410
3	7	0.001005533	0.002323947	-0.001872149
4	6	0.000147427	-0.002546854	-0.000703678
5	7	0.002395499	-0.008898569	-0.010186368
6	6	0.002375110	0.009217778	-0.001216363
7	1	0.000528655	-0.000216589	-0.000337411
8	1	0.002968575	-0.000700621	-0.004081030
9	1	-0.000707456	0.000266795	0.002014293
10	1	0.000332855	-0.000803893	0.000154132
11	35	-0.001244790	0.003165119	0.003392203
12	1	-0.000503917	0.000882948	0.001818081
13	6	0.001017972	0.001458455	0.000893716
14	6	-0.000693130	0.000484462	-0.000378768
15	1	-0.000498040	-0.001219403	0.000830904
16	1	0.000279674	0.000139211	0.000049507
17	1	0.000481825	-0.000764256	-0.000509160
18	6	-0.001145530	0.001760004	-0.000134657
19	6	0.000736309	-0.001005735	-0.001968355
20	8	0.005164989	-0.006673724	0.005129180
21	1	0.000297276	-0.000019504	-0.000059031
22	1	-0.000046335	-0.000353477	0.000979933
23	1	-0.000559714	-0.000663472	-0.000774977
24	6	-0.000723201	-0.000091095	0.000590240
25	1	0.000385151	0.000209131	0.000099020
26	1	0.000078794	-0.000081840	0.000021165
27	1	0.000285955	-0.000018782	-0.000223804
28	6	-0.002900601	-0.010178413	0.003832513
29	1	-0.000759770	0.004400025	-0.000908686
30	1	-0.001920752	-0.000435778	-0.001691043
31	6	0.004103693	-0.009090558	0.007491026
32	8	-0.002055140	0.012154284	-0.003035707
33	8	-0.000566974	0.001122790	-0.011206530
34	1	-0.005581312	0.002320190	0.005854851

Cartesian Forces: Max 0.012154284 RMS 0.003497928

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.011570463 RMS 0.002514157

Search for a local minimum.

Step number 2 out of a maximum of 175
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 1 2
DE= -1.61D-02 DEPred=-2.02D-02 R= 7.97D-01
TightC=F SS= 1.41D+00 RLast= 5.04D-01 DXNew= 5.0454D-01 1.5125D+00
Trust test= 7.97D-01 RLast= 5.04D-01 DXMaxT set to 5.05D-01
ITU= 1 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00227	0.00233	0.00244	0.00478	0.00698
Eigenvalues ---	0.00767	0.00873	0.01269	0.01303	0.01428
Eigenvalues ---	0.01546	0.01630	0.01812	0.01910	0.02124
Eigenvalues ---	0.02198	0.02264	0.02277	0.02354	0.02481
Eigenvalues ---	0.02644	0.03013	0.03057	0.03060	0.03589
Eigenvalues ---	0.03777	0.04098	0.05079	0.05329	0.05357
Eigenvalues ---	0.05791	0.05877	0.08805	0.09316	0.10257
Eigenvalues ---	0.11975	0.12544	0.12589	0.13380	0.13619
Eigenvalues ---	0.15470	0.15869	0.15975	0.15997	0.15998
Eigenvalues ---	0.16000	0.16000	0.16000	0.16000	0.16000
Eigenvalues ---	0.16232	0.16936	0.21167	0.22002	0.22375
Eigenvalues ---	0.22793	0.23372	0.23915	0.24782	0.24949
Eigenvalues ---	0.24992	0.25000	0.27578	0.28430	0.29083
Eigenvalues ---	0.31847	0.32209	0.32617	0.34497	0.34563
Eigenvalues ---	0.34611	0.34764	0.34885	0.34923	0.34962
Eigenvalues ---	0.35027	0.35090	0.35531	0.35686	0.35765
Eigenvalues ---	0.36542	0.36582	0.36788	0.37098	0.37351
Eigenvalues ---	0.37725	0.41074	0.42559	0.45623	0.49303
Eigenvalues ---	0.52453	0.53568	0.55498	0.56156	0.60279
Eigenvalues ---	0.88096				

RFO step: Lambda=-1.34556305D-02 EMin= 2.27455378D-03
Quartic linear search produced a step of 0.19577.
Iteration 1 RMS(Cart)= 0.48495849 RMS(Int)= 0.01425357
Iteration 2 RMS(Cart)= 0.06467144 RMS(Int)= 0.00050601
Iteration 3 RMS(Cart)= 0.00110187 RMS(Int)= 0.00037242
Iteration 4 RMS(Cart)= 0.00000096 RMS(Int)= 0.00037242

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.57220	-0.00204	0.00208	-0.00298	-0.00098	2.57122
R2	2.62162	-0.00218	-0.00065	-0.00551	-0.00611	2.61551
R3	2.03220	0.00034	-0.00004	0.00097	0.00092	2.03312
R4	2.61944	0.00012	-0.00222	-0.00105	-0.00339	2.61605
R5	2.03268	-0.00239	0.00029	-0.00686	-0.00658	2.02610
R6	2.53960	-0.00144	0.00059	-0.00225	-0.00162	2.53797
R7	2.69874	-0.00068	-0.00047	-0.00207	-0.00255	2.69620

R8	2.52792	-0.00064	0.00014	-0.00105	-0.00079	2.52713
R9	2.03479	-0.00052	-0.00217	-0.00289	-0.00505	2.02974
R10	2.77473	-0.00125	0.00236	-0.00225	0.00012	2.77485
R11	2.06202	0.00022	0.00090	0.00121	0.00211	2.06413
R12	2.06080	-0.00005	-0.00062	-0.00052	-0.00114	2.05966
R13	2.92345	-0.00596	0.00260	-0.02071	-0.01811	2.90534
R14	5.72363	-0.00477	-0.02424	-0.20616	-0.23040	5.49323
R15	2.50168	-0.00050	-0.00106	-0.00157	-0.00263	2.49905
R16	2.04556	-0.00072	-0.00193	-0.00338	-0.00531	2.04025
R17	2.04373	-0.00031	-0.00015	-0.00103	-0.00119	2.04255
R18	2.04553	-0.00018	-0.00052	-0.00086	-0.00139	2.04415
R19	2.78077	-0.00077	-0.00050	-0.00305	-0.00350	2.77727
R20	2.74056	-0.00109	-0.00096	-0.00378	-0.00475	2.73581
R21	2.05102	0.00017	-0.00114	-0.00017	-0.00131	2.04971
R22	2.04994	0.00044	-0.00172	0.00031	-0.00141	2.04853
R23	2.73444	0.00032	0.00082	0.00186	0.00264	2.73708
R24	2.05751	-0.00046	-0.00021	-0.00153	-0.00174	2.05577
R25	2.84412	-0.00005	-0.00003	-0.00018	-0.00020	2.84392
R26	3.11199	0.00877	0.02492	0.10307	0.12799	3.23998
R27	2.06607	0.00032	0.00059	0.00134	0.00193	2.06800
R28	2.06709	0.00011	0.00041	0.00060	0.00101	2.06810
R29	2.06301	0.00025	0.00048	0.00107	0.00155	2.06456
R30	2.05296	0.00396	0.00606	0.01511	0.02117	2.07413
R31	2.05360	0.00246	0.00619	0.01085	0.01703	2.07064
R32	2.86369	0.00095	-0.00910	-0.00186	-0.01096	2.85272
R33	2.28572	-0.01027	-0.00767	-0.01719	-0.02486	2.26086
R34	2.55076	-0.00360	-0.00266	-0.00895	-0.01160	2.53916
R35	1.87777	0.00361	0.00833	0.01251	0.02084	1.89861
A1	1.87808	-0.00087	0.00152	-0.00293	-0.00192	1.87616
A2	2.27862	0.00046	-0.00063	0.00193	0.00096	2.27958
A3	2.12643	0.00042	-0.00076	0.00157	0.00052	2.12695
A4	1.86380	0.00024	-0.00093	0.00109	-0.00027	1.86353
A5	2.29900	-0.00187	0.00240	-0.01078	-0.00840	2.29060
A6	2.12036	0.00163	-0.00130	0.00961	0.00830	2.12866
A7	1.89395	0.00047	-0.00008	0.00318	0.00289	1.89683
A8	2.22024	-0.00161	-0.00268	-0.00884	-0.01149	2.20875
A9	2.16387	0.00116	0.00327	0.00654	0.00986	2.17373
A10	1.90028	-0.00177	0.00152	-0.00644	-0.00509	1.89519
A11	2.18656	0.00098	0.00069	0.00457	0.00507	2.19163
A12	2.19536	0.00080	-0.00129	0.00222	0.00072	2.19608
A13	1.88680	0.00205	-0.00229	0.00879	0.00566	1.89246
A14	2.22279	-0.00838	0.00044	-0.03493	-0.03540	2.18739
A15	2.17124	0.00642	0.00329	0.02971	0.03210	2.20333
A16	1.85969	0.00455	-0.00646	0.03326	0.02720	1.88689

A17	1.86958	0.00153	-0.00782	-0.02427	-0.03298	1.83660
A18	2.05874	-0.01157	0.01208	-0.05185	-0.04023	2.01851
A19	1.87530	-0.00167	-0.00159	0.00391	0.00208	1.87738
A20	1.87543	0.00407	0.00299	0.03887	0.04208	1.91751
A21	1.91712	0.00368	-0.00001	0.00515	0.00363	1.92075
A22	1.62161	-0.00331	0.00558	-0.01074	-0.00516	1.61645
A23	2.14908	0.00001	0.00030	0.00016	0.00043	2.14951
A24	1.96790	0.00138	0.00330	0.01067	0.01394	1.98184
A25	2.16554	-0.00141	-0.00365	-0.01122	-0.01490	2.15065
A26	2.08692	-0.00006	0.00064	-0.00014	0.00037	2.08729
A27	2.14300	0.00010	-0.00104	-0.00009	-0.00126	2.14174
A28	2.05303	-0.00005	0.00036	-0.00026	-0.00003	2.05300
A29	2.07506	0.00064	0.00255	0.00290	0.00551	2.08057
A30	2.13085	-0.00139	-0.00131	-0.01007	-0.01147	2.11939
A31	1.98768	0.00009	0.00016	0.00169	0.00184	1.98953
A32	1.99420	-0.00039	0.00009	0.00198	0.00209	1.99629
A33	2.00960	0.00054	-0.00126	0.00334	0.00205	2.01165
A34	2.05842	-0.00067	0.00082	-0.00747	-0.00663	2.05179
A35	2.13011	0.00059	-0.00118	0.00322	0.00202	2.13213
A36	1.96022	-0.00013	-0.00008	0.00029	0.00019	1.96041
A37	2.03195	0.00038	0.00121	0.00383	0.00504	2.03699
A38	2.01695	0.00005	-0.00007	0.00177	0.00167	2.01863
A39	2.36138	-0.00052	-0.00359	-0.01167	-0.01507	2.34631
A40	2.63083	0.00127	0.00214	0.01374	0.01585	2.64668
A41	1.93154	0.00043	-0.00001	0.00308	0.00306	1.93460
A42	1.92207	-0.00014	0.00052	-0.00110	-0.00058	1.92149
A43	1.93256	0.00027	0.00036	0.00205	0.00240	1.93496
A44	1.88488	-0.00018	-0.00023	-0.00153	-0.00176	1.88313
A45	1.89634	-0.00024	-0.00011	-0.00074	-0.00086	1.89548
A46	1.89531	-0.00015	-0.00055	-0.00193	-0.00248	1.89283
A47	1.86116	-0.00179	-0.00969	-0.02001	-0.02953	1.83163
A48	1.93595	0.00247	0.00496	0.00942	0.01431	1.95026
A49	1.97588	-0.00436	0.01277	-0.01404	-0.00131	1.97457
A50	1.91434	-0.00070	0.00072	-0.00100	-0.00015	1.91418
A51	1.89182	0.00487	-0.00368	0.04225	0.03881	1.93063
A52	1.88388	-0.00036	-0.00524	-0.01513	-0.02065	1.86323
A53	2.17996	-0.00824	-0.01767	-0.04531	-0.06313	2.11684
A54	1.94123	0.00615	-0.00366	0.02390	0.02002	1.96125
A55	2.15967	0.00209	0.02087	0.02117	0.04175	2.20142
A56	1.85375	0.00066	-0.01502	-0.00424	-0.01926	1.83449
A57	2.56549	0.00597	0.01155	0.03206	0.04362	2.60911
D1	0.02978	-0.00185	0.00335	-0.05835	-0.05476	-0.02498
D2	-3.10481	-0.00154	0.01390	-0.04487	-0.03108	-3.13589
D3	-3.12364	-0.00005	-0.00728	-0.00225	-0.00890	-3.13254

D4	0.02495	0.00026	0.00327	0.01123	0.01478	0.03973
D5	-0.05448	0.00208	-0.00526	0.06744	0.06221	0.00772
D6	-3.12434	0.00040	-0.01985	0.01146	-0.00673	-3.13108
D7	3.09769	0.00047	0.00424	0.01727	0.02121	3.11890
D8	0.02783	-0.00121	-0.01035	-0.03871	-0.04773	-0.01990
D9	0.00518	0.00093	-0.00024	0.02885	0.02845	0.03362
D10	3.04070	0.00117	0.00471	0.03849	0.04303	3.08374
D11	3.14065	0.00064	-0.00960	0.01696	0.00738	-3.13516
D12	-0.10701	0.00089	-0.00464	0.02659	0.02196	-0.08505
D13	-1.71314	-0.00017	-0.03369	-0.00451	-0.03806	-1.75120
D14	1.43631	0.00019	-0.02181	0.01066	-0.01129	1.42502
D15	-0.03965	0.00044	-0.00311	0.01350	0.01043	-0.02923
D16	3.05649	0.00050	0.00926	0.02158	0.03141	3.08790
D17	-3.07939	0.00041	-0.00733	0.00539	-0.00221	-3.08160
D18	0.01675	0.00047	0.00503	0.01347	0.01877	0.03552
D19	0.56515	-0.00084	-0.00633	-0.03446	-0.04092	0.52423
D20	-2.53868	-0.00046	-0.00450	-0.02311	-0.02760	-2.56628
D21	-2.69780	-0.00063	-0.00098	-0.02384	-0.02482	-2.72263
D22	0.48155	-0.00026	0.00085	-0.01248	-0.01150	0.47005
D23	0.05809	-0.00153	0.00515	-0.04973	-0.04468	0.01340
D24	3.13058	-0.00067	0.01893	0.00094	0.02159	-3.13101
D25	-3.03777	-0.00159	-0.00746	-0.05793	-0.06588	-3.10364
D26	0.03473	-0.00073	0.00633	-0.00726	0.00040	0.03513
D27	-2.73759	0.00212	0.02004	0.10378	0.12374	-2.61386
D28	-0.73465	0.00309	0.01080	0.11272	0.12297	-0.61167
D29	1.43729	0.00083	0.01323	0.06070	0.07447	1.51176
D30	0.48665	0.00050	0.00371	0.04069	0.04437	0.53102
D31	2.48960	0.00147	-0.00554	0.04963	0.04360	2.53320
D32	-1.62165	-0.00079	-0.00311	-0.00240	-0.00490	-1.62655
D33	-3.10891	0.00229	0.00345	0.13063	0.13401	-2.97490
D34	1.09072	0.00284	0.00558	0.13872	0.14430	1.23501
D35	-1.03008	0.00459	0.00041	0.16143	0.16158	-0.86851
D36	1.07412	0.00085	0.00181	0.09072	0.09272	1.16684
D37	-1.00944	0.00140	0.00393	0.09882	0.10301	-0.90643
D38	-3.13024	0.00315	-0.00124	0.12153	0.12029	-3.00995
D39	-0.96075	-0.00141	0.00203	0.06153	0.06356	-0.89719
D40	-3.04431	-0.00085	0.00415	0.06962	0.07385	-2.97045
D41	1.11808	0.00089	-0.00102	0.09233	0.09113	1.20921
D42	-3.08387	0.00022	0.00153	0.00745	0.00892	-3.07495
D43	0.03380	-0.00070	-0.00265	-0.01726	-0.01997	0.01384
D44	0.01567	-0.00013	-0.00038	-0.00469	-0.00501	0.01066
D45	3.13335	-0.00105	-0.00456	-0.02940	-0.03390	3.09945
D46	-2.74122	0.00005	-0.00148	0.00515	0.00365	-2.73757
D47	-0.03138	-0.00001	-0.00260	-0.00111	-0.00371	-0.03509

D48	-0.00542	-0.00042	-0.00179	-0.00498	-0.00678	-0.01219
D49	2.70442	-0.00048	-0.00290	-0.01124	-0.01414	2.69028
D50	0.67239	0.00064	-0.00225	0.01000	0.00783	0.68022
D51	-1.68681	0.00013	-0.00057	0.00089	0.00036	-1.68645
D52	2.04777	0.00114	0.00547	0.02482	0.03032	2.07809
D53	-0.33369	0.00078	0.00433	0.01740	0.02175	-0.31194
D54	2.54355	0.00010	0.00006	0.00344	0.00350	2.54705
D55	-1.65683	0.00006	0.00010	0.00279	0.00288	-1.65395
D56	0.43961	-0.00005	-0.00002	0.00099	0.00095	0.44056
D57	1.33663	0.00018	0.00038	0.00224	0.00264	1.33927
D58	-2.86375	0.00014	0.00041	0.00159	0.00202	-2.86173
D59	-0.76731	0.00002	0.00029	-0.00021	0.00009	-0.76722
D60	-1.02029	-0.00012	-0.00082	-0.00482	-0.00565	-1.02594
D61	1.06252	-0.00017	-0.00078	-0.00547	-0.00626	1.05625
D62	-3.12423	-0.00028	-0.00091	-0.00728	-0.00819	-3.13242
D63	1.80352	-0.00202	0.00038	-0.11524	-0.11480	1.68873
D64	-2.50233	-0.00131	-0.00460	-0.11975	-0.12441	-2.62674
D65	1.80015	0.00261	0.01372	0.13830	0.15239	1.95254
D66	-1.27037	0.00254	0.02762	0.14080	0.16799	-1.10237
D67	-2.42196	0.00096	0.00720	0.13290	0.14052	-2.28145
D68	0.79071	0.00090	0.02110	0.13541	0.15612	0.94683
D69	-0.34967	0.00262	0.00287	0.14659	0.14988	-0.19979
D70	2.86300	0.00256	0.01677	0.14910	0.16548	3.02849
D71	3.08441	-0.00562	-0.01119	-0.17122	-0.18353	2.90087
D72	0.01291	-0.00518	0.00252	-0.16554	-0.16190	-0.14899
D73	-1.31825	-0.00044	0.01573	-0.01520	0.00053	-1.31772

Item	Value	Threshold	Converged?
Maximum Force	0.011570	0.000450	NO
RMS Force	0.002514	0.000300	NO
Maximum Displacement	1.792002	0.001800	NO
RMS Displacement	0.532256	0.001200	NO

Predicted change in Energy=-9.526170D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.580094	1.449873	1.329393
2	6	0	-1.273991	0.297844	1.535923
3	7	0	-2.408876	0.368034	0.746276
4	6	0	-2.377180	1.515174	0.048557
5	7	0	-1.278581	2.194509	0.394899

6	6	0	-0.869504	3.506078	-0.123364
7	1	0	0.354480	1.787941	1.741465
8	1	0	-1.080629	-0.538181	2.178741
9	1	0	-1.771604	4.067672	-0.376204
10	1	0	-0.393004	4.010194	0.717318
11	35	0	-0.013541	-2.137757	-0.001330
12	1	0	-3.101547	1.821856	-0.682818
13	6	0	-3.399318	-0.646966	0.589866
14	6	0	-3.700344	-1.516340	1.539823
15	1	0	-3.843109	-0.668679	-0.394121
16	1	0	-4.416410	-2.300514	1.338329
17	1	0	-3.222900	-1.510301	2.510453
18	6	0	2.881558	-0.708197	0.224042
19	6	0	3.730931	-0.368994	1.374448
20	8	0	2.896359	0.639045	0.753793
21	1	0	3.332780	-0.800946	-0.757935
22	1	0	1.939148	-1.228637	0.351103
23	1	0	3.374340	-0.649089	2.363310
24	6	0	5.219376	-0.188014	1.245557
25	1	0	5.578926	0.583120	1.933780
26	1	0	5.734230	-1.122554	1.488988
27	1	0	5.489540	0.100443	0.227027
28	6	0	0.083313	3.477399	-1.329612
29	1	0	0.408747	4.517727	-1.458048
30	1	0	-0.423052	3.134347	-2.238757
31	6	0	1.272218	2.569947	-1.124878
32	8	0	1.400820	1.562284	-1.756891
33	8	0	2.057356	2.976144	-0.112949
34	1	0	2.662635	2.197252	0.077804

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.360632	0.000000			
3	N	2.203371	1.384353	0.000000		
4	C	2.207787	2.216118	1.343036	0.000000	
5	N	1.384069	2.213435	2.176475	1.337299	0.000000
6	C	2.534214	3.634503	3.601841	2.503266	1.468385
7	H	1.075882	2.216879	3.262311	3.225260	2.155325
8	H	2.219073	1.072166	2.153467	3.230324	3.269384
9	H	3.343895	4.256226	3.918342	2.657516	2.084805
10	H	2.639107	3.902281	4.162921	3.257195	2.045706
11	Br	3.868190	3.143888	3.546200	4.351227	4.530546
12	H	3.247321	3.253519	2.153068	1.074091	2.150244

13	C	3.590495	2.510917	1.426767	2.452067	3.550988
14	C	4.310296	3.029598	2.418361	3.628321	4.576700
15	H	4.255118	3.355533	2.105304	2.667232	3.923927
16	H	5.364960	4.082316	3.391440	4.514582	5.562487
17	H	4.140284	2.831491	2.702424	3.991200	4.688450
18	C	4.226359	4.472331	5.423993	5.712136	5.075594
19	C	4.679236	5.051732	6.215709	6.528177	5.711941
20	O	3.615866	4.256756	5.312158	5.392140	4.469720
21	H	4.973300	5.262268	6.049445	6.214377	5.618401
22	H	3.805004	3.749428	4.648746	5.123546	4.698258
23	H	4.594799	4.815416	6.090561	6.566742	5.797445
24	C	6.026903	6.517990	7.664770	7.876631	6.973054
25	H	6.249006	6.870382	8.078454	8.229363	7.210418
26	H	6.820084	7.150867	8.311657	8.650284	7.834504
27	H	6.314795	6.891845	7.919987	7.994910	7.086660
28	C	3.409001	4.490339	4.493158	3.435652	2.544504
29	H	4.261380	5.440853	5.478868	4.364237	3.417283
30	H	3.948900	4.797714	4.528400	3.416451	2.924272
31	C	3.272472	4.327297	4.679753	3.975877	2.992866
32	O	3.669034	4.426743	4.712310	4.187499	3.494152
33	O	3.371350	4.581479	5.242875	4.671790	3.463717
34	H	3.555326	4.607699	5.432598	5.085845	3.953953

		6	7	8	9	10
6	C	0.000000				
7	H	2.815620	0.000000			
8	H	4.658357	2.767958	0.000000		
9	H	1.092292	3.768545	5.312163	0.000000	
10	H	1.089923	2.558519	4.826624	1.760578	0.000000
11	Br	5.709679	4.310902	2.906894	6.460547	6.201431
12	H	2.851598	4.221661	4.224027	2.628013	3.753054
13	C	4.914919	4.620168	2.812948	5.080409	5.544665
14	C	6.000377	5.234551	2.868434	6.210667	6.492887
15	H	5.132664	5.311823	3.777293	5.169573	5.918647
16	H	6.959425	6.295980	3.865171	7.105521	7.509893
17	H	6.135106	4.926194	2.375789	6.446149	6.457516
18	C	5.652546	3.862565	4.421389	6.694860	5.764486
19	C	6.198679	4.023368	4.881252	7.281942	6.051111
20	O	4.813627	2.959157	4.385519	5.901039	4.710189
21	H	6.050812	4.671146	5.307664	7.064269	6.261382
22	H	5.525502	3.680221	3.596672	6.507653	5.746164
23	H	6.438880	3.930059	4.460170	7.498901	6.213782
24	C	7.252222	5.274234	6.378363	8.343547	7.028712
25	H	7.372773	5.365018	6.757736	8.456265	6.992036
26	H	8.223941	6.121800	6.874559	9.314233	8.030166

27	H	7.222088	5.613378	6.883615	8.296204	7.080315
28	C	1.537438	3.515582	5.457856	2.167516	2.168103
29	H	2.106831	4.206133	6.403645	2.475250	2.373312
30	H	2.193716	4.273117	5.782228	2.481691	3.083243
31	C	2.542901	3.109613	5.109818	3.473981	2.870707
32	O	3.406041	3.658448	5.104777	4.271714	3.915581
33	O	2.974466	2.783966	5.239205	3.990197	2.786192
34	H	3.772201	2.874523	5.090045	4.833950	3.610079

		11	12	13	14	15
11	Br	0.000000				
12	H	5.067419	0.000000			
13	C	3.746392	2.793470	0.000000		
14	C	4.043986	4.054904	1.322439	0.000000	
15	H	4.120445	2.614580	1.079654	2.116376	0.000000
16	H	4.605044	4.775755	2.080599	1.080870	2.448048
17	H	4.123437	4.616815	2.113084	1.081716	3.086994
18	C	3.236670	6.559049	6.291819	6.760607	6.753136
19	C	4.363755	7.464243	7.178669	7.521143	7.783555
20	O	4.092476	6.279950	6.427772	6.984269	6.960480
21	H	3.682035	6.948763	6.867418	7.433459	7.186324
22	H	2.182591	5.981899	5.375367	5.770589	5.856912
23	H	4.391513	7.571102	7.001968	7.175054	7.726279
24	C	5.721857	8.774735	8.655776	9.022884	9.222159
25	H	6.513333	9.150501	9.161227	9.521963	9.785749
26	H	6.023998	9.563328	9.190011	9.442925	9.771260
27	H	5.945215	8.808965	8.927601	9.422918	9.384866
28	C	5.770935	3.647259	5.729180	6.891092	5.786355
29	H	6.826112	4.493425	6.735678	7.891883	6.790363
30	H	5.741851	3.364211	5.581899	6.829875	5.437139
31	C	5.007795	4.459247	5.925548	6.965970	6.098301
32	O	4.332749	4.635982	5.781815	6.809414	5.859449
33	O	5.518429	5.317087	6.587577	7.487668	6.941130
34	H	5.095143	5.826257	6.715583	7.511043	7.124674

		16	17	18	19	20
16	H	0.000000				
17	H	1.850075	0.000000			
18	C	7.552314	6.567758	0.000000		
19	C	8.373246	7.137846	1.469669	0.000000	
20	O	7.903118	6.719440	1.447728	1.448401	0.000000
21	H	8.166577	7.359516	1.084658	2.211823	2.132923
22	H	6.520480	5.602577	1.084038	2.235331	2.136972
23	H	8.029544	6.654841	2.196086	1.087869	2.116199
24	C	9.865071	8.638311	2.603743	1.504937	2.514412
25	H	10.420012	9.065710	3.444778	2.152779	2.931154

26	H	10.219872	9.023519	3.147938	2.143403	3.420125
27	H	10.253167	9.149597	2.730472	2.151662	2.700400
28	C	7.794209	7.110155	5.269083	5.950782	4.506669
29	H	8.808534	8.079293	6.021171	6.552860	5.111225
30	H	7.634145	7.208807	5.634800	6.525658	5.118630
31	C	7.883480	7.076025	3.893044	4.574852	3.145730
32	O	7.638178	7.002127	3.357345	4.354828	3.064725
33	O	8.476967	7.408882	3.790415	4.025314	2.630057
34	H	8.481256	7.369074	2.917353	3.067272	1.714525

		21	22	23	24	25
21	H	0.000000				
22	H	1.831691	0.000000			
23	H	3.125213	2.538627	0.000000		
24	C	2.819381	3.555677	2.205928	0.000000	
25	H	3.769103	4.362948	2.561842	1.094338	0.000000
26	H	3.304399	3.963418	2.560798	1.094394	1.769543
27	H	2.536585	3.793036	3.098318	1.092521	1.775943
28	C	5.402785	5.330639	6.441773	6.815123	7.016291
29	H	6.109698	6.215774	7.077676	7.252285	7.329146
30	H	5.637875	5.596695	7.064955	7.417245	7.742258
31	C	3.967805	4.129474	5.191200	5.367063	5.643633
32	O	3.211734	3.538739	5.075530	5.163294	5.660069
33	O	4.038456	4.231962	4.583516	4.675020	4.724100
34	H	3.183825	3.512099	3.719101	3.686470	3.815078

		26	27	28	29	30
26	H	0.000000				
27	H	1.774300	0.000000			
28	C	7.812614	6.561574	0.000000		
29	H	8.298105	6.940197	1.097581	0.000000	
30	H	8.362380	7.088258	1.095734	1.793080	0.000000
31	C	6.354243	5.070690	1.509597	2.156486	2.105520
32	O	6.043386	4.773943	2.363485	3.131798	2.455623
33	O	5.734539	4.490560	2.372419	2.627485	3.270552
34	H	4.737852	3.522820	3.205075	3.580986	3.970651

		31	32	33	34
31	C	0.000000			
32	O	1.196396	0.000000		
33	O	1.343666	2.265521	0.000000	
34	H	1.875795	2.315484	1.004701	0.000000

Stoichiometry C11H17BrN2O3

Framework group C1[X(C11H17BrN2O3)]

Deg. of freedom 96

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.707565	0.976107	1.274882
2	6	0	-1.576900	-0.069640	1.230289
3	7	0	-2.655321	0.339728	0.464875
4	6	0	-2.421024	1.586333	0.023481
5	7	0	-1.246301	1.997874	0.512385
6	6	0	-0.621413	3.306818	0.283617
7	1	0	0.250461	1.070382	1.755318
8	1	0	-1.539266	-1.039949	1.684848
9	1	0	-1.416373	4.043490	0.147766
10	1	0	-0.107482	3.545380	1.214689
11	35	0	-0.642727	-2.303908	-0.774554
12	1	0	-3.060292	2.147375	-0.632445
13	6	0	-3.782074	-0.452165	0.092051
14	6	0	-4.249987	-1.440013	0.836404
15	1	0	-4.184334	-0.200473	-0.877737
16	1	0	-5.068761	-2.042949	0.469856
17	1	0	-3.816356	-1.709397	1.790084
18	6	0	2.425357	-1.426121	-0.233828
19	6	0	3.269945	-1.469413	0.968138
20	8	0	2.624514	-0.236456	0.566765
21	1	0	2.895970	-1.384545	-1.210188
22	1	0	1.410224	-1.806350	-0.225436
23	1	0	2.835578	-1.887408	1.873712
24	6	0	4.772516	-1.502731	0.890649
25	1	0	5.217817	-0.956448	1.727821
26	1	0	5.128518	-2.536594	0.936337
27	1	0	5.124000	-1.056924	-0.042794
28	6	0	0.363245	3.377394	-0.895019
29	1	0	0.848562	4.357264	-0.800115
30	1	0	-0.152852	3.313194	-1.859465
31	6	0	1.390533	2.271398	-0.876695
32	8	0	1.388911	1.408147	-1.705041
33	8	0	2.187447	2.331460	0.203471
34	1	0	2.658608	1.444512	0.230937

Rotational constants (GHZ): 0.3665767 0.2862239 0.1865301

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 538 symmetry adapted cartesian basis functions of A symmetry.

```
 There are      519 symmetry adapted basis functions of A      symmetry.
    519 basis functions,      823 primitive gaussians,      538 cartesian basis functions
     78 alpha electrons              78 beta electrons
          nuclear repulsion energy           1633.9445801731 Hartrees.
 NAtoms=       34 NActive=       34 NUniq=       34 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      519 RedAO= T EigKep=    2.69D-06    NBF=      519
 NBsUse=      519 1.00D-06 EigRej= -1.00D+00 NBFU=      519
 Initial guess from the checkpoint file:    "./coohpo.chk"
 B after Tr=          0.000000        0.000000        0.000000
             Rot=        0.996578      -0.046056        0.023200      -0.064592 Ang=    -9.48 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn=                5 AccDes=
0.00D+00
 Harris functional with IExCor=    402 and IRadAn=             5 diagonalized for initial guess.
 HarFok:    IExCor=    402 AccDes= 0.00D+00 IRadAn=                5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=    3500011 ScaDFX=    1.000000    1.000000    1.000000    1.000000
 FoFCou: FMM=F IPFlag=                  0 FMFlag=           100000 FMFlg1=                  0
             NFxFlg=                  0 DoJE=T BraDBF=F KetDBF=T FulRan=T
             wScrn=      0.000000  ICntrl=             500  IOpCl=      0  I1Cent=        200000004  NGrid=
0
             NMat0=         1 NMatS0=            1 NMatT0=         0 NMatD0=         1 NMtDS0=         0
NMtDT0=        0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                       energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3338.88086252          A.U. after      15 cycles
                  NFock= 15    Conv=0.15D-08         -V/T= 2.0018
 Calling FoFJK, ICntrl=             2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center         Atomic                             Forces (Hartrees/Bohr)
 Number         Number                       X                      Y                      Z
 -------------------------------------------------------------------
        1              6               -0.000281692        0.001549930        0.004163428
        2              6               -0.001999995        0.002395943        0.001908772
        3              7               -0.000584563       -0.000912278       -0.001422735
        4              6                0.003816740       -0.001505367       -0.001237123
```

5	7	-0.002571440	-0.004100786	-0.002651601
6	6	0.001211942	0.004037302	0.002810751
7	1	0.000695252	-0.000910834	-0.001363403
8	1	0.002153580	-0.001523819	-0.002181281
9	1	0.000005575	-0.001360288	0.000384341
10	1	0.000699800	0.001459419	-0.000971653
11	35	-0.015975594	-0.007827192	-0.000044348
12	1	-0.001364048	0.000579184	-0.000381459
13	6	0.000652749	0.001700616	0.000276139
14	6	0.000338703	-0.001274930	0.000795264
15	1	-0.000716677	0.000638838	-0.001118185
16	1	-0.000283913	0.000105020	0.000051363
17	1	-0.000163002	-0.000253499	0.000369439
18	6	0.007365863	-0.001294448	0.001695330
19	6	0.002083168	-0.001054484	-0.005421507
20	8	0.002456886	0.007375003	0.005546806
21	1	0.002475284	0.000859697	-0.000931832
22	1	0.002443076	0.000251849	0.000261375
23	1	-0.000546184	-0.000482657	0.000109003
24	6	-0.000177686	0.001757014	0.001321066
25	1	0.000868584	0.000092892	0.000058225
26	1	-0.000252579	-0.000075355	-0.000024448
27	1	-0.000189737	-0.000145892	0.000148950
28	6	-0.006094118	0.006165513	-0.002097553
29	1	0.000190518	-0.002533524	-0.002647137
30	1	0.000311714	0.002730997	0.003402880
31	6	-0.008849877	0.007086835	0.007185562
32	8	0.009280913	-0.008511054	-0.006941240
33	8	0.007677452	-0.012016919	-0.004613847
34	1	-0.004676693	0.006997271	0.003560658

Cartesian Forces: Max 0.015975594 RMS 0.003797136

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.097556897 RMS 0.018789897
Search for a local minimum.
Step number 3 out of a maximum of 175
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 2 3

DE= -2.27D-03 DEPred=-9.53D-03 R= 2.38D-01

Trust test= 2.38D-01 RLast= 7.17D-01 DXMaxT set to 5.05D-01

ITU= 0 1 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00207	0.00231	0.00304	0.00447	0.00698
Eigenvalues ---	0.00758	0.00937	0.01302	0.01397	0.01428
Eigenvalues ---	0.01524	0.01587	0.01811	0.01914	0.02100
Eigenvalues ---	0.02258	0.02265	0.02348	0.02464	0.02507
Eigenvalues ---	0.03014	0.03045	0.03063	0.03320	0.03777
Eigenvalues ---	0.03844	0.04969	0.05115	0.05339	0.05761
Eigenvalues ---	0.05871	0.06744	0.07596	0.09265	0.09982
Eigenvalues ---	0.11970	0.12497	0.12589	0.13409	0.13623
Eigenvalues ---	0.15454	0.15768	0.15986	0.15992	0.15999
Eigenvalues ---	0.16000	0.16000	0.16000	0.16000	0.16069
Eigenvalues ---	0.16868	0.18521	0.20051	0.22003	0.22346
Eigenvalues ---	0.22883	0.23433	0.23926	0.24837	0.24996
Eigenvalues ---	0.25000	0.26311	0.28386	0.29120	0.29659
Eigenvalues ---	0.31847	0.32543	0.34497	0.34561	0.34610
Eigenvalues ---	0.34764	0.34884	0.34890	0.34959	0.35006
Eigenvalues ---	0.35072	0.35531	0.35675	0.35763	0.36484
Eigenvalues ---	0.36545	0.36651	0.36895	0.37255	0.37714
Eigenvalues ---	0.41070	0.42302	0.45522	0.48976	0.52358
Eigenvalues ---	0.53359	0.55363	0.56069	0.60279	0.87024
Eigenvalues ---	1.16247				

RFO step: Lambda=-5.50374567D-02 EMin= 2.07086409D-03

Quartic linear search produced a step of -0.34606.

Iteration 1 RMS(Cart)= 0.33233717 RMS(Int)= 0.01694148

Iteration 2 RMS(Cart)= 0.03506752 RMS(Int)= 0.00079470

Iteration 3 RMS(Cart)= 0.00108939 RMS(Int)= 0.00051587

Iteration 4 RMS(Cart)= 0.00000146 RMS(Int)= 0.00051587

Iteration 5 RMS(Cart)= 0.00000000 RMS(Int)= 0.00051587

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.57122	0.02001	0.00034	0.00463	0.00479	2.57601
R2	2.61551	0.00836	0.00211	-0.00314	-0.00087	2.61465
R3	2.03312	-0.00020	-0.00032	0.00142	0.00110	2.03423
R4	2.61605	-0.00795	0.00117	-0.00549	-0.00455	2.61149
R5	2.02610	0.00347	0.00228	-0.00874	-0.00646	2.01964
R6	2.53797	-0.01081	0.00056	-0.00977	-0.00920	2.52877
R7	2.69620	-0.00058	0.00088	-0.00348	-0.00260	2.69360
R8	2.52713	0.00064	0.00027	-0.00169	-0.00116	2.52596
R9	2.02974	0.00135	0.00175	-0.00280	-0.00105	2.02869
R10	2.77485	0.01364	-0.00004	0.00465	0.00461	2.77945
R11	2.06413	-0.00079	-0.00073	0.00101	0.00028	2.06441

R12	2.05966	0.00023	0.00040	-0.00043	-0.00003	2.05962
R13	2.90534	0.00828	0.00627	-0.02693	-0.02066	2.88467
R14	5.49323	-0.00153	0.07973	-0.29567	-0.21594	5.27729
R15	2.49905	0.00183	0.00091	-0.00125	-0.00034	2.49871
R16	2.04025	0.00130	0.00184	-0.00370	-0.00187	2.03838
R17	2.04255	0.00010	0.00041	-0.00152	-0.00111	2.04144
R18	2.04415	0.00026	0.00048	-0.00099	-0.00051	2.04364
R19	2.77727	-0.00310	0.00121	-0.00829	-0.00713	2.77015
R20	2.73581	0.00131	0.00164	-0.00390	-0.00224	2.73357
R21	2.04971	0.00180	0.00045	0.00145	0.00190	2.05161
R22	2.04853	-0.00221	0.00049	-0.00038	0.00011	2.04864
R23	2.73708	0.00085	-0.00091	0.00368	0.00279	2.73987
R24	2.05577	0.00041	0.00060	-0.00207	-0.00147	2.05430
R25	2.84392	0.00031	0.00007	-0.00004	0.00003	2.84395
R26	3.23998	-0.00326	-0.04429	0.14608	0.10178	3.34177
R27	2.06800	0.00039	-0.00067	0.00218	0.00152	2.06951
R28	2.06810	-0.00006	-0.00035	0.00076	0.00040	2.06851
R29	2.06456	-0.00023	-0.00054	0.00136	0.00082	2.06539
R30	2.07413	-0.00204	-0.00732	0.02031	0.01298	2.08711
R31	2.07064	-0.00382	-0.00590	0.01226	0.00637	2.07701
R32	2.85272	0.01549	0.00379	0.01344	0.01724	2.86996
R33	2.26086	0.01184	0.00860	-0.02071	-0.01211	2.24875
R34	2.53916	0.01341	0.00402	-0.00676	-0.00275	2.53641
R35	1.89861	-0.00273	-0.00721	0.01512	0.00791	1.90652
A1	1.87616	-0.00780	0.00066	-0.01198	-0.01116	1.86500
A2	2.27958	0.00416	-0.00033	0.00571	0.00529	2.28487
A3	2.12695	0.00389	-0.00018	0.00492	0.00460	2.13155
A4	1.86353	0.00239	0.00009	0.00415	0.00399	1.86751
A5	2.29060	0.01545	0.00291	0.00326	0.00625	2.29685
A6	2.12866	-0.01789	-0.00287	-0.00815	-0.01092	2.11774
A7	1.89683	-0.00012	-0.00100	0.00152	0.00047	1.89730
A8	2.20875	0.00122	0.00398	-0.01030	-0.00629	2.20246
A9	2.17373	-0.00118	-0.00341	0.00964	0.00625	2.17999
A10	1.89519	0.01002	0.00176	-0.00381	-0.00198	1.89321
A11	2.19163	-0.00492	-0.00175	0.00409	0.00179	2.19342
A12	2.19608	-0.00484	-0.00025	0.00102	0.00021	2.19629
A13	1.89246	-0.00460	-0.00196	0.00860	0.00627	1.89873
A14	2.18739	0.05422	0.01225	-0.00627	0.00469	2.19208
A15	2.20333	-0.04959	-0.01111	-0.00204	-0.01420	2.18914
A16	1.88689	-0.04356	-0.00941	-0.01192	-0.02159	1.86529
A17	1.83660	0.00062	0.01141	-0.00787	0.00379	1.84040
A18	2.01851	0.06806	0.01392	-0.01221	0.00185	2.02037
A19	1.87738	0.00823	-0.00072	0.00101	0.00034	1.87772
A20	1.91751	-0.00979	-0.01456	0.04318	0.02862	1.94613

A21	1.92075	-0.02635	-0.00126	-0.01375	-0.01441	1.90634
A22	1.61645	0.01798	0.00179	-0.00221	-0.00042	1.61603
A23	2.14951	0.00073	-0.00015	0.00086	0.00071	2.15021
A24	1.98184	-0.00075	-0.00482	0.01473	0.00990	1.99174
A25	2.15065	0.00004	0.00515	-0.01632	-0.01117	2.13948
A26	2.08729	-0.00029	-0.00013	-0.00103	-0.00120	2.08609
A27	2.14174	0.00055	0.00044	0.00062	0.00102	2.14276
A28	2.05300	-0.00025	0.00001	-0.00110	-0.00113	2.05187
A29	2.08057	-0.00539	-0.00191	-0.00315	-0.00501	2.07555
A30	2.11939	0.00380	0.00397	-0.01076	-0.00690	2.11249
A31	1.98953	-0.00091	-0.00064	0.00167	0.00104	1.99057
A32	1.99629	0.00029	-0.00072	0.00341	0.00267	1.99896
A33	2.01165	0.00125	-0.00071	0.00720	0.00645	2.01810
A34	2.05179	0.00171	0.00230	-0.00847	-0.00615	2.04564
A35	2.13213	-0.00174	-0.00070	0.00320	0.00247	2.13460
A36	1.96041	-0.00059	-0.00007	-0.00102	-0.00107	1.95934
A37	2.03699	0.00005	-0.00174	0.00577	0.00400	2.04099
A38	2.01863	-0.00006	-0.00058	0.00193	0.00135	2.01998
A39	2.34631	0.00080	0.00522	-0.01981	-0.01459	2.33172
A40	2.64668	-0.00473	-0.00549	0.00896	0.00324	2.64992
A41	1.93460	0.00130	-0.00106	0.00661	0.00554	1.94014
A42	1.92149	-0.00057	0.00020	-0.00266	-0.00246	1.91903
A43	1.93496	-0.00036	-0.00083	0.00255	0.00171	1.93667
A44	1.88313	-0.00029	0.00061	-0.00258	-0.00197	1.88115
A45	1.89548	-0.00030	0.00030	-0.00145	-0.00116	1.89432
A46	1.89283	0.00020	0.00086	-0.00277	-0.00191	1.89092
A47	1.83163	-0.01053	0.01022	-0.04925	-0.03890	1.79273
A48	1.95026	-0.01893	-0.00495	0.00836	0.00243	1.95269
A49	1.97457	0.05553	0.00045	0.03497	0.03506	2.00964
A50	1.91418	0.00545	0.00005	-0.00813	-0.00823	1.90595
A51	1.93063	-0.03734	-0.01343	0.00051	-0.01244	1.91819
A52	1.86323	0.00399	0.00715	0.01215	0.01864	1.88187
A53	2.11684	0.03352	0.02185	-0.03129	-0.01226	2.10457
A54	1.96125	-0.04741	-0.00693	-0.00231	-0.01210	1.94915
A55	2.20142	0.01641	-0.01445	0.04434	0.02696	2.22838
A56	1.83449	0.09756	0.00666	0.12688	0.13355	1.96804
A57	2.60911	0.08163	-0.01509	0.12277	0.10768	2.71679
D1	-0.02498	0.00453	0.01895	-0.06490	-0.04601	-0.07099
D2	-3.13589	0.00697	0.01075	-0.03684	-0.02581	3.12149
D3	-3.13254	-0.00446	0.00308	-0.01855	-0.01589	3.13476
D4	0.03973	-0.00202	-0.00512	0.00951	0.00432	0.04405
D5	0.00772	-0.00946	-0.02153	0.06061	0.03910	0.04682
D6	-3.13108	-0.01712	0.00233	-0.04758	-0.04655	3.10556
D7	3.11890	-0.00139	-0.00734	0.01923	0.01227	3.13117

D8	-0.01990	-0.00905	0.01652	-0.08895	-0.07337	-0.09327
D9	0.03362	0.00195	-0.00984	0.04711	0.03749	0.07112
D10	3.08374	0.00082	-0.01489	0.05791	0.04310	3.12684
D11	-3.13516	0.00047	-0.00255	0.02246	0.02014	-3.11502
D12	-0.08505	-0.00067	-0.00760	0.03326	0.02575	-0.05930
D13	-1.75120	-0.04897	0.01317	-0.25133	-0.23824	-1.98944
D14	1.42502	-0.04663	0.00391	-0.21988	-0.21589	1.20913
D15	-0.02923	-0.00802	-0.00361	-0.00950	-0.01311	-0.04233
D16	3.08790	0.00340	-0.01087	0.04619	0.03495	3.12285
D17	-3.08160	-0.00706	0.00077	-0.01876	-0.01782	-3.09942
D18	0.03552	0.00436	-0.00650	0.03694	0.03024	0.06576
D19	0.52423	0.00028	0.01416	-0.04858	-0.03435	0.48988
D20	-2.56628	0.00008	0.00955	-0.03272	-0.02307	-2.58935
D21	-2.72263	-0.00095	0.00859	-0.03679	-0.02831	-2.75093
D22	0.47005	-0.00115	0.00398	-0.02093	-0.01703	0.45302
D23	0.01340	0.01070	0.01546	-0.03138	-0.01610	-0.00269
D24	-3.13101	0.01866	-0.00747	0.07806	0.06941	-3.06160
D25	-3.10364	-0.00076	0.02280	-0.08730	-0.06428	3.11526
D26	0.03513	0.00721	-0.00014	0.02213	0.02122	0.05635
D27	-2.61386	-0.00210	-0.04282	0.11780	0.07479	-2.53907
D28	-0.61167	-0.01200	-0.04256	0.10977	0.06736	-0.54431
D29	1.51176	-0.00306	-0.02577	0.07905	0.05299	1.56475
D30	0.53102	-0.01123	-0.01535	-0.00947	-0.02480	0.50622
D31	2.53320	-0.02113	-0.01509	-0.01750	-0.03223	2.50098
D32	-1.62655	-0.01219	0.00170	-0.04823	-0.04659	-1.67314
D33	-2.97490	-0.02695	-0.04637	0.06661	0.02049	-2.95441
D34	1.23501	-0.01723	-0.04994	0.10160	0.05173	1.28674
D35	-0.86851	-0.04828	-0.05592	0.05468	-0.00135	-0.86986
D36	1.16684	-0.01126	-0.03209	0.05684	0.02483	1.19167
D37	-0.90643	-0.00154	-0.03565	0.09183	0.05607	-0.85036
D38	-3.00995	-0.03259	-0.04163	0.04491	0.00299	-3.00696
D39	-0.89719	0.00060	-0.02200	0.03767	0.01590	-0.88128
D40	-2.97045	0.01032	-0.02556	0.07266	0.04714	-2.92331
D41	1.20921	-0.02073	-0.03154	0.02574	-0.00594	1.20327
D42	-3.07495	-0.00036	-0.00309	0.00935	0.00624	-3.06871
D43	0.01384	-0.00001	0.00691	-0.02516	-0.01827	-0.00443
D44	0.01066	-0.00017	0.00173	-0.00708	-0.00533	0.00532
D45	3.09945	0.00018	0.01173	-0.04159	-0.02985	3.06960
D46	-2.73757	0.00065	-0.00126	0.00812	0.00683	-2.73074
D47	-0.03509	0.00044	0.00128	-0.00014	0.00112	-0.03397
D48	-0.01219	-0.00009	0.00235	-0.00876	-0.00642	-0.01862
D49	2.69028	-0.00030	0.00489	-0.01702	-0.01213	2.67815
D50	0.68022	-0.00269	-0.00271	0.00200	-0.00062	0.67960
D51	-1.68645	-0.00395	-0.00013	-0.01477	-0.01483	-1.70128

D52	2.07809	0.00333	-0.01049	0.05382	0.04337	2.12146
D53	-0.31194	0.00406	-0.00753	0.04536	0.03787	-0.27406
D54	2.54705	0.00025	-0.00121	0.00520	0.00400	2.55104
D55	-1.65395	0.00035	-0.00100	0.00446	0.00346	-1.65049
D56	0.44056	-0.00001	-0.00033	0.00091	0.00057	0.44113
D57	1.33927	-0.00051	-0.00091	0.00222	0.00131	1.34058
D58	-2.86173	-0.00041	-0.00070	0.00148	0.00078	-2.86095
D59	-0.76722	-0.00077	-0.00003	-0.00208	-0.00211	-0.76933
D60	-1.02594	0.00046	0.00195	-0.00535	-0.00340	-1.02933
D61	1.05625	0.00056	0.00217	-0.00609	-0.00393	1.05232
D62	-3.13242	0.00021	0.00284	-0.00965	-0.00682	-3.13924
D63	1.68873	0.01939	0.03973	-0.06854	-0.02886	1.65987
D64	-2.62674	0.00765	0.04305	-0.10968	-0.06658	-2.69332
D65	1.95254	0.01742	-0.05274	0.26632	0.21327	2.16581
D66	-1.10237	-0.01276	-0.05814	0.13765	0.08038	-1.02199
D67	-2.28145	0.01468	-0.04863	0.22695	0.17776	-2.10369
D68	0.94683	-0.01550	-0.05403	0.09827	0.04487	0.99170
D69	-0.19979	0.00288	-0.05187	0.22473	0.17196	-0.02783
D70	3.02849	-0.02729	-0.05727	0.09605	0.03907	3.06755
D71	2.90087	0.05759	0.06351	-0.02047	0.04456	2.94543
D72	-0.14899	0.02488	0.05603	-0.15195	-0.09744	-0.24642
D73	-1.31772	0.00449	-0.00018	0.00148	0.00130	-1.31642

Item	Value	Threshold	Converged?
Maximum Force	0.097557	0.000450	NO
RMS Force	0.018790	0.000300	NO
Maximum Displacement	2.053764	0.001800	NO
RMS Displacement	0.348720	0.001200	NO

Predicted change in Energy=-3.247864D-02

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.756236	1.359494	1.339199
2	6	0	-1.535134	0.255690	1.521284
3	7	0	-2.655920	0.416885	0.729058
4	6	0	-2.519851	1.541487	0.016701
5	7	0	-1.372347	2.129671	0.368831
6	6	0	-0.900952	3.436611	-0.113883
7	1	0	0.191757	1.632277	1.770100
8	1	0	-1.422165	-0.595305	2.157887
9	1	0	-1.789567	4.030383	-0.340203

10	1	0	-0.404269	3.899139	0.738918
11	35	0	-1.100346	-2.330326	-0.006571
12	1	0	-3.225576	1.918409	-0.699092
13	6	0	-3.732622	-0.507642	0.595979
14	6	0	-4.084844	-1.351170	1.551371
15	1	0	-4.199695	-0.503286	-0.376310
16	1	0	-4.866334	-2.072809	1.362894
17	1	0	-3.575878	-1.402088	2.504204
18	6	0	3.437306	-0.822290	0.176893
19	6	0	4.200358	-0.403861	1.356522
20	8	0	3.188391	0.464975	0.788023
21	1	0	3.907414	-0.764809	-0.800021
22	1	0	2.617996	-1.527063	0.262267
23	1	0	3.897779	-0.815744	2.315982
24	6	0	5.628321	0.062773	1.266743
25	1	0	5.837638	0.840146	2.009178
26	1	0	6.307477	-0.774012	1.458329
27	1	0	5.847216	0.462934	0.273511
28	6	0	0.062891	3.398556	-1.297003
29	1	0	0.425702	4.440437	-1.348612
30	1	0	-0.450665	3.147664	-2.235802
31	6	0	1.237919	2.448967	-1.141782
32	8	0	1.441788	1.600636	-1.951006
33	8	0	1.976621	2.746682	-0.061403
34	1	0	2.648900	2.028300	0.161801

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.363166	0.000000			
3	N	2.206713	1.381944	0.000000		
4	C	2.211890	2.210590	1.338169	0.000000	
5	N	1.383611	2.206004	2.170475	1.336683	0.000000
6	C	2.539056	3.632384	3.592939	2.495873	1.470822
7	H	1.076466	2.222399	3.266530	3.230398	2.158096
8	H	2.221475	1.068746	2.142016	3.217992	3.260169
9	H	3.319911	4.216417	3.866685	2.618262	2.071112
10	H	2.633251	3.894313	4.146821	3.248970	2.050648
11	Br	3.942624	3.034940	3.241625	4.123891	4.484026
12	H	3.250331	3.248429	2.149114	1.073535	2.149313
13	C	3.591301	2.503561	1.425393	2.450573	3.546536
14	C	4.297946	3.013954	2.417444	3.629308	4.568620
15	H	4.274380	3.358093	2.109927	2.675338	3.934666
16	H	5.354827	4.067418	3.389138	4.514572	5.554903

17	H	4.115088	2.806955	2.702985	3.995935	4.678535
18	C	4.867950	5.262564	6.242423	6.410992	5.646563
19	C	5.260946	5.775640	6.933678	7.123251	6.200755
20	O	4.082161	4.784679	5.844806	5.859849	4.873116
21	H	5.553248	6.004266	6.841918	6.877192	6.133523
22	H	4.569184	4.691676	5.640126	5.989472	5.413492
23	H	5.229305	5.594288	6.854829	7.213127	6.343587
24	C	6.515314	7.170572	8.309222	8.375077	7.354432
25	H	6.648141	7.411976	8.599906	8.620294	7.505831
26	H	7.379843	7.910170	9.071525	9.239131	8.282395
27	H	6.748711	7.489926	8.515455	8.440204	7.410074
28	C	3.431953	4.513760	4.515221	3.441668	2.538696
29	H	4.255997	5.439971	5.477415	4.352501	3.394440
30	H	4.008934	4.863669	4.594637	3.454722	2.944472
31	C	3.364353	4.426308	4.774032	4.035645	3.032719
32	O	3.964203	4.767362	5.037382	4.423794	3.685224
33	O	3.369642	4.587195	5.245305	4.655841	3.432403
34	H	3.664495	4.743046	5.573111	5.193653	4.027849

		6	7	8	9	10
6	C	0.000000				
7	H	2.828255	0.000000			
8	H	4.657140	2.777993	0.000000		
9	H	1.092439	3.758981	5.269955	0.000000	
10	H	1.089906	2.560712	4.821785	1.760903	0.000000
11	Br	5.771382	4.530819	2.792624	6.406634	6.312410
12	H	2.837479	4.225748	4.211101	2.579023	3.735095
13	C	4.907076	4.621533	2.790243	5.024497	5.524318
14	C	5.986074	5.219014	2.833558	6.148777	6.463161
15	H	5.145227	5.334094	3.761023	5.134605	5.918643
16	H	6.946858	6.283134	3.831100	7.043862	7.480878
17	H	6.117403	4.892990	2.325793	6.386963	6.424822
18	C	6.086318	4.369988	5.252649	7.150945	6.112729
19	C	6.552456	4.515062	5.682570	7.643337	6.332443
20	O	5.134859	3.362570	4.925236	6.226162	4.970220
21	H	6.422079	5.114455	6.097735	7.460623	6.535392
22	H	6.096109	4.259298	4.558997	7.118623	6.229362
23	H	6.856718	4.474974	5.326856	7.930080	6.574562
24	C	7.477989	5.680927	7.136986	8.564419	7.168573
25	H	7.527125	5.706189	7.401849	8.594851	7.066286
26	H	8.494860	6.579472	7.763291	9.585356	8.209958
27	H	7.384484	5.965849	7.583842	8.451260	7.148788
28	C	1.526504	3.541676	5.485671	2.178594	2.147974
29	H	2.071770	4.203196	6.408498	2.468289	2.310765
30	H	2.188330	4.330861	5.853044	2.482971	3.068522

31	C	2.570367	3.200077	5.218377	3.508430	2.887354
32	O	3.497751	3.925584	5.468765	4.352013	3.990831
33	O	2.959591	2.789631	5.257934	3.988708	2.763568
34	H	3.828941	2.963277	5.238439	4.894930	3.626974

		11	12	13	14	15
11	Br	0.000000				
12	H	4.800827	0.000000			
13	C	3.257932	2.796431	0.000000		
14	C	3.506160	4.061165	1.322260	0.000000	
15	H	3.616731	2.630152	1.078666	2.109040	0.000000
16	H	4.015521	4.782645	2.079233	1.080284	2.435702
17	H	3.646077	4.627041	2.113273	1.081448	3.081290
18	C	4.785198	7.257601	7.189054	7.664961	7.663652
19	C	5.802306	8.047545	7.970029	8.341458	8.577498
20	O	5.180575	6.742622	6.991658	7.535318	7.541684
21	H	5.306418	7.621640	7.770786	8.351590	8.122385
22	H	3.813604	6.851483	6.440570	6.827941	6.923641
23	H	5.715721	8.204173	7.827922	8.037013	8.539037
24	C	7.254187	9.257396	9.402264	9.819665	9.980478
25	H	7.889915	9.520463	9.767474	10.171877	10.404009
26	H	7.709986	10.138179	10.080585	10.408750	10.669575
27	H	7.493289	9.240126	9.634278	10.176921	10.114162
28	C	5.986521	3.655455	5.766081	6.919309	5.851640
29	H	7.069168	4.484901	6.749561	7.892884	6.839595
30	H	5.949784	3.401864	5.670228	6.912990	5.553590
31	C	5.440389	4.516664	6.038843	7.072899	6.234532
32	O	5.069096	4.842784	6.140561	7.177984	6.223542
33	O	5.936897	5.306179	6.604410	7.492315	6.986296
34	H	5.751767	5.938239	6.880650	7.661268	7.321321

		16	17	18	19	20
16	H	0.000000				
17	H	1.848710	0.000000			
18	C	8.480614	7.411969	0.000000		
19	C	9.219019	7.923602	1.465898	0.000000	
20	O	8.464597	7.224025	1.446544	1.449878	0.000000
21	H	9.130593	8.205102	1.085665	2.206078	2.133365
22	H	7.584485	6.588321	1.084095	2.227744	2.137753
23	H	8.904957	7.498985	2.188100	1.087090	2.116160
24	C	10.710170	9.401830	2.602242	1.504955	2.518770
25	H	11.112065	9.689527	3.447109	2.157360	2.941171
26	H	11.249445	9.958365	3.143611	2.141804	3.422440
27	H	11.063313	9.861491	2.732912	2.153228	2.708151
28	C	7.829952	7.122920	5.601302	6.214355	4.766757
29	H	8.819313	8.061757	6.252457	6.710663	5.291687

30	H	7.726712	7.275634	6.057883	6.866596	5.439031
31	C	7.998860	7.162156	4.156600	4.812089	3.385958
32	O	8.016766	7.351341	3.792178	4.750522	3.441311
33	O	8.490121	7.390864	3.863670	4.108703	2.719576
34	H	8.645257	7.483467	2.957647	3.122466	1.768386

		21	22	23	24	25
21	H	0.000000				
22	H	1.836325	0.000000			
23	H	3.116435	2.522214	0.000000		
24	C	2.813881	3.549452	2.206235	0.000000	
25	H	3.767392	4.361361	2.568881	1.095140	0.000000
26	H	3.295532	3.950939	2.558115	1.094608	1.769092
27	H	2.534296	3.793162	3.099518	1.092956	1.776210
28	C	5.688669	5.763819	6.746877	6.976694	7.129095
29	H	6.286322	6.558364	7.287798	7.285003	7.316140
30	H	6.030071	6.124549	7.438837	7.664101	7.930148
31	C	4.191820	4.436753	5.448791	5.547121	5.802954
32	O	3.605469	4.008060	5.484339	5.499636	5.965308
33	O	4.074811	4.333708	4.694006	4.722527	4.778037
34	H	3.210984	3.556917	3.780051	3.736462	3.872023

		26	27	28	29	30
26	H	0.000000				
27	H	1.773603	0.000000			
28	C	7.999814	6.674040	0.000000		
29	H	8.346536	6.916981	1.104450	0.000000	
30	H	8.642836	7.291621	1.099105	1.796214	0.000000
31	C	6.545883	5.214691	1.518718	2.160655	2.129876
32	O	6.398237	5.064646	2.358304	3.075675	2.460850
33	O	5.784564	4.506571	2.369390	2.632691	3.283369
34	H	4.787392	3.562594	3.270039	3.611421	4.075387

		31	32	33	34
31	C	0.000000			
32	O	1.189988	0.000000		
33	O	1.342213	2.273778	0.000000	
34	H	1.966509	2.470621	1.008887	0.000000

Stoichiometry C11H17BrN2O3
Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	6	0	-0.532991	0.982337	1.304135
2	6	0	-1.559655	0.086073	1.274269
3	7	0	-2.585468	0.670522	0.556011
4	6	0	-2.162240	1.849402	0.085038
5	7	0	-0.917443	2.058929	0.524696
6	6	0	-0.131573	3.283239	0.308385
7	1	0	0.440045	0.924770	1.760936
8	1	0	-1.673222	-0.877948	1.721464
9	1	0	-0.844198	4.107247	0.227150
10	1	0	0.437223	3.429107	1.226583
11	35	0	-1.716777	-2.162821	-0.757639
12	1	0	-2.735625	2.522800	-0.523439
13	6	0	-3.848846	0.080271	0.260666
14	6	0	-4.421055	-0.829005	1.031488
15	1	0	-4.273065	0.394542	-0.679968
16	1	0	-5.347589	-1.286789	0.716873
17	1	0	-3.966848	-1.193631	1.942681
18	6	0	3.043311	-1.865006	-0.369075
19	6	0	3.850540	-1.891651	0.854251
20	8	0	3.094288	-0.707385	0.496838
21	1	0	3.541225	-1.725741	-1.323725
22	1	0	2.076300	-2.353228	-0.411395
23	1	0	3.430317	-2.404140	1.715953
24	6	0	5.350820	-1.775520	0.830530
25	1	0	5.719806	-1.239079	1.711105
26	1	0	5.802714	-2.772492	0.832779
27	1	0	5.688004	-1.247088	-0.064802
28	6	0	0.828241	3.254445	-0.878267
29	1	0	1.432588	4.165964	-0.724296
30	1	0	0.296502	3.330932	-1.837138
31	6	0	1.735085	2.038041	-0.945352
32	8	0	1.751780	1.348022	-1.914716
33	8	0	2.492468	1.922872	0.156756
34	1	0	2.965297	1.033501	0.214232

Rotational constants (GHZ): 0.3760964 0.2228585 0.1607386

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 538 symmetry adapted cartesian basis functions of A symmetry.

There are 519 symmetry adapted basis functions of A symmetry.

519 basis functions, 823 primitive gaussians, 538 cartesian basis functions

78 alpha electrons 78 beta electrons

nuclear repulsion energy 1577.1627809505 Hartrees.

NAtoms= 34 NActive= 34 NUniq= 34 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 519 RedAO= T EigKep= 3.56D-06 NBF= 519

NBsUse= 519 1.00D-06 EigRej= -1.00D+00 NBFU= 519

Initial guess from the checkpoint file: "./coohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.997074 -0.000424 -0.027763 0.071221 Ang= -8.77 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3338.88255236 A.U. after 15 cycles

NFock= 15 Conv=0.41D-08 -V/T= 2.0018

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000193190	-0.004364016	0.000771276
2	6	-0.002063898	0.004715968	0.005521588
3	7	-0.002183270	-0.001482813	-0.001827040
4	6	0.002847586	-0.001210506	0.001722398
5	7	-0.002813112	0.003982243	-0.002657611
6	6	-0.000604093	-0.001185889	0.008430111
7	1	-0.000350840	-0.000514909	-0.001690832
8	1	0.002311619	-0.002702171	0.000280219

9	1	0.001969835	0.000513178	-0.001843935
10	1	-0.000418498	0.001058245	0.000299595
11	35	0.006804415	-0.004838945	-0.002376128
12	1	-0.001013668	0.000313680	-0.001397817
13	6	-0.002467856	0.000844244	0.000230193
14	6	-0.000367345	0.000605196	0.002200622
15	1	0.000007016	0.001766527	-0.001695428
16	1	-0.000396732	-0.000003561	-0.000022518
17	1	-0.000616814	-0.000024936	0.000477191
18	6	-0.001650101	-0.000997645	-0.002257298
19	6	0.001712603	0.001238678	-0.000886882
20	8	0.001226834	0.001561882	0.002357134
21	1	0.000123241	0.000157146	-0.000338941
22	1	-0.001643661	-0.000168325	0.000395161
23	1	-0.000599692	-0.000084219	0.000402021
24	6	0.000213425	0.000921801	0.000246484
25	1	-0.000489567	-0.000646766	-0.000500185
26	1	-0.000279590	0.000056670	0.000042542
27	1	-0.000217828	-0.000172535	0.000392684
28	6	-0.006653738	0.010850829	-0.001824180
29	1	0.001640792	-0.006508949	-0.005475623
30	1	0.003330718	0.000996166	0.005313316
31	6	-0.006183952	0.019174827	0.003462965
32	8	0.011976268	-0.019503667	-0.008111533
33	8	0.010369680	-0.011875485	0.008612238
34	1	-0.013326586	0.007528056	-0.008251787

Cartesian Forces: Max 0.019503667 RMS 0.004715553

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.021477997 RMS 0.004473308
Search for a local minimum.
Step number 4 out of a maximum of 175
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 3 4
DE= -1.69D-03 DEPred=-3.25D-02 R= 5.20D-02
Trust test= 5.20D-02 RLast= 6.28D-01 DXMaxT set to 2.52D-01
ITU= -1 0 1 0
Use linear search instead of GDIIS.

```
 Eigenvalues ---     0.00222   0.00232   0.00349   0.00520   0.00698
 Eigenvalues ---     0.00788   0.00963   0.01302   0.01383   0.01430
 Eigenvalues ---     0.01543   0.01598   0.01816   0.01920   0.02091
 Eigenvalues ---     0.02256   0.02259   0.02352   0.02467   0.02499
 Eigenvalues ---     0.03012   0.03049   0.03072   0.03211   0.03710
 Eigenvalues ---     0.03822   0.04875   0.05051   0.05381   0.05725
 Eigenvalues ---     0.05874   0.06971   0.07592   0.09534   0.10032
 Eigenvalues ---     0.11949   0.12536   0.12743   0.13427   0.13643
 Eigenvalues ---     0.15431   0.15787   0.15950   0.15992   0.15999
 Eigenvalues ---     0.15999   0.16000   0.16000   0.16000   0.16035
 Eigenvalues ---     0.16882   0.19169   0.20205   0.22005   0.22353
 Eigenvalues ---     0.22907   0.23421   0.23884   0.24771   0.24875
 Eigenvalues ---     0.24962   0.26308   0.28402   0.29129   0.29725
 Eigenvalues ---     0.31847   0.32513   0.34497   0.34560   0.34609
 Eigenvalues ---     0.34763   0.34882   0.34889   0.34957   0.35005
 Eigenvalues ---     0.35066   0.35530   0.35667   0.35763   0.36488
 Eigenvalues ---     0.36546   0.36710   0.36886   0.37244   0.37712
 Eigenvalues ---     0.41070   0.42232   0.45583   0.48849   0.52093
 Eigenvalues ---     0.53177   0.55366   0.56076   0.60276   0.87005
 Eigenvalues ---     1.15474
RFO step:  Lambda=-5.74740856D-02 EMin= 2.22384152D-03
Quartic linear search produced a step of -0.61923.
Maximum step size (   0.252) exceeded in Quadratic search.
    -- Step size scaled by   0.587
Iteration  1 RMS(Cart)=  0.19892677 RMS(Int)=  0.01701779
Iteration  2 RMS(Cart)=  0.05065070 RMS(Int)=  0.00294470
Iteration  3 RMS(Cart)=  0.00577565 RMS(Int)=  0.00073395
Iteration  4 RMS(Cart)=  0.00004488 RMS(Int)=  0.00073314
Iteration  5 RMS(Cart)=  0.00000001 RMS(Int)=  0.00073314
Variable       Old X    -DE/DX   Delta X   Delta X   Delta X     New X
                                 (Linear)    (Quad)   (Total)
    R1         2.57601  -0.00142  -0.00296   0.00671   0.00366   2.57967
    R2         2.61465   0.00233   0.00054   0.00802   0.00864   2.62328
    R3         2.03423  -0.00111  -0.00068  -0.00166  -0.00234   2.03189
    R4         2.61149   0.00699   0.00282   0.00459   0.00727   2.61877
    R5         2.01964   0.00572   0.00400   0.01046   0.01446   2.03410
    R6         2.52877   0.00280   0.00570  -0.00148   0.00426   2.53304
    R7         2.69360   0.00071   0.00161   0.00161   0.00321   2.69682
    R8         2.52596  -0.00091   0.00072  -0.00053   0.00030   2.52627
    R9         2.02869   0.00171   0.00065   0.00478   0.00543   2.03412
   R10         2.77945   0.00258  -0.00285   0.00871   0.00585   2.78530
   R11         2.06441  -0.00094  -0.00017  -0.00236  -0.00253   2.06188
   R12         2.05962   0.00049   0.00002   0.00116   0.00118   2.06081
   R13         2.88467   0.00466   0.01280   0.01932   0.03212   2.91679
```

R14	5.27729	0.00563	0.13372	0.17732	0.31103	5.58833
R15	2.49871	0.00193	0.00021	0.00313	0.00334	2.50205
R16	2.03838	0.00153	0.00116	0.00472	0.00588	2.04426
R17	2.04144	0.00029	0.00069	0.00091	0.00159	2.04303
R18	2.04364	0.00014	0.00031	0.00092	0.00124	2.04488
R19	2.77015	0.00244	0.00441	0.00334	0.00779	2.77793
R20	2.73357	-0.00009	0.00139	0.00265	0.00402	2.73759
R21	2.05161	0.00036	-0.00118	0.00184	0.00066	2.05227
R22	2.04864	0.00139	-0.00007	0.00107	0.00101	2.04965
R23	2.73987	-0.00176	-0.00173	-0.00300	-0.00475	2.73512
R24	2.05430	0.00055	0.00091	0.00160	0.00251	2.05681
R25	2.84395	-0.00070	-0.00002	-0.00054	-0.00056	2.84339
R26	3.34177	-0.00218	-0.06303	-0.07305	-0.13608	3.20569
R27	2.06951	-0.00089	-0.00094	-0.00168	-0.00261	2.06690
R28	2.06851	-0.00021	-0.00025	-0.00073	-0.00098	2.06753
R29	2.06539	-0.00046	-0.00051	-0.00133	-0.00184	2.06355
R30	2.08711	-0.00535	-0.00804	-0.01630	-0.02433	2.06277
R31	2.07701	-0.00632	-0.00394	-0.01610	-0.02004	2.05696
R32	2.86996	0.00227	-0.01067	0.01573	0.00506	2.87502
R33	2.24875	0.02148	0.00750	0.02426	0.03175	2.28051
R34	2.53641	-0.00290	0.00170	0.00806	0.00976	2.54618
R35	1.90652	-0.01849	-0.00490	-0.02456	-0.02946	1.87706
A1	1.86500	0.00416	0.00691	0.00444	0.01090	1.87590
A2	2.28487	-0.00166	-0.00327	-0.00038	-0.00389	2.28098
A3	2.13155	-0.00260	-0.00285	-0.00226	-0.00532	2.12623
A4	1.86751	-0.00296	-0.00247	-0.00158	-0.00439	1.86313
A5	2.29685	-0.00639	-0.00387	0.00176	-0.00195	2.29490
A6	2.11774	0.00932	0.00676	-0.00001	0.00693	2.12467
A7	1.89730	-0.00101	-0.00029	-0.00285	-0.00335	1.89395
A8	2.20246	0.00623	0.00389	0.01519	0.01923	2.22169
A9	2.17999	-0.00508	-0.00387	-0.01203	-0.01581	2.16418
A10	1.89321	0.00196	0.00122	0.01041	0.01161	1.90482
A11	2.19342	-0.00107	-0.00111	-0.00622	-0.00727	2.18615
A12	2.19629	-0.00090	-0.00013	-0.00405	-0.00414	2.19215
A13	1.89873	-0.00225	-0.00388	-0.00817	-0.01284	1.88588
A14	2.19208	-0.00340	-0.00290	0.04567	0.04190	2.23397
A15	2.18914	0.00572	0.00879	-0.03394	-0.02592	2.16322
A16	1.86529	0.00562	0.01337	-0.03262	-0.01838	1.84691
A17	1.84040	0.00113	-0.00235	0.02053	0.01738	1.85778
A18	2.02037	-0.00757	-0.00115	0.05296	0.05155	2.07191
A19	1.87772	-0.00089	-0.00021	0.00102	0.00050	1.87822
A20	1.94613	-0.00142	-0.01772	-0.03055	-0.04804	1.89809
A21	1.90634	0.00357	0.00892	-0.01148	-0.00400	1.90234
A22	1.61603	0.01536	0.00026	0.03477	0.03503	1.65105

A23	2.15021	0.00075	-0.00044	0.00152	0.00102	2.15123
A24	1.99174	-0.00220	-0.00613	-0.01119	-0.01738	1.97435
A25	2.13948	0.00154	0.00692	0.01053	0.01739	2.15687
A26	2.08609	-0.00042	0.00074	-0.00081	-0.00018	2.08591
A27	2.14276	0.00078	-0.00063	0.00252	0.00177	2.14453
A28	2.05187	-0.00031	0.00070	-0.00043	0.00015	2.05202
A29	2.07555	0.00074	0.00310	-0.00424	-0.00110	2.07445
A30	2.11249	-0.00048	0.00427	0.00847	0.01264	2.12514
A31	1.99057	0.00039	-0.00065	-0.00206	-0.00270	1.98787
A32	1.99896	-0.00023	-0.00166	-0.00294	-0.00457	1.99439
A33	2.01810	0.00014	-0.00399	-0.00021	-0.00426	2.01384
A34	2.04564	-0.00048	0.00381	0.00456	0.00841	2.05405
A35	2.13460	0.00054	-0.00153	-0.00156	-0.00312	2.13148
A36	1.95934	-0.00027	0.00066	-0.00147	-0.00082	1.95852
A37	2.04099	0.00012	-0.00248	-0.00235	-0.00482	2.03617
A38	2.01998	0.00008	-0.00084	-0.00081	-0.00168	2.01830
A39	2.33172	-0.00119	0.00904	0.00821	0.01743	2.34915
A40	2.64992	0.00030	-0.00200	-0.00836	-0.01041	2.63950
A41	1.94014	-0.00043	-0.00343	-0.00177	-0.00521	1.93494
A42	1.91903	-0.00017	0.00152	-0.00013	0.00139	1.92042
A43	1.93667	-0.00005	-0.00106	-0.00153	-0.00259	1.93408
A44	1.88115	0.00026	0.00122	0.00119	0.00241	1.88357
A45	1.89432	0.00024	0.00072	0.00052	0.00123	1.89555
A46	1.89092	0.00018	0.00118	0.00190	0.00309	1.89401
A47	1.79273	0.00695	0.02409	0.02913	0.05331	1.84604
A48	1.95269	0.00236	-0.00150	-0.01781	-0.01868	1.93401
A49	2.00964	-0.00773	-0.02171	0.02393	0.00239	2.01203
A50	1.90595	-0.00234	0.00510	-0.00049	0.00453	1.91048
A51	1.91819	0.00019	0.00770	-0.04472	-0.03757	1.88062
A52	1.88187	0.00081	-0.01154	0.00791	-0.00342	1.87845
A53	2.10457	0.01152	0.00759	0.06487	0.07008	2.17465
A54	1.94915	0.00263	0.00749	-0.03345	-0.02805	1.92110
A55	2.22838	-0.01389	-0.01670	-0.02807	-0.04657	2.18181
A56	1.96804	-0.01922	-0.08270	0.03406	-0.04863	1.91941
A57	2.71679	-0.00677	-0.06668	0.01610	-0.05057	2.66621
D1	-0.07099	-0.00108	0.02849	0.03502	0.06383	-0.00716
D2	3.12149	-0.00081	0.01598	0.03091	0.04687	-3.11483
D3	3.13476	0.00075	0.00984	0.00246	0.01315	-3.13528
D4	0.04405	0.00103	-0.00267	-0.00165	-0.00382	0.04024
D5	0.04682	0.00091	-0.02421	-0.04295	-0.06707	-0.02025
D6	3.10556	0.00218	0.02882	0.00017	0.03141	3.13697
D7	3.13117	-0.00071	-0.00760	-0.01385	-0.02185	3.10932
D8	-0.09327	0.00055	0.04543	0.02927	0.07663	-0.01664
D9	0.07112	0.00084	-0.02322	-0.01559	-0.03904	0.03208

D10	3.12684	0.00232	-0.02669	-0.01247	-0.03915	3.08769
D11	-3.11502	0.00009	-0.01247	-0.01193	-0.02437	-3.13939
D12	-0.05930	0.00157	-0.01594	-0.00881	-0.02447	-0.08378
D13	-1.98944	0.01529	0.14753	0.17947	0.32718	-1.66225
D14	1.20913	0.01597	0.13369	0.17490	0.30840	1.51753
D15	-0.04233	-0.00046	0.00812	-0.01151	-0.00321	-0.04554
D16	3.12285	-0.00011	-0.02164	-0.01736	-0.03819	3.08466
D17	-3.09942	-0.00260	0.01103	-0.01623	-0.00522	-3.10464
D18	0.06576	-0.00225	-0.01873	-0.02208	-0.04020	0.02556
D19	0.48988	0.00086	0.02127	0.02892	0.04998	0.53985
D20	-2.58935	-0.00068	0.01428	0.01314	0.02739	-2.56196
D21	-2.75093	0.00289	0.01753	0.03326	0.05082	-2.70012
D22	0.45302	0.00135	0.01054	0.01748	0.02824	0.48126
D23	-0.00269	-0.00014	0.00997	0.03380	0.04348	0.04079
D24	-3.06160	-0.00086	-0.04298	-0.01394	-0.05404	-3.11565
D25	3.11526	-0.00049	0.03981	0.03963	0.07856	-3.08937
D26	0.05635	-0.00122	-0.01314	-0.00812	-0.01897	0.03738
D27	-2.53907	-0.00096	-0.04631	-0.05740	-0.10377	-2.64283
D28	-0.54431	0.00103	-0.04171	-0.06120	-0.10356	-0.64787
D29	1.56475	0.00176	-0.03282	-0.02851	-0.06111	1.50364
D30	0.50622	0.00005	0.01535	-0.00517	0.01045	0.51667
D31	2.50098	0.00204	0.01996	-0.00898	0.01065	2.51163
D32	-1.67314	0.00277	0.02885	0.02371	0.05310	-1.62004
D33	-2.95441	0.00208	-0.01269	-0.05451	-0.06767	-3.02208
D34	1.28674	-0.00019	-0.03203	-0.06226	-0.09450	1.19225
D35	-0.86986	0.00289	0.00084	-0.07724	-0.07649	-0.94634
D36	1.19167	0.00149	-0.01538	-0.02622	-0.04147	1.15020
D37	-0.85036	-0.00077	-0.03472	-0.03398	-0.06830	-0.91866
D38	-3.00696	0.00231	-0.00185	-0.04895	-0.05029	-3.05725
D39	-0.88128	0.00118	-0.00985	-0.00136	-0.01152	-0.89280
D40	-2.92331	-0.00109	-0.02919	-0.00912	-0.03835	-2.96166
D41	1.20327	0.00199	0.00368	-0.02409	-0.02034	1.18293
D42	-3.06871	-0.00101	-0.00387	-0.01021	-0.01416	-3.08287
D43	-0.00443	-0.00028	0.01131	0.00977	0.02100	0.01657
D44	0.00532	0.00052	0.00330	0.00610	0.00948	0.01480
D45	3.06960	0.00125	0.01848	0.02607	0.04464	3.11424
D46	-2.73074	-0.00058	-0.00423	-0.00529	-0.00956	-2.74030
D47	-0.03397	-0.00021	-0.00069	0.00014	-0.00056	-0.03454
D48	-0.01862	0.00049	0.00398	0.00523	0.00920	-0.00941
D49	2.67815	0.00086	0.00751	0.01066	0.01820	2.69634
D50	0.67960	0.00078	0.00038	-0.00194	-0.00148	0.67813
D51	-1.70128	0.00038	0.00918	0.00403	0.01325	-1.68803
D52	2.12146	0.00014	-0.02685	-0.02117	-0.04798	2.07348
D53	-0.27406	0.00020	-0.02345	-0.01541	-0.03883	-0.31290

D54	2.55104	-0.00008	-0.00247	-0.00254	-0.00502	2.54602
D55	-1.65049	-0.00014	-0.00215	-0.00226	-0.00442	-1.65490
D56	0.44113	-0.00006	-0.00035	-0.00096	-0.00132	0.43981
D57	1.34058	-0.00007	-0.00081	-0.00217	-0.00297	1.33761
D58	-2.86095	-0.00013	-0.00048	-0.00189	-0.00236	-2.86331
D59	-0.76933	-0.00004	0.00131	-0.00059	0.00073	-0.76860
D60	-1.02933	0.00015	0.00210	0.00410	0.00619	-1.02314
D61	1.05232	0.00009	0.00243	0.00437	0.00680	1.05912
D62	-3.13924	0.00018	0.00422	0.00568	0.00990	-3.12935
D63	1.65987	-0.00341	0.01787	0.03491	0.05282	1.71269
D64	-2.69332	-0.00179	0.04123	0.04393	0.08513	-2.60819
D65	2.16581	-0.00320	-0.13206	-0.12316	-0.25653	1.90928
D66	-1.02199	0.00191	-0.04978	-0.05256	-0.10118	-1.12317
D67	-2.10369	0.00093	-0.11007	-0.10220	-0.21376	-2.31745
D68	0.99170	0.00603	-0.02778	-0.03160	-0.05841	0.93329
D69	-0.02783	-0.00131	-0.10648	-0.12350	-0.23089	-0.25872
D70	3.06755	0.00380	-0.02419	-0.05290	-0.07553	2.99202
D71	2.94543	-0.00698	-0.02759	0.04721	0.02351	2.96894
D72	-0.24642	-0.00055	0.06034	0.12703	0.18347	-0.06295
D73	-1.31642	-0.00307	-0.00081	-0.00726	-0.00807	-1.32449

Item	Value	Threshold	Converged?
Maximum Force	0.021478	0.000450	NO
RMS Force	0.004473	0.000300	NO
Maximum Displacement	0.956342	0.001800	NO
RMS Displacement	0.216280	0.001200	NO

Predicted change in Energy=-8.656585D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.830715	1.158852	1.376800
2	6	0	-1.713073	0.130505	1.542475
3	7	0	-2.810937	0.414014	0.745773
4	6	0	-2.576150	1.558801	0.089207
5	7	0	-1.394999	2.051400	0.475696
6	6	0	-0.830357	3.319592	-0.019590
7	1	0	0.140499	1.325414	1.807049
8	1	0	-1.675695	-0.748172	2.163089
9	1	0	-1.686051	3.953530	-0.257098
10	1	0	-0.306629	3.773916	0.822169
11	35	0	-0.594272	-2.494954	0.036026

12	1	0	-3.231340	2.002027	-0.640815
13	6	0	-3.964817	-0.400606	0.541928
14	6	0	-4.446636	-1.220612	1.463061
15	1	0	-4.379822	-0.308054	-0.452781
16	1	0	-5.292384	-1.850706	1.225302
17	1	0	-4.007335	-1.322068	2.446761
18	6	0	3.521925	-0.739736	0.200244
19	6	0	4.332354	-0.247479	1.323564
20	8	0	3.314145	0.592545	0.729871
21	1	0	3.958483	-0.754746	-0.794047
22	1	0	2.686684	-1.414930	0.351579
23	1	0	4.061670	-0.576834	2.325019
24	6	0	5.759749	0.194565	1.147116
25	1	0	5.997519	1.022007	1.821733
26	1	0	6.439062	-0.632047	1.375756
27	1	0	5.941413	0.518917	0.120364
28	6	0	0.114722	3.284211	-1.239412
29	1	0	0.500344	4.299875	-1.345498
30	1	0	-0.427951	3.006284	-2.141128
31	6	0	1.306091	2.346729	-1.111308
32	8	0	1.437415	1.317391	-1.727396
33	8	0	2.116706	2.762146	-0.118453
34	1	0	2.803454	2.069940	0.070934

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.365101	0.000000			
3	N	2.207772	1.385791	0.000000		
4	C	2.205539	2.212899	1.340426	0.000000	
5	N	1.388181	2.220141	2.181480	1.336842	0.000000
6	C	2.572683	3.659168	3.598730	2.481938	1.473920
7	H	1.075227	2.221156	3.266180	3.222675	2.158080
8	H	2.229122	1.076398	2.155977	3.230160	3.280806
9	H	3.348350	4.225484	3.846984	2.578164	2.059077
10	H	2.724122	3.971318	4.191221	3.254949	2.066798
11	Br	3.899216	3.227095	3.725512	4.512604	4.637219
12	H	3.247263	3.251844	2.149686	1.076408	2.149694
13	C	3.598821	2.520620	1.427094	2.443895	3.552560
14	C	4.329455	3.050278	2.421161	3.620957	4.581860
15	H	4.253862	3.359305	2.102216	2.651816	3.916409
16	H	5.383947	4.103324	3.393595	4.504817	5.565784
17	H	4.170215	2.862051	2.709005	3.988202	4.699965
18	C	4.892280	5.473948	6.460177	6.517831	5.660606

19	C	5.351437	6.061186	7.197084	7.246634	6.229469
20	O	4.233094	5.113387	6.127704	6.003306	4.936486
21	H	5.595610	6.197544	7.040035	6.988137	6.176282
22	H	4.477447	4.812948	5.807259	6.050565	5.356396
23	H	5.277041	5.870295	7.120992	7.322599	6.332681
24	C	6.664595	7.483548	8.582884	8.512786	7.422200
25	H	6.844083	7.766981	8.894731	8.763424	7.584246
26	H	7.487122	8.189420	9.330253	9.366381	8.329676
27	H	6.917360	7.795153	8.775293	8.580863	7.503179
28	C	3.500795	4.585367	4.553951	3.461656	2.596281
29	H	4.364476	5.533828	5.517056	4.363105	3.459005
30	H	3.993876	4.846708	4.553316	3.418240	2.948687
31	C	3.488219	4.590159	4.912642	4.139307	3.146694
32	O	3.847802	4.693221	4.998114	4.412145	3.662642
33	O	3.673366	4.934716	5.526506	4.849130	3.631837
34	H	3.967688	5.130873	5.892273	5.403863	4.217959

		6	7	8	9	10
6	C	0.000000				
7	H	2.873311	0.000000			
8	H	4.693121	2.779404	0.000000		
9	H	1.091100	3.808410	5.288045	0.000000	
10	H	1.090532	2.676766	4.911384	1.760649	0.000000
11	Br	5.819602	4.274532	2.957215	6.546819	6.324515
12	H	2.808312	4.221273	4.224395	2.518634	3.719388
13	C	4.896938	4.629610	2.826489	4.978927	5.557652
14	C	5.990758	5.257603	2.896783	6.111589	6.518874
15	H	5.093738	5.311153	3.787979	5.045372	5.905834
16	H	6.942004	6.319999	3.895569	6.992303	7.527061
17	H	6.141748	4.962148	2.417926	6.366407	6.504119
18	C	5.955572	4.275595	5.555906	7.025591	5.951275
19	C	6.417292	4.503265	6.087048	7.507873	6.159803
20	O	5.017507	3.430662	5.361916	6.105104	4.820751
21	H	6.335061	5.066534	6.363070	7.370003	6.427450
22	H	5.909572	4.013843	4.770376	6.950659	6.008785
23	H	6.679166	4.388898	5.742207	7.760659	6.345835
24	C	7.386237	5.769775	7.563517	8.458225	7.051119
25	H	7.435675	5.864892	7.882150	8.482489	6.950857
26	H	8.390882	6.609808	8.153691	9.471600	8.076096
27	H	7.329409	6.094747	7.987401	8.373605	7.079942
28	C	1.543500	3.621944	5.571600	2.157710	2.160431
29	H	2.118904	4.349191	6.521358	2.466758	2.372050
30	H	2.181976	4.328575	5.846289	2.455537	3.063512
31	C	2.588961	3.304315	5.402883	3.502056	2.894142
32	O	3.473931	3.764884	5.393874	4.343621	3.946705

33	O	3.000950	3.110812	5.648900	3.987428	2.789444
34	H	3.843749	3.264926	5.690488	4.879669	3.624983

		11	12	13	14	15
11	Br	0.000000				
12	H	5.256908	0.000000			
13	C	4.000350	2.776602	0.000000		
14	C	4.301289	4.035920	1.324027	0.000000	
15	H	4.399074	2.586666	1.081777	2.123129	0.000000
16	H	4.888935	4.751195	2.081400	1.081127	2.455303
17	H	4.340081	4.602706	2.116432	1.082102	3.094239
18	C	4.477816	7.336978	7.502204	8.082322	7.940428
19	C	5.566016	8.131945	8.335312	8.833862	8.891629
20	O	5.028896	6.834383	7.348806	8.003427	7.836253
21	H	4.944180	7.701742	8.042942	8.715365	8.357231
22	H	3.468530	6.905320	6.731088	7.222009	7.197755
23	H	5.531408	8.284606	8.224048	8.576054	8.890849
24	C	6.988678	9.343624	9.761540	10.308873	10.277314
25	H	7.681763	9.601897	10.144450	10.688235	10.706618
26	H	7.398182	10.223580	10.439805	10.901948	10.977102
27	H	7.197618	9.323004	9.957742	10.617927	10.370162
28	C	5.960550	3.632966	5.778726	6.957211	5.807243
29	H	7.019721	4.438710	6.752374	7.926941	6.770965
30	H	5.918723	3.334436	5.595990	6.856141	5.427028
31	C	5.326316	4.574763	6.169562	7.242042	6.309606
32	O	4.665981	4.842175	6.106181	7.158389	6.173083
33	O	5.916955	5.426991	6.886509	7.838431	7.193244
34	H	5.690695	6.077000	7.220451	8.082670	7.584759

		16	17	18	19	20
16	H	0.000000				
17	H	1.850073	0.000000			
18	C	8.942989	7.878813	0.000000		
19	C	9.757846	8.483320	1.470020	0.000000	
20	O	8.960316	7.759995	1.448672	1.447363	0.000000
21	H	9.531916	8.618523	1.086012	2.209383	2.133703
22	H	8.038583	7.014862	1.084627	2.239626	2.137000
23	H	9.504234	8.104260	2.198302	1.088419	2.114412
24	C	11.240058	9.969212	2.603333	1.504658	2.512660
25	H	11.664910	10.294778	3.444058	2.152335	2.928668
26	H	11.795533	10.523801	3.146921	2.142158	3.417880
27	H	11.534045	10.381663	2.728463	2.150377	2.698047
28	C	7.853597	7.197015	5.465693	6.068780	4.621629
29	H	8.831442	8.142888	6.075932	6.518176	5.095972
30	H	7.654144	7.252264	5.925893	6.726928	5.298307
31	C	8.161990	7.372409	4.019497	4.670844	3.240275

32	O	8.002840	7.350892	3.506102	4.487520	3.175795
33	O	8.830554	7.795190	3.786738	4.005789	2.619290
34	H	9.068992	7.971017	2.902964	3.045824	1.696378

		21	22	23	24	25
21	H	0.000000				
22	H	1.834604	0.000000			
23	H	3.125840	2.547049	0.000000		
24	C	2.813160	3.559085	2.205898	0.000000	
25	H	3.762556	4.365964	2.560684	1.093756	0.000000
26	H	3.297935	3.967643	2.560496	1.094089	1.769111
27	H	2.527919	3.792952	3.097516	1.091982	1.775079
28	C	5.593391	5.588217	6.572004	6.863509	7.006817
29	H	6.149147	6.349736	7.066685	7.122361	7.141058
30	H	5.933024	5.954970	7.276119	7.550228	7.805657
31	C	4.093285	4.265695	5.286661	5.437588	5.689211
32	O	3.394212	3.653544	5.186219	5.310944	5.786028
33	O	4.027046	4.241906	4.571895	4.633131	4.674732
34	H	3.171929	3.498101	3.697218	3.662633	3.790187

		26	27	28	29	30
26	H	0.000000				
27	H	1.774368	0.000000			
28	C	7.885015	6.591371	0.000000		
29	H	8.185197	6.785987	1.091573	0.000000	
30	H	8.530053	7.202092	1.088498	1.779926	0.000000
31	C	6.434749	5.132653	1.521395	2.125759	2.121896
32	O	6.200511	4.933333	2.419923	3.149469	2.550122
33	O	5.695259	4.440439	2.353092	2.546149	3.259769
34	H	4.713910	3.500700	3.228117	3.504740	4.026405

		31	32	33	34
31	C	0.000000			
32	O	1.206792	0.000000		
33	O	1.347379	2.266594	0.000000	
34	H	1.927798	2.380416	0.993297	0.000000

Stoichiometry C11H17BrN2O3
Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.814039	0.889324	1.240395
2	6	0	-1.876872	0.032719	1.229726
3	7	0	-2.873808	0.642515	0.484954
4	6	0	-2.407656	1.812975	0.027279
5	7	0	-1.170478	2.005380	0.495804
6	6	0	-0.363372	3.207270	0.219256
7	1	0	0.155047	0.798394	1.697253
8	1	0	-2.025194	-0.925450	1.697215
9	1	0	-1.077813	4.020940	0.085039
10	1	0	0.204658	3.413262	1.127094
11	35	0	-1.209670	-2.479333	-0.683014
12	1	0	-2.942706	2.483335	-0.623101
13	6	0	-4.150396	0.103606	0.143638
14	6	0	-4.808592	-0.748211	0.914504
15	1	0	-4.504917	0.431547	-0.824355
16	1	0	-5.747199	-1.160974	0.571754
17	1	0	-4.431461	-1.087585	1.870298
18	6	0	3.151608	-1.581172	-0.210363
19	6	0	3.998050	-1.437775	0.982924
20	8	0	3.175010	-0.336505	0.530520
21	1	0	3.613451	-1.518019	-1.191247
22	1	0	2.200924	-2.102214	-0.176725
23	1	0	3.635113	-1.866969	1.914978
24	6	0	5.488021	-1.250186	0.889166
25	1	0	5.850312	-0.601922	1.692162
26	1	0	5.993907	-2.215846	0.981963
27	1	0	5.763523	-0.804990	-0.069126
28	6	0	0.602242	3.191123	-0.984788
29	1	0	1.172753	4.119484	-0.920017
30	1	0	0.050420	3.169244	-1.922787
31	6	0	1.594107	2.037709	-1.006763
32	8	0	1.554810	1.114857	-1.783389
33	8	0	2.431221	2.127619	0.045181
34	1	0	2.970701	1.297087	0.121454

Rotational constants (GHZ): 0.3713439 0.2189097 0.1561099

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 538 symmetry adapted cartesian basis functions of A symmetry.

There are 519 symmetry adapted basis functions of A symmetry.

519 basis functions, 823 primitive gaussians, 538 cartesian basis functions

78 alpha electrons 78 beta electrons

nuclear repulsion energy 1555.1715730412 Hartrees.

NAtoms= 34 NActive= 34 NUniq= 34 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 519 RedAO= T EigKep= 3.65D-06 NBF= 519
NBsUse= 519 1.00D-06 EigRej= -1.00D+00 NBFU= 519
Initial guess from the checkpoint file: "./coohpo.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.998653 0.027911 0.013358 -0.041652 Ang= 5.95 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3338.88347927 A.U. after 15 cycles
NFock= 15 Conv=0.38D-08 -V/T= 2.0019
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.002450413	0.003494264	0.003470217
2	6	0.000707777	0.000744769	0.002202284
3	7	0.001276465	-0.001637550	-0.001104612
4	6	-0.000196992	0.001540735	-0.003304025
5	7	0.001341503	-0.007240603	-0.007913672
6	6	0.004906469	0.005415033	0.004971316
7	1	0.000877192	-0.000671050	-0.000788198
8	1	0.003063747	-0.000143573	-0.004246840
9	1	0.000837055	0.001165346	0.000081864
10	1	-0.000579246	-0.000553631	0.000568522

11	35	-0.001070154	0.003067657	0.002988498
12	1	-0.000339900	0.000466803	0.000905306
13	6	0.001147891	0.000663875	0.000981755
14	6	0.000481171	-0.000706629	-0.000640599
15	1	-0.000541382	-0.000108470	0.000257094
16	1	-0.000187524	0.000145871	0.000075008
17	1	0.000170820	-0.000203025	-0.000024999
18	6	-0.001571859	-0.000143451	-0.000760262
19	6	0.000437756	-0.000426409	-0.001774699
20	8	0.002738520	-0.000730018	0.003193034
21	1	0.000336703	0.000182423	0.000107697
22	1	-0.001155281	-0.000531010	0.000877545
23	1	-0.000459885	-0.000583892	-0.000627729
24	6	-0.000364028	0.000323821	0.000460461
25	1	0.000165012	0.000056410	0.000057423
26	1	0.000000207	-0.000070732	-0.000004573
27	1	0.000219541	-0.000020015	-0.000117591
28	6	-0.002401290	-0.006077838	-0.003355471
29	1	-0.001980832	0.002046860	-0.001424041
30	1	-0.000703972	0.000277643	-0.001309634
31	6	-0.004039815	-0.011689963	0.013247414
32	8	0.001820849	0.010965351	-0.001708402
33	8	0.003191084	0.001828977	-0.004673251
34	1	-0.005677189	-0.000847984	-0.000666842

Cartesian Forces: Max 0.013247414 RMS 0.003013479

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.018682720 RMS 0.003555331
Search for a local minimum.
Step number 5 out of a maximum of 175
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 2 3 4 5
DE= -9.27D-04 DEPred=-8.66D-03 R= 1.07D-01
Trust test= 1.07D-01 RLast= 8.30D-01 DXMaxT set to 2.52D-01
ITU= 0 -1 0 1 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00201	0.00236	0.00280	0.00651	0.00698
Eigenvalues ---	0.00823	0.01137	0.01302	0.01411	0.01554
Eigenvalues ---	0.01597	0.01713	0.01832	0.01973	0.02154

Eigenvalues ---	0.02256	0.02267	0.02378	0.02474	0.02616
Eigenvalues ---	0.03010	0.03051	0.03070	0.03355	0.03602
Eigenvalues ---	0.03793	0.04888	0.05231	0.05278	0.05739
Eigenvalues ---	0.05813	0.05880	0.07829	0.09707	0.10382
Eigenvalues ---	0.11969	0.12570	0.12950	0.13592	0.13602
Eigenvalues ---	0.15456	0.15750	0.15997	0.15998	0.16000
Eigenvalues ---	0.16000	0.16000	0.16000	0.16001	0.16116
Eigenvalues ---	0.16899	0.18250	0.19794	0.22002	0.22484
Eigenvalues ---	0.22875	0.23338	0.24063	0.24683	0.24989
Eigenvalues ---	0.25021	0.26312	0.28615	0.29115	0.29621
Eigenvalues ---	0.31848	0.32563	0.34497	0.34561	0.34611
Eigenvalues ---	0.34764	0.34884	0.34892	0.34957	0.35001
Eigenvalues ---	0.35070	0.35531	0.35669	0.35765	0.36540
Eigenvalues ---	0.36559	0.36621	0.36981	0.37243	0.37710
Eigenvalues ---	0.41081	0.42341	0.45555	0.49047	0.51932
Eigenvalues ---	0.53179	0.55398	0.56095	0.60268	0.87005
Eigenvalues ---	1.48695				

RFO step: Lambda=-7.45369823D-03 EMin= 2.00551446D-03

Quartic linear search produced a step of -0.51249.

Iteration 1 RMS(Cart)= 0.15075099 RMS(Int)= 0.02806450

Iteration 2 RMS(Cart)= 0.08264103 RMS(Int)= 0.00254326

Iteration 3 RMS(Cart)= 0.00522008 RMS(Int)= 0.00062800

Iteration 4 RMS(Cart)= 0.00001313 RMS(Int)= 0.00062796

Iteration 5 RMS(Cart)= 0.00000001 RMS(Int)= 0.00062796

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.57967	-0.00563	-0.00187	0.00285	0.00081	2.58047
R2	2.62328	-0.00304	-0.00443	0.00357	-0.00074	2.62254
R3	2.03189	0.00037	0.00120	-0.00168	-0.00048	2.03141
R4	2.61877	0.00094	-0.00373	0.00777	0.00384	2.62261
R5	2.03410	-0.00304	-0.00741	0.00811	0.00070	2.03480
R6	2.53304	0.00276	-0.00219	-0.00020	-0.00235	2.53069
R7	2.69682	-0.00085	-0.00165	-0.00100	-0.00265	2.69417
R8	2.52627	-0.00066	-0.00015	-0.00230	-0.00222	2.52405
R9	2.03412	-0.00021	-0.00278	0.00319	0.00041	2.03453
R10	2.78530	-0.00356	-0.00300	0.01047	0.00747	2.79278
R11	2.06188	0.00000	0.00130	-0.00221	-0.00091	2.06097
R12	2.06081	-0.00007	-0.00061	0.00091	0.00030	2.06111
R13	2.91679	-0.00686	-0.01646	0.00070	-0.01576	2.90103
R14	5.58833	-0.00436	-0.15940	-0.09370	-0.25310	5.33523
R15	2.50205	-0.00011	-0.00171	0.00286	0.00115	2.50320
R16	2.04426	-0.00004	-0.00301	0.00294	-0.00007	2.04419
R17	2.04303	0.00004	-0.00082	0.00039	-0.00042	2.04261
R18	2.04488	0.00007	-0.00063	0.00023	-0.00040	2.04447

R19	2.77793	0.00016	-0.00399	0.00169	-0.00226	2.77568
R20	2.73759	-0.00020	-0.00206	-0.00012	-0.00220	2.73539
R21	2.05227	0.00003	-0.00034	0.00211	0.00177	2.05403
R22	2.04965	0.00135	-0.00052	0.00332	0.00280	2.05245
R23	2.73512	-0.00033	0.00244	-0.00318	-0.00077	2.73435
R24	2.05681	-0.00028	-0.00129	0.00056	-0.00073	2.05609
R25	2.84339	0.00005	0.00029	-0.00142	-0.00113	2.84226
R26	3.20569	0.00237	0.06974	0.03335	0.10309	3.30878
R27	2.06690	0.00011	0.00134	-0.00097	0.00037	2.06727
R28	2.06753	0.00005	0.00050	-0.00016	0.00034	2.06787
R29	2.06355	0.00014	0.00094	-0.00056	0.00038	2.06393
R30	2.06277	0.00134	0.01247	-0.00471	0.00776	2.07053
R31	2.05696	0.00137	0.01027	-0.00966	0.00061	2.05757
R32	2.87502	-0.00171	-0.00259	0.01500	0.01240	2.88742
R33	2.28051	-0.00828	-0.01627	0.01236	-0.00392	2.27659
R34	2.54618	-0.00448	-0.00500	-0.00490	-0.00990	2.53628
R35	1.87706	-0.00158	0.01510	-0.02649	-0.01139	1.86567
A1	1.87590	0.00054	-0.00558	0.00555	-0.00004	1.87586
A2	2.28098	-0.00039	0.00200	-0.00094	0.00071	2.28169
A3	2.12623	-0.00017	0.00273	-0.00494	-0.00258	2.12366
A4	1.86313	0.00021	0.00225	-0.00613	-0.00402	1.85911
A5	2.29490	-0.00231	0.00100	-0.01897	-0.01802	2.27688
A6	2.12467	0.00213	-0.00355	0.02452	0.02085	2.14552
A7	1.89395	0.00043	0.00172	-0.00017	0.00145	1.89540
A8	2.22169	-0.00164	-0.00985	0.01390	0.00369	2.22537
A9	2.16418	0.00122	0.00810	-0.01039	-0.00265	2.16154
A10	1.90482	-0.00416	-0.00595	0.00477	-0.00119	1.90363
A11	2.18615	0.00209	0.00372	-0.00173	0.00116	2.18731
A12	2.19215	0.00206	0.00212	-0.00253	-0.00124	2.19091
A13	1.88588	0.00304	0.00658	-0.00457	0.00181	1.88770
A14	2.23397	-0.01287	-0.02147	0.00658	-0.01604	2.21794
A15	2.16322	0.00983	0.01328	-0.00128	0.01089	2.17411
A16	1.84691	0.00942	0.00942	0.00090	0.01014	1.85705
A17	1.85778	0.00253	-0.00891	0.00562	-0.00306	1.85472
A18	2.07191	-0.01868	-0.02642	-0.00844	-0.03477	2.03715
A19	1.87822	-0.00249	-0.00026	0.00247	0.00223	1.88045
A20	1.89809	0.00316	0.02462	-0.00304	0.02151	1.91959
A21	1.90234	0.00696	0.00205	0.00343	0.00585	1.90819
A22	1.65105	-0.00262	-0.01795	0.05777	0.03981	1.69087
A23	2.15123	0.00006	-0.00052	0.00374	0.00325	2.15448
A24	1.97435	0.00051	0.00891	-0.00402	0.00492	1.97928
A25	2.15687	-0.00058	-0.00891	0.00090	-0.00798	2.14889
A26	2.08591	0.00000	0.00009	-0.00204	-0.00189	2.08402
A27	2.14453	0.00001	-0.00091	0.00383	0.00298	2.14751

A28	2.05202	-0.00001	-0.00008	-0.00172	-0.00174	2.05027
A29	2.07445	0.00083	0.00057	-0.00129	-0.00060	2.07385
A30	2.12514	-0.00135	-0.00648	-0.00295	-0.00951	2.11562
A31	1.98787	-0.00008	0.00138	-0.00127	0.00014	1.98800
A32	1.99439	-0.00017	0.00234	-0.00355	-0.00123	1.99315
A33	2.01384	0.00054	0.00218	0.00577	0.00798	2.02183
A34	2.05405	-0.00092	-0.00431	-0.00664	-0.01090	2.04314
A35	2.13148	0.00083	0.00160	0.00528	0.00684	2.13832
A36	1.95852	-0.00001	0.00042	-0.00235	-0.00190	1.95663
A37	2.03617	-0.00005	0.00247	0.00104	0.00347	2.03964
A38	2.01830	0.00010	0.00086	0.00145	0.00231	2.02062
A39	2.34915	-0.00054	-0.00893	-0.01704	-0.02575	2.32340
A40	2.63950	0.00146	0.00534	0.00821	0.01335	2.65286
A41	1.93494	0.00018	0.00267	0.00147	0.00413	1.93907
A42	1.92042	-0.00017	-0.00071	-0.00244	-0.00315	1.91727
A43	1.93408	0.00025	0.00133	0.00102	0.00234	1.93642
A44	1.88357	-0.00005	-0.00124	-0.00023	-0.00146	1.88210
A45	1.89555	-0.00013	-0.00063	0.00035	-0.00028	1.89527
A46	1.89401	-0.00010	-0.00158	-0.00020	-0.00179	1.89222
A47	1.84604	0.00114	-0.02732	0.01672	-0.01065	1.83540
A48	1.93401	0.00578	0.00957	0.00804	0.01755	1.95156
A49	2.01203	-0.01439	-0.00123	0.00194	0.00064	2.01267
A50	1.91048	-0.00246	-0.00232	-0.01553	-0.01769	1.89279
A51	1.88062	0.00839	0.01926	-0.01678	0.00258	1.88320
A52	1.87845	0.00189	0.00175	0.00358	0.00529	1.88373
A53	2.17465	-0.00670	-0.03591	0.03763	-0.00234	2.17231
A54	1.92110	0.01037	0.01438	-0.00885	0.00160	1.92270
A55	2.18181	-0.00355	0.02387	-0.01702	0.00304	2.18485
A56	1.91941	-0.01470	0.02492	-0.00752	0.01741	1.93681
A57	2.66621	-0.00557	0.02592	0.06579	0.09171	2.75792
D1	-0.00716	-0.00056	-0.03271	-0.02337	-0.05612	-0.06327
D2	-3.11483	-0.00132	-0.02402	-0.00346	-0.02791	3.14044
D3	-3.13528	0.00112	-0.00674	0.00526	-0.00136	-3.13663
D4	0.04024	0.00036	0.00196	0.02517	0.02685	0.06708
D5	-0.02025	0.00119	0.03437	0.01492	0.04927	0.02902
D6	3.13697	0.00124	-0.01610	-0.03658	-0.05276	3.08421
D7	3.10932	-0.00031	0.01120	-0.01060	0.00055	3.10987
D8	-0.01664	-0.00027	-0.03927	-0.06210	-0.10148	-0.11812
D9	0.03208	-0.00031	0.02001	0.02373	0.04374	0.07582
D10	3.08769	-0.00003	0.02006	0.06554	0.08575	-3.10975
D11	-3.13939	0.00026	0.01249	0.00525	0.01730	-3.12209
D12	-0.08378	0.00054	0.01254	0.04705	0.05931	-0.02447
D13	-1.66225	0.00197	-0.16768	0.04410	-0.12362	-1.78587
D14	1.51753	0.00116	-0.15805	0.06717	-0.09084	1.42669

D15	-0.04554	0.00122	0.00165	-0.01498	-0.01344	-0.05899
D16	3.08466	0.00024	0.01957	0.03137	0.05090	3.13556
D17	-3.10464	0.00112	0.00267	-0.05654	-0.05394	3.12460
D18	0.02556	0.00014	0.02060	-0.01019	0.01040	0.03597
D19	0.53985	-0.00106	-0.02561	-0.02591	-0.05148	0.48837
D20	-2.56196	-0.00081	-0.01404	-0.04273	-0.05687	-2.61883
D21	-2.70012	-0.00081	-0.02604	0.02265	-0.00329	-2.70340
D22	0.48126	-0.00056	-0.01447	0.00583	-0.00868	0.47258
D23	0.04079	-0.00150	-0.02228	0.00008	-0.02198	0.01881
D24	-3.11565	-0.00179	0.02770	0.04910	0.07657	-3.03908
D25	-3.08937	-0.00052	-0.04026	-0.04647	-0.08651	3.10731
D26	0.03738	-0.00081	0.00972	0.00255	0.01204	0.04942
D27	-2.64283	0.00030	0.05318	0.05904	0.11225	-2.53058
D28	-0.64787	0.00287	0.05307	0.06474	0.11800	-0.52987
D29	1.50364	0.00106	0.03132	0.06811	0.09937	1.60301
D30	0.51667	0.00046	-0.00535	0.00003	-0.00540	0.51127
D31	2.51163	0.00302	-0.00546	0.00573	0.00035	2.51198
D32	-1.62004	0.00122	-0.02721	0.00910	-0.01828	-1.63833
D33	-3.02208	0.00345	0.03468	-0.00837	0.02639	-2.99569
D34	1.19225	0.00266	0.04843	-0.00389	0.04463	1.23688
D35	-0.94634	0.00633	0.03920	-0.01659	0.02261	-0.92373
D36	1.15020	0.00159	0.02125	-0.00091	0.02031	1.17051
D37	-0.91866	0.00080	0.03500	0.00357	0.03855	-0.88011
D38	-3.05725	0.00447	0.02578	-0.00913	0.01653	-3.04072
D39	-0.89280	-0.00109	0.00590	-0.00406	0.00186	-0.89094
D40	-2.96166	-0.00187	0.01965	0.00042	0.02010	-2.94156
D41	1.18293	0.00179	0.01042	-0.01228	-0.00192	1.18102
D42	-3.08287	-0.00010	0.00726	-0.01617	-0.00885	-3.09172
D43	0.01657	-0.00009	-0.01076	-0.01406	-0.02476	-0.00819
D44	0.01480	-0.00035	-0.00486	0.00230	-0.00262	0.01219
D45	3.11424	-0.00034	-0.02288	0.00441	-0.01853	3.09572
D46	-2.74030	-0.00013	0.00490	-0.00116	0.00372	-2.73658
D47	-0.03454	-0.00010	0.00029	-0.00073	-0.00047	-0.03501
D48	-0.00941	0.00007	-0.00472	0.00446	-0.00029	-0.00971
D49	2.69634	0.00010	-0.00932	0.00489	-0.00448	2.69187
D50	0.67813	0.00110	0.00076	0.00538	0.00625	0.68438
D51	-1.68803	0.00054	-0.00679	0.00172	-0.00495	-1.69298
D52	2.07348	0.00071	0.02459	0.03518	0.05983	2.13331
D53	-0.31290	0.00061	0.01990	0.03446	0.05443	-0.25846
D54	2.54602	0.00018	0.00257	0.00135	0.00392	2.54994
D55	-1.65490	0.00013	0.00226	0.00043	0.00268	-1.65222
D56	0.43981	0.00005	0.00068	-0.00076	-0.00009	0.43972
D57	1.33761	0.00002	0.00152	-0.00101	0.00052	1.33814
D58	-2.86331	-0.00004	0.00121	-0.00193	-0.00071	-2.86402

D59	-0.76860	-0.00011	-0.00037	-0.00312	-0.00348	-0.77208
D60	-1.02314	-0.00003	-0.00317	-0.00013	-0.00330	-1.02644
D61	1.05912	-0.00009	-0.00348	-0.00105	-0.00454	1.05459
D62	-3.12935	-0.00016	-0.00507	-0.00224	-0.00731	-3.13666
D63	1.71269	-0.00357	-0.02707	-0.12615	-0.15320	1.55949
D64	-2.60819	-0.00170	-0.04363	-0.14781	-0.19146	-2.79966
D65	1.90928	0.00271	0.13147	0.28161	0.41368	2.32296
D66	-1.12317	0.00165	0.05185	0.16966	0.22081	-0.90236
D67	-2.31745	0.00125	0.10955	0.29212	0.40244	-1.91502
D68	0.93329	0.00019	0.02993	0.18018	0.20957	1.14286
D69	-0.25872	0.00380	0.11833	0.26687	0.38579	0.12707
D70	2.99202	0.00273	0.03871	0.15493	0.19292	-3.09824
D71	2.96894	-0.00596	-0.01205	-0.00725	-0.02155	2.94739
D72	-0.06295	-0.00679	-0.09403	-0.12393	-0.21570	-0.27866
D73	-1.32449	-0.00201	0.00414	-0.08200	-0.07786	-1.40235

Item	Value	Threshold	Converged?
Maximum Force	0.018683	0.000450	NO
RMS Force	0.003555	0.000300	NO
Maximum Displacement	0.651907	0.001800	NO
RMS Displacement	0.140725	0.001200	NO

Predicted change in Energy=-5.262263D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.831512	1.266370	1.386843
2	6	0	-1.653444	0.187589	1.545981
3	7	0	-2.735003	0.387288	0.699572
4	6	0	-2.519158	1.499719	-0.014093
5	7	0	-1.378045	2.063484	0.390920
6	6	0	-0.875586	3.371194	-0.079762
7	1	0	0.109388	1.505469	1.848480
8	1	0	-1.579919	-0.654402	2.213124
9	1	0	-1.754177	3.965530	-0.333322
10	1	0	-0.393488	3.840269	0.778816
11	35	0	-0.631306	-2.511803	0.310204
12	1	0	-3.186337	1.901765	-0.757297
13	6	0	-3.877364	-0.450357	0.538453
14	6	0	-4.348521	-1.234562	1.496416
15	1	0	-4.303665	-0.409242	-0.454893
16	1	0	-5.191780	-1.878088	1.288714

17	1	0	-3.896183	-1.305364	2.476652
18	6	0	3.464842	-0.799293	0.196992
19	6	0	4.314221	-0.367116	1.314681
20	8	0	3.235474	0.474844	0.844485
21	1	0	3.849326	-0.715551	-0.816228
22	1	0	2.667797	-1.522578	0.342637
23	1	0	4.102638	-0.796140	2.291916
24	6	0	5.713698	0.146502	1.115056
25	1	0	5.956835	0.921935	1.847396
26	1	0	6.430842	-0.670336	1.241186
27	1	0	5.837640	0.562818	0.112966
28	6	0	0.102538	3.349642	-1.262779
29	1	0	0.465932	4.379366	-1.352920
30	1	0	-0.393332	3.076583	-2.192876
31	6	0	1.315762	2.436833	-1.090946
32	8	0	1.709846	1.662365	-1.925360
33	8	0	1.931295	2.699571	0.072423
34	1	0	2.603819	2.007408	0.280552

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.365528	0.000000			
3	N	2.206447	1.387825	0.000000		
4	C	2.205725	2.214718	1.339182	0.000000	
5	N	1.387787	2.220133	2.178586	1.335667	0.000000
6	C	2.565766	3.658339	3.601179	2.491598	1.477874
7	H	1.074974	2.221686	3.265100	3.221563	2.155996
8	H	2.220860	1.076770	2.170294	3.237731	3.278427
9	H	3.331027	4.220753	3.851325	2.601409	2.069729
10	H	2.680768	3.939302	4.172775	3.259655	2.068037
11	Br	3.933679	3.139845	3.603037	4.445386	4.636528
12	H	3.247502	3.254727	2.149375	1.076625	2.148133
13	C	3.597796	2.523472	1.425692	2.439842	3.547924
14	C	4.316945	3.047689	2.422560	3.620013	4.574161
15	H	4.272647	3.373926	2.104269	2.650075	3.922885
16	H	5.376726	4.105244	3.393342	4.499977	5.557572
17	H	4.146530	2.850428	2.715037	3.996060	4.694724
18	C	4.913386	5.384288	6.332348	6.413912	5.629090
19	C	5.399264	5.997852	7.116112	7.207343	6.258039
20	O	4.178641	4.947336	5.972877	5.907903	4.900414
21	H	5.540016	6.056086	6.845969	6.790319	6.041991
22	H	4.594971	4.800608	5.741536	6.013820	5.406571
23	H	5.423923	5.886988	7.119648	7.378132	6.467544

24	C	6.645882	7.379849	8.462338	8.419388	7.381871
25	H	6.812664	7.651566	8.783586	8.697208	7.564715
26	H	7.517568	8.135393	9.242544	9.294480	8.317178
27	H	6.826078	7.636143	8.594482	8.410113	7.375322
28	C	3.497566	4.579430	4.547307	3.443069	2.565355
29	H	4.345159	5.519635	5.513202	4.358393	3.435773
30	H	4.035252	4.890114	4.591512	3.428226	2.944831
31	C	3.481409	4.563843	4.880091	4.091993	3.097081
32	O	4.193567	5.053404	5.317214	4.643691	3.880866
33	O	3.378589	4.618634	5.245408	4.610170	3.384934
34	H	3.684361	4.799723	5.594943	5.156497	3.983788

		6	7	8	9	10
6	C	0.000000				
7	H	2.858185	0.000000			
8	H	4.686025	2.766183	0.000000		
9	H	1.090619	3.779554	5.278117	0.000000	
10	H	1.090691	2.616936	4.864866	1.761821	0.000000
11	Br	5.900966	4.365020	2.823280	6.605362	6.373772
12	H	2.820965	4.220063	4.235324	2.547540	3.730609
13	C	4.898685	4.629862	2.850335	4.976743	5.532146
14	C	5.979849	5.244489	2.918117	6.092578	6.473881
15	H	5.117044	5.333543	3.820629	5.064908	5.905071
16	H	6.932331	6.313809	3.923962	6.971082	7.482192
17	H	6.126129	4.933557	2.420388	6.345586	6.452059
18	C	6.025684	4.392996	5.434647	7.086813	6.062241
19	C	6.546261	4.633804	5.969140	7.636307	6.336542
20	O	5.113110	3.441309	5.131898	6.202317	4.949724
21	H	6.290363	5.101053	6.217509	7.317443	6.426596
22	H	6.056648	4.240530	4.721816	7.080261	6.190464
23	H	6.911891	4.630344	5.684871	7.991724	6.633318
24	C	7.432691	5.813175	7.419168	8.511870	7.145257
25	H	7.509646	5.876491	7.708518	8.571972	7.070017
26	H	8.453565	6.712952	8.069524	9.537550	8.193340
27	H	7.279528	6.059165	7.804645	8.331465	7.071916
28	C	1.535161	3.616760	5.562817	2.165779	2.157513
29	H	2.106422	4.316871	6.499307	2.477847	2.360832
30	H	2.187376	4.365053	5.894155	2.469832	3.068251
31	C	2.587958	3.311043	5.371925	3.512184	2.896062
32	O	3.607047	4.102189	5.772089	4.454056	4.059538
33	O	2.890124	2.810624	5.306634	3.917905	2.684175
34	H	3.754464	2.988734	5.322004	4.816971	3.548450

		11	12	13	14	15
11	Br	0.000000				
12	H	5.210310	0.000000			

13	C	3.852084	2.772899	0.000000		
14	C	4.105622	4.033167	1.324634	0.000000	
15	H	4.300274	2.584691	1.081739	2.119144	0.000000
16	H	4.707123	4.742916	2.080623	1.080904	2.446717
17	H	4.099807	4.609554	2.118491	1.081889	3.092415
18	C	4.441163	7.241862	7.358420	7.932628	7.805561
19	C	5.483329	8.105510	8.228702	8.707961	8.797791
20	O	4.915028	6.770633	7.179284	7.801542	7.701208
21	H	4.956958	7.506956	7.849028	8.533603	8.166740
22	H	3.444372	6.870726	6.635295	7.116381	7.104706
23	H	5.411183	8.348985	8.177691	8.499830	8.852151
24	C	6.926287	9.262683	9.626900	10.163711	10.154859
25	H	7.586640	9.557305	10.015388	10.534420	10.599548
26	H	7.357422	10.153806	10.334474	10.797136	10.870809
27	H	7.165156	9.164186	9.776957	10.435630	10.203599
28	C	6.113047	3.628851	5.789996	6.959885	5.847778
29	H	7.173431	4.453352	6.765186	7.925519	6.818084
30	H	6.127976	3.352903	5.660207	6.916672	5.519263
31	C	5.499390	4.546044	6.161118	7.228947	6.331087
32	O	5.282273	5.039275	6.461493	7.536878	6.528104
33	O	5.812218	5.245482	6.624180	7.545942	6.986952
34	H	5.557893	5.883383	6.936343	7.766834	7.354890

		16	17	18	19	20
16	H	0.000000				
17	H	1.848724	0.000000			
18	C	8.791630	7.722542	0.000000		
19	C	9.625372	8.345132	1.468827	0.000000	
20	O	8.760835	7.529518	1.447508	1.446954	0.000000
21	H	9.355420	8.437053	1.086948	2.208689	2.133500
22	H	7.924292	6.905581	1.086109	2.233982	2.136305
23	H	9.410804	8.017143	2.189863	1.088034	2.112446
24	C	11.093177	9.813852	2.606669	1.504058	2.514481
25	H	11.508426	10.121205	3.449128	2.154905	2.934540
26	H	11.685302	10.420033	3.147082	2.139492	3.417482
27	H	11.357312	10.189428	2.737258	2.151674	2.704465
28	C	7.865690	7.186251	5.536215	6.180280	4.745557
29	H	8.839890	8.124643	6.181763	6.667422	5.267281
30	H	7.726275	7.299035	5.968198	6.806106	5.400263
31	C	8.162685	7.341401	4.092657	4.758144	3.358659
32	O	8.396280	7.720925	3.693799	4.625952	3.377838
33	O	8.554094	7.468556	3.822216	4.077513	2.691910
34	H	8.768400	7.618881	2.936990	3.103749	1.750931

		21	22	23	24	25
21	H	0.000000				

22	H	1.841269	0.000000			
23	H	3.119491	2.527088	0.000000		
24	C	2.819375	3.558086	2.206601	0.000000	
25	H	3.770656	4.365514	2.566598	1.093953	0.000000
26	H	3.301396	3.961592	2.557420	1.094271	1.768474
27	H	2.539886	3.801254	3.099165	1.092184	1.775224
28	C	5.546497	5.735542	6.769355	6.884717	7.059727
29	H	6.139509	6.523501	7.300433	7.179631	7.235044
30	H	5.854536	6.078784	7.438083	7.538143	7.828852
31	C	4.053634	4.422679	5.446333	5.427145	5.698099
32	O	3.385563	4.025586	5.436462	5.250981	5.728773
33	O	4.016417	4.294414	4.675562	4.681007	4.745049
34	H	3.188843	3.531111	3.761904	3.718967	3.856937

		26	27	28	29	30
26	H	0.000000				
27	H	1.773538	0.000000			
28	C	7.904271	6.523071	0.000000		
29	H	8.234624	6.750564	1.095679	0.000000	
30	H	8.508909	7.103586	1.088820	1.772316	0.000000
31	C	6.423191	5.040706	1.527959	2.136416	2.131790
32	O	6.144617	4.733124	2.422676	3.042549	2.548516
33	O	5.741795	4.452740	2.355782	2.645865	3.267660
34	H	4.768567	3.545776	3.231079	3.586778	4.030371

		31	32	33	34
31	C	0.000000			
32	O	1.204720	0.000000		
33	O	1.342140	2.261852	0.000000	
34	H	1.929898	2.405055	0.987268	0.000000

Stoichiometry C11H17BrN2O3
Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.792283	0.936654	1.262291
2	6	0	-1.819222	0.041187	1.171739
3	7	0	-2.795391	0.638336	0.386523
4	6	0	-2.326991	1.811291	-0.058659
5	7	0	-1.118496	2.026737	0.467774

6	6	0	-0.343013	3.274166	0.304507
7	1	0	0.152857	0.871028	1.770202
8	1	0	-1.948297	-0.922919	1.633555
9	1	0	-1.071988	4.076730	0.186452
10	1	0	0.178769	3.435331	1.248633
11	35	0	-1.293079	-2.473909	-0.632726
12	1	0	-2.862570	2.493991	-0.695994
13	6	0	-4.071856	0.108576	0.036394
14	6	0	-4.737218	-0.752234	0.792011
15	1	0	-4.430807	0.452164	-0.924470
16	1	0	-5.680000	-1.147942	0.441399
17	1	0	-4.358024	-1.126621	1.733568
18	6	0	3.062137	-1.655184	-0.339954
19	6	0	3.922986	-1.661121	0.850153
20	8	0	3.058264	-0.533951	0.575525
21	1	0	3.506212	-1.432828	-1.306810
22	1	0	2.130905	-2.213638	-0.363868
23	1	0	3.581314	-2.240494	1.705375
24	6	0	5.404887	-1.414437	0.777313
25	1	0	5.760057	-0.884416	1.665945
26	1	0	5.938044	-2.368350	0.720555
27	1	0	5.659509	-0.823790	-0.105392
28	6	0	0.669718	3.311431	-0.848623
29	1	0	1.234633	4.239042	-0.703987
30	1	0	0.177030	3.355724	-1.818585
31	6	0	1.667025	2.154257	-0.880010
32	8	0	1.940872	1.516797	-1.864896
33	8	0	2.263012	2.024634	0.315539
34	1	0	2.773145	1.180909	0.366424

Rotational constants (GHZ): 0.3607105 0.2247632 0.1557018

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 538 symmetry adapted cartesian basis functions of A symmetry.

There are 519 symmetry adapted basis functions of A symmetry.

519 basis functions, 823 primitive gaussians, 538 cartesian basis functions

78 alpha electrons 78 beta electrons

nuclear repulsion energy 1556.3641117261 Hartrees.

NAtoms= 34 NActive= 34 NUniq= 34 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 519 RedAO= T EigKep= 3.69D-06 NBF= 519

NBsUse= 519 1.00D-06 EigRej= -1.00D+00 NBFU= 519
Initial guess from the checkpoint file: "./coohpo.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999819 -0.015959 0.003872 0.009556 Ang= -2.18 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3338.88864346 A.U. after 16 cycles
NFock= 16 Conv=0.17D-08 -V/T= 2.0019
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000033446	-0.000847584	-0.000894480
2	6	-0.001314174	0.004760711	0.005774824
3	7	0.001702056	-0.004595421	-0.000497034
4	6	-0.000883901	0.003383288	-0.002056125
5	7	-0.000591719	-0.000545959	-0.002097123
6	6	0.002758547	0.000294938	0.004824123
7	1	0.000758187	-0.000592980	-0.000765806
8	1	0.000543046	-0.000226991	-0.004579733
9	1	0.000524021	0.001055619	-0.000603079
10	1	-0.000882907	-0.000875804	0.000022056
11	35	0.000458827	0.002021795	0.001296010
12	1	0.000171465	-0.000448786	0.000088880
13	6	0.000575883	-0.000724220	0.000732119
14	6	0.001541097	-0.000880240	-0.000948182
15	1	-0.000220377	0.000545518	0.000098692

16	1	-0.000317039	0.000055457	-0.000032317
17	1	0.000058064	0.000320611	0.000084960
18	6	-0.001433200	-0.001077245	-0.001628050
19	6	-0.000239878	-0.000062871	-0.000792837
20	8	0.000838918	0.002239165	0.002191924
21	1	-0.000228049	0.000122009	0.000456651
22	1	-0.000649063	-0.000014046	0.000360392
23	1	-0.000151478	-0.000118389	-0.000049550
24	6	0.000193800	0.000014132	-0.000086532
25	1	-0.000246676	-0.000069090	0.000051694
26	1	0.000066629	0.000004076	0.000052147
27	1	-0.000092972	0.000014736	-0.000046158
28	6	-0.002656859	-0.005551282	0.000077681
29	1	0.000799317	-0.001056581	-0.002295320
30	1	-0.000431820	-0.000576653	-0.000724816
31	6	0.005732527	0.007046781	-0.004521949
32	8	-0.004314473	0.001292439	0.003991835
33	8	-0.002956138	-0.001928186	0.005129169
34	1	0.000854895	-0.002978947	-0.002614066

Cartesian Forces: Max 0.007046781 RMS 0.002059820

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.015769712 RMS 0.003154536
Search for a local minimum.
Step number 6 out of a maximum of 175
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 4 5 6
DE= -5.16D-03 DEPred=-5.26D-03 R= 9.81D-01
TightC=F SS= 1.41D+00 RLast= 9.74D-01 DXNew= 4.2426D-01 2.9222D+00
Trust test= 9.81D-01 RLast= 9.74D-01 DXMaxT set to 4.24D-01
ITU= 1 0 -1 0 1 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00153	0.00236	0.00291	0.00698	0.00768
Eigenvalues ---	0.00970	0.01091	0.01308	0.01483	0.01583
Eigenvalues ---	0.01673	0.01790	0.01955	0.02053	0.02250
Eigenvalues ---	0.02257	0.02379	0.02470	0.02496	0.02993
Eigenvalues ---	0.03050	0.03072	0.03104	0.03328	0.03745
Eigenvalues ---	0.03799	0.04792	0.04994	0.05275	0.05489

Eigenvalues ---	0.05737	0.05888	0.07819	0.09580	0.10138
Eigenvalues ---	0.11941	0.12557	0.12812	0.13443	0.13625
Eigenvalues ---	0.15409	0.15796	0.15943	0.15967	0.15999
Eigenvalues ---	0.16000	0.16000	0.16000	0.16007	0.16284
Eigenvalues ---	0.16911	0.18061	0.19844	0.21886	0.22021
Eigenvalues ---	0.22740	0.23043	0.23714	0.24486	0.24971
Eigenvalues ---	0.25286	0.26246	0.28648	0.29165	0.29751
Eigenvalues ---	0.31847	0.32525	0.34497	0.34575	0.34609
Eigenvalues ---	0.34763	0.34879	0.34895	0.34959	0.35012
Eigenvalues ---	0.35058	0.35530	0.35666	0.35764	0.36506
Eigenvalues ---	0.36558	0.36628	0.37020	0.37284	0.37705
Eigenvalues ---	0.41087	0.42423	0.45719	0.48974	0.51020
Eigenvalues ---	0.53624	0.55401	0.56092	0.60280	0.85107
Eigenvalues ---	1.20648				

RFO step: Lambda=-7.06363040D-03 EMin= 1.53330347D-03

Quartic linear search produced a step of 0.09126.

Iteration 1 RMS(Cart)= 0.27756100 RMS(Int)= 0.01066680

Iteration 2 RMS(Cart)= 0.03988832 RMS(Int)= 0.00082083

Iteration 3 RMS(Cart)= 0.00111713 RMS(Int)= 0.00073039

Iteration 4 RMS(Cart)= 0.00000102 RMS(Int)= 0.00073039

Iteration 5 RMS(Cart)= 0.00000000 RMS(Int)= 0.00073039

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.58047	-0.00504	0.00007	-0.00606	-0.00590	2.57458
R2	2.62254	-0.00182	-0.00007	0.00119	0.00113	2.62367
R3	2.03141	0.00020	-0.00004	-0.00137	-0.00141	2.02999
R4	2.62261	-0.00070	0.00035	0.00724	0.00760	2.63021
R5	2.03480	-0.00337	0.00006	0.00217	0.00224	2.03704
R6	2.53069	0.00363	-0.00021	0.00613	0.00587	2.53655
R7	2.69417	-0.00091	-0.00024	-0.00168	-0.00192	2.69225
R8	2.52405	0.00012	-0.00020	-0.00105	-0.00131	2.52273
R9	2.03453	-0.00033	0.00004	0.00351	0.00355	2.03807
R10	2.79278	-0.00407	0.00068	0.00026	0.00094	2.79372
R11	2.06097	0.00029	-0.00008	-0.00184	-0.00192	2.05905
R12	2.06111	-0.00075	0.00003	-0.00053	-0.00050	2.06061
R13	2.90103	-0.00274	-0.00144	-0.00140	-0.00284	2.89820
R14	5.33523	-0.00205	-0.02310	-0.10255	-0.12564	5.20958
R15	2.50320	-0.00081	0.00010	0.00208	0.00218	2.50538
R16	2.04419	0.00002	-0.00001	0.00398	0.00398	2.04817
R17	2.04261	0.00022	-0.00004	0.00106	0.00102	2.04363
R18	2.04447	0.00008	-0.00004	0.00071	0.00067	2.04515
R19	2.77568	0.00088	-0.00021	0.00423	0.00407	2.77975
R20	2.73539	0.00024	-0.00020	0.00177	0.00157	2.73696
R21	2.05403	-0.00050	0.00016	0.00107	0.00123	2.05526

R22	2.05245	0.00054	0.00026	0.00445	0.00471	2.05716
R23	2.73435	-0.00078	-0.00007	-0.00514	-0.00525	2.72910
R24	2.05609	0.00003	-0.00007	0.00103	0.00097	2.05705
R25	2.84226	-0.00009	-0.00010	-0.00151	-0.00161	2.84064
R26	3.30878	-0.00143	0.00941	-0.01081	-0.00140	3.30738
R27	2.06727	-0.00007	0.00003	-0.00161	-0.00158	2.06569
R28	2.06787	0.00005	0.00003	-0.00033	-0.00030	2.06757
R29	2.06393	0.00004	0.00003	-0.00086	-0.00083	2.06310
R30	2.07053	-0.00054	0.00071	-0.01104	-0.01033	2.06020
R31	2.05757	0.00096	0.00006	-0.01137	-0.01132	2.04626
R32	2.88742	-0.00446	0.00113	0.00494	0.00608	2.89350
R33	2.27659	-0.00500	-0.00036	0.01358	0.01322	2.28981
R34	2.53628	0.00001	-0.00090	-0.00148	-0.00238	2.53389
R35	1.86567	0.00019	-0.00104	-0.02832	-0.02936	1.83630
A1	1.87586	0.00062	0.00000	0.00497	0.00492	1.88078
A2	2.28169	-0.00045	0.00007	-0.00218	-0.00260	2.27909
A3	2.12366	-0.00027	-0.00024	-0.00508	-0.00572	2.11794
A4	1.85911	0.00106	-0.00037	-0.00228	-0.00278	1.85633
A5	2.27688	-0.00085	-0.00164	-0.01658	-0.01874	2.25814
A6	2.14552	-0.00007	0.00190	0.02173	0.02314	2.16866
A7	1.89540	-0.00003	0.00013	0.00032	0.00040	1.89580
A8	2.22537	-0.00172	0.00034	0.00929	0.00942	2.23480
A9	2.16154	0.00175	-0.00024	-0.00859	-0.00904	2.15249
A10	1.90363	-0.00321	-0.00011	-0.00159	-0.00171	1.90192
A11	2.18731	0.00141	0.00011	-0.00078	-0.00078	2.18653
A12	2.19091	0.00192	-0.00011	0.00230	0.00211	2.19302
A13	1.88770	0.00171	0.00017	0.00013	0.00024	1.88794
A14	2.21794	-0.01007	-0.00146	-0.01728	-0.01893	2.19900
A15	2.17411	0.00850	0.00099	0.01683	0.01755	2.19166
A16	1.85705	0.00829	0.00093	0.02418	0.02447	1.88152
A17	1.85472	0.00199	-0.00028	0.01581	0.01570	1.87042
A18	2.03715	-0.01577	-0.00317	-0.05443	-0.05763	1.97952
A19	1.88045	-0.00199	0.00020	0.00313	0.00304	1.88349
A20	1.91959	0.00231	0.00196	-0.00798	-0.00605	1.91355
A21	1.90819	0.00583	0.00053	0.02322	0.02392	1.93211
A22	1.69087	-0.00268	0.00363	0.04266	0.04629	1.73716
A23	2.15448	-0.00050	0.00030	0.00128	0.00157	2.15605
A24	1.97928	0.00007	0.00045	-0.00742	-0.00698	1.97229
A25	2.14889	0.00042	-0.00073	0.00641	0.00567	2.15456
A26	2.08402	0.00008	-0.00017	-0.00161	-0.00181	2.08221
A27	2.14751	-0.00027	0.00027	0.00283	0.00308	2.15059
A28	2.05027	0.00020	-0.00016	-0.00057	-0.00075	2.04952
A29	2.07385	0.00095	-0.00005	0.00032	0.00035	2.07421
A30	2.11562	-0.00090	-0.00087	-0.00314	-0.00411	2.11151

A31	1.98800	0.00006	0.00001	-0.00215	-0.00212	1.98588
A32	1.99315	-0.00007	-0.00011	-0.00453	-0.00466	1.98849
A33	2.02183	0.00014	0.00073	0.00602	0.00674	2.02857
A34	2.04314	-0.00021	-0.00100	-0.00630	-0.00726	2.03588
A35	2.13832	0.00014	0.00062	0.00619	0.00679	2.14511
A36	1.95663	0.00012	-0.00017	-0.00210	-0.00224	1.95439
A37	2.03964	-0.00026	0.00032	-0.00160	-0.00130	2.03834
A38	2.02062	0.00009	0.00021	0.00136	0.00156	2.02218
A39	2.32340	-0.00078	-0.00235	-0.01936	-0.02148	2.30192
A40	2.65286	0.00120	0.00122	0.00919	0.01025	2.66311
A41	1.93907	-0.00038	0.00038	-0.00128	-0.00090	1.93817
A42	1.91727	0.00015	-0.00029	-0.00127	-0.00156	1.91571
A43	1.93642	-0.00008	0.00021	-0.00016	0.00005	1.93648
A44	1.88210	0.00009	-0.00013	0.00059	0.00045	1.88256
A45	1.89527	0.00018	-0.00003	0.00124	0.00121	1.89648
A46	1.89222	0.00004	-0.00016	0.00098	0.00082	1.89304
A47	1.83540	0.00399	-0.00097	0.04007	0.03886	1.87426
A48	1.95156	0.00360	0.00160	0.01579	0.01727	1.96883
A49	2.01267	-0.01083	0.00006	-0.03420	-0.03394	1.97873
A50	1.89279	-0.00187	-0.00161	-0.02007	-0.02207	1.87072
A51	1.88320	0.00407	0.00024	-0.01371	-0.01306	1.87015
A52	1.88373	0.00147	0.00048	0.01108	0.01172	1.89546
A53	2.17231	-0.00488	-0.00021	0.03536	0.03054	2.20285
A54	1.92270	0.00809	0.00015	0.01337	0.00906	1.93176
A55	2.18485	-0.00258	0.00028	-0.03473	-0.03878	2.14607
A56	1.93681	-0.01231	0.00159	-0.04472	-0.04313	1.89368
A57	2.75792	-0.01038	0.00837	0.01171	0.02008	2.77800
D1	-0.06327	0.00067	-0.00512	0.01347	0.00842	-0.05485
D2	3.14044	-0.00185	-0.00255	-0.04049	-0.04229	3.09816
D3	-3.13663	0.00241	-0.00012	0.05302	0.05281	-3.08382
D4	0.06708	-0.00011	0.00245	-0.00094	0.00210	0.06919
D5	0.02902	0.00065	0.00450	-0.00279	0.00171	0.03073
D6	3.08421	0.00296	-0.00481	-0.00575	-0.01036	3.07386
D7	3.10987	-0.00091	0.00005	-0.03791	-0.03766	3.07221
D8	-0.11812	0.00140	-0.00926	-0.04088	-0.04972	-0.16784
D9	0.07582	-0.00179	0.00399	-0.01953	-0.01563	0.06018
D10	-3.10975	-0.00170	0.00782	0.00594	0.01378	-3.09597
D11	-3.12209	0.00045	0.00158	0.02778	0.03001	-3.09208
D12	-0.02447	0.00055	0.00541	0.05325	0.05942	0.03495
D13	-1.78587	0.00471	-0.01128	-0.10844	-0.11967	-1.90555
D14	1.42669	0.00181	-0.00829	-0.16906	-0.17740	1.24930
D15	-0.05899	0.00236	-0.00123	0.01807	0.01693	-0.04206
D16	3.13556	-0.00011	0.00464	0.01935	0.02401	-3.12362
D17	3.12460	0.00238	-0.00492	-0.00680	-0.01134	3.11326

D18	0.03597	-0.00009	0.00095	-0.00552	-0.00427	0.03170
D19	0.48837	-0.00108	-0.00470	-0.04402	-0.04868	0.43969
D20	-2.61883	-0.00076	-0.00519	-0.05304	-0.05816	-2.67699
D21	-2.70340	-0.00103	-0.00030	-0.01465	-0.01501	-2.71842
D22	0.47258	-0.00071	-0.00079	-0.02367	-0.02450	0.44808
D23	0.01881	-0.00183	-0.00201	-0.00938	-0.01144	0.00736
D24	-3.03908	-0.00294	0.00699	-0.00444	0.00279	-3.03629
D25	3.10731	0.00062	-0.00789	-0.01078	-0.01866	3.08864
D26	0.04942	-0.00049	0.00110	-0.00584	-0.00442	0.04499
D27	-2.53058	-0.00120	0.01024	-0.02036	-0.01037	-2.54095
D28	-0.52987	0.00123	0.01077	0.00147	0.01238	-0.51749
D29	1.60301	-0.00007	0.00907	0.00795	0.01718	1.62019
D30	0.51127	0.00094	-0.00049	-0.02494	-0.02572	0.48556
D31	2.51198	0.00337	0.00003	-0.00311	-0.00296	2.50901
D32	-1.63833	0.00207	-0.00167	0.00337	0.00183	-1.63650
D33	-2.99569	0.00352	0.00241	-0.06464	-0.06170	-3.05739
D34	1.23688	0.00154	0.00407	-0.07253	-0.06835	1.16852
D35	-0.92373	0.00517	0.00206	-0.07355	-0.07134	-0.99507
D36	1.17051	0.00210	0.00185	-0.05069	-0.04875	1.12176
D37	-0.88011	0.00012	0.00352	-0.05858	-0.05540	-0.93551
D38	-3.04072	0.00375	0.00151	-0.05960	-0.05839	-3.09911
D39	-0.89094	-0.00035	0.00017	-0.06370	-0.06334	-0.95428
D40	-2.94156	-0.00233	0.00183	-0.07159	-0.06999	-3.01155
D41	1.18102	0.00130	-0.00017	-0.07262	-0.07298	1.10804
D42	-3.09172	-0.00002	-0.00081	-0.01468	-0.01550	-3.10722
D43	-0.00819	0.00038	-0.00226	-0.00117	-0.00344	-0.01163
D44	0.01219	-0.00039	-0.00024	-0.00507	-0.00529	0.00690
D45	3.09572	0.00002	-0.00169	0.00844	0.00676	3.10248
D46	-2.73658	-0.00035	0.00034	-0.00336	-0.00304	-2.73962
D47	-0.03501	-0.00027	-0.00004	0.00003	-0.00004	-0.03505
D48	-0.00971	0.00021	-0.00003	0.00686	0.00681	-0.00290
D49	2.69187	0.00029	-0.00041	0.01025	0.00981	2.70168
D50	0.68438	0.00085	0.00057	0.00541	0.00608	0.69046
D51	-1.69298	0.00063	-0.00045	0.00344	0.00310	-1.68988
D52	2.13331	0.00016	0.00546	0.03803	0.04354	2.17685
D53	-0.25846	0.00017	0.00497	0.04014	0.04516	-0.21330
D54	2.54994	-0.00003	0.00036	-0.00019	0.00014	2.55008
D55	-1.65222	-0.00005	0.00024	-0.00109	-0.00086	-1.65309
D56	0.43972	0.00005	-0.00001	-0.00079	-0.00082	0.43890
D57	1.33814	-0.00003	0.00005	-0.00236	-0.00230	1.33584
D58	-2.86402	-0.00005	-0.00006	-0.00326	-0.00330	-2.86732
D59	-0.77208	0.00005	-0.00032	-0.00296	-0.00326	-0.77534
D60	-1.02644	-0.00002	-0.00030	0.00135	0.00105	-1.02539
D61	1.05459	-0.00004	-0.00041	0.00046	0.00005	1.05463

D62	-3.13666	0.00006	-0.00067	0.00075	0.00009	-3.13657
D63	1.55949	-0.00356	-0.01398	-0.09067	-0.10461	1.45488
D64	-2.79966	-0.00203	-0.01747	-0.11377	-0.13128	-2.93094
D65	2.32296	-0.00378	0.03775	0.03607	0.07284	2.39580
D66	-0.90236	0.00410	0.02015	0.21031	0.23120	-0.67116
D67	-1.91502	-0.00247	0.03673	0.05632	0.09233	-1.82268
D68	1.14286	0.00540	0.01912	0.23057	0.25069	1.39354
D69	0.12707	-0.00174	0.03521	0.03133	0.06566	0.19273
D70	-3.09824	0.00613	0.01761	0.20557	0.22401	-2.87423
D71	2.94739	-0.00968	-0.00197	-0.13850	-0.13749	2.80991
D72	-0.27866	-0.00186	-0.01968	0.04141	0.01874	-0.25992
D73	-1.40235	-0.00397	-0.00711	-0.18212	-0.18923	-1.59158

Item	Value	Threshold	Converged?
Maximum Force	0.015770	0.000450	NO
RMS Force	0.003155	0.000300	NO
Maximum Displacement	1.134381	0.001800	NO
RMS Displacement	0.287250	0.001200	NO

Predicted change in Energy=-4.833901D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.629785	1.368951	1.320498
2	6	0	-1.357869	0.231169	1.497982
3	7	0	-2.468504	0.342749	0.666551
4	6	0	-2.361813	1.478361	-0.041075
5	7	0	-1.257380	2.124635	0.339332
6	6	0	-0.851800	3.473087	-0.110959
7	1	0	0.317228	1.664060	1.732856
8	1	0	-1.166061	-0.609672	2.144650
9	1	0	-1.756091	4.025947	-0.363620
10	1	0	-0.382222	3.968638	0.739310
11	35	0	-0.506049	-2.500980	0.250648
12	1	0	-3.084851	1.836689	-0.756604
13	6	0	-3.556856	-0.566189	0.528610
14	6	0	-3.933180	-1.408076	1.481145
15	1	0	-4.030226	-0.515513	-0.445077
16	1	0	-4.749676	-2.091326	1.291345
17	1	0	-3.435525	-1.479929	2.439493
18	6	0	2.977495	-0.771519	0.398099
19	6	0	3.991144	-0.387989	1.392682

20	8	0	2.962716	0.546280	0.998827
21	1	0	3.249038	-0.770429	-0.655056
22	1	0	2.127520	-1.392682	0.675142
23	1	0	3.842564	-0.753611	2.407165
24	6	0	5.404828	-0.034726	1.023464
25	1	0	5.802739	0.737292	1.687209
26	1	0	6.043194	-0.918475	1.115980
27	1	0	5.461041	0.326230	-0.005352
28	6	0	0.094588	3.453751	-1.317643
29	1	0	0.397284	4.483133	-1.510797
30	1	0	-0.380993	3.085799	-2.218176
31	6	0	1.372132	2.645432	-1.074753
32	8	0	1.891624	1.876329	-1.853766
33	8	0	1.815794	2.825918	0.177662
34	1	0	2.421021	2.098377	0.398219

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.362408	0.000000			
3	N	2.204909	1.391848	0.000000		
4	C	2.205849	2.220831	1.342287	0.000000	
5	N	1.388387	2.222112	2.179222	1.334972	0.000000
6	C	2.554553	3.654425	3.607945	2.502789	1.478371
7	H	1.074226	2.216820	3.262388	3.218474	2.152540
8	H	2.209473	1.077954	2.188206	3.250708	3.277796
9	H	3.341323	4.245525	3.890338	2.638395	2.087544
10	H	2.675338	3.936514	4.183890	3.275554	2.079959
11	Br	4.016996	3.121871	3.480086	4.400468	4.687076
12	H	3.249689	3.262410	2.153395	1.078501	2.150265
13	C	3.597165	2.531997	1.424678	2.435746	3.544566
14	C	4.318577	3.052808	2.423680	3.621860	4.576427
15	H	4.269831	3.387404	2.100311	2.631037	3.908241
16	H	5.380322	4.115949	3.393941	4.496654	5.556688
17	H	4.152161	2.851483	2.720406	4.007188	4.706152
18	C	4.294753	4.583722	5.565300	5.810597	5.130821
19	C	4.944193	5.385758	6.541277	6.774879	5.913530
20	O	3.699504	4.360723	5.445180	5.504615	4.553609
21	H	4.850261	5.182891	5.972947	6.075827	5.447752
22	H	3.955481	3.932161	4.912762	5.376798	4.893039
23	H	5.068336	5.370373	6.637870	7.033482	6.210448
24	C	6.202830	6.784537	7.890452	7.983946	7.036754
25	H	6.473859	7.180966	8.343313	8.378309	7.320299
26	H	7.057110	7.499556	8.616361	8.816334	7.947458

27	H	6.320072	6.983308	7.957978	7.907321	6.963495
28	C	3.439606	4.519116	4.492749	3.400837	2.517922
29	H	4.332347	5.496591	5.486016	4.336052	3.423946
30	H	3.941024	4.786756	4.494850	3.353695	2.869275
31	C	3.372581	4.461002	4.804683	4.046343	3.030710
32	O	4.085448	4.949745	5.264464	4.640684	3.845460
33	O	3.067520	4.306751	4.975977	4.395014	3.156317
34	H	3.269568	4.356140	5.202085	4.842819	3.678966

		6	7	8	9	10
6	C	0.000000				
7	H	2.835288	0.000000			
8	H	4.674982	2.745829	0.000000		
9	H	1.089603	3.777879	5.303633	0.000000	
10	H	1.090427	2.605272	4.852866	1.762740	0.000000
11	Br	5.994979	4.496919	2.756793	6.673882	6.489228
12	H	2.842740	4.219165	4.252495	2.590924	3.753287
13	C	4.903277	4.629551	2.886066	5.012639	5.539617
14	C	5.987942	5.250461	2.955442	6.137710	6.486036
15	H	5.111062	5.328629	3.862512	5.079683	5.900704
16	H	6.937044	6.322291	3.970608	7.008672	7.490164
17	H	6.141075	4.946428	2.448417	6.402547	6.473033
18	C	5.739278	3.845860	4.499521	6.782531	5.820070
19	C	6.373614	4.221882	5.216451	7.456416	6.207530
20	O	4.934405	2.964260	4.438010	6.019260	4.792546
21	H	5.926241	4.497151	5.230420	6.938405	6.130992
22	H	5.759340	3.706695	3.690560	6.747073	5.920023
23	H	6.800219	4.327565	5.017564	7.865517	6.552114
24	C	7.262029	5.410434	6.690606	8.348163	7.042558
25	H	7.416257	5.563436	7.112506	8.494532	7.042291
26	H	8.266325	6.311633	7.288819	9.352292	8.081567
27	H	7.054489	5.591956	7.029716	8.118082	6.925705
28	C	1.533659	3.543742	5.485263	2.159301	2.173364
29	H	2.130716	4.298240	6.460883	2.482349	2.436251
30	H	2.193631	4.256702	5.771230	2.492820	3.086443
31	C	2.561208	3.155723	5.234758	3.492465	2.849467
32	O	3.621241	3.922709	5.613998	4.488565	4.033879
33	O	2.760106	2.452396	4.956186	3.806759	2.540183
34	H	3.586146	2.528998	4.821899	4.663066	3.387091

		11	12	13	14	15
11	Br	0.000000				
12	H	5.145887	0.000000			
13	C	3.623272	2.765572	0.000000		
14	C	3.801814	4.031834	1.325788	0.000000	
15	H	4.104381	2.554141	1.083843	2.125187	0.000000

16	H	4.388535	4.732340	2.081015	1.081444	2.452745
17	H	3.796764	4.619303	2.121583	1.082245	3.099115
18	C	3.892024	6.699860	6.538879	7.023932	7.062906
19	C	5.098403	7.722586	7.599387	7.990201	8.230189
20	O	4.677381	6.428046	6.630499	7.183698	7.218969
21	H	4.232704	6.850221	6.911076	7.520252	7.286752
22	H	2.888633	6.296630	5.746015	6.114078	6.319980
23	H	5.158904	8.044139	7.636459	7.857991	8.376920
24	C	6.451210	8.873866	8.991058	9.449548	9.560754
25	H	7.235394	9.282789	9.520685	9.971619	10.139200
26	H	6.793062	9.716929	9.624451	9.995053	10.201621
27	H	6.607936	8.710806	9.077665	9.667931	9.538660
28	C	6.187012	3.610884	5.735993	6.906047	5.790554
29	H	7.259238	4.438213	6.729789	7.900062	6.762031
30	H	6.109242	3.317728	5.564887	6.818938	5.424963
31	C	5.636472	4.540924	6.097558	7.149117	6.290750
32	O	5.416478	5.096140	6.428651	7.472435	6.540154
33	O	5.811379	5.086034	6.363562	7.257856	6.762315
34	H	5.453770	5.631760	6.546139	7.337834	7.011573

		16	17	18	19	20
16	H	0.000000				
17	H	1.849066	0.000000			
18	C	7.889801	6.767271	0.000000		
19	C	8.905817	7.579153	1.470978	0.000000	
20	O	8.156196	6.864294	1.448339	1.444176	0.000000
21	H	8.337426	7.400203	1.087599	2.211383	2.133315
22	H	6.940002	5.836781	1.088602	2.235480	2.135860
23	H	8.767047	7.314312	2.187468	1.088546	2.108854
24	C	10.364136	9.068936	2.612641	1.503203	2.510396
25	H	10.932121	9.530348	3.452582	2.152877	2.928495
26	H	10.857826	9.587128	3.152056	2.137495	3.413001
27	H	10.572831	9.401509	2.745146	2.150630	2.701560
28	C	7.811631	7.135752	5.395167	6.106389	4.695272
29	H	8.807196	8.115006	6.157332	6.713707	5.327144
30	H	7.629204	7.202077	5.744844	6.649894	5.289485
31	C	8.093938	7.244453	4.052411	4.706284	3.352034
32	O	8.351100	7.620699	3.641581	4.480464	3.324690
33	O	8.277981	7.157691	3.786779	4.066648	2.680764
34	H	8.352855	7.160321	2.923349	3.104233	1.750192

		21	22	23	24	25
21	H	0.000000				
22	H	1.847817	0.000000			
23	H	3.119256	2.519860	0.000000		
24	C	2.829509	3.564565	2.207283	0.000000	

25	H	3.778997	4.366728	2.565817	1.093117	0.000000
26	H	3.311464	3.968843	2.556778	1.094112	1.767961
27	H	2.552986	3.811837	3.099318	1.091747	1.774963
28	C	5.313499	5.620668	6.754511	6.771182	6.999377
29	H	6.038601	6.503633	7.392149	7.204792	7.312832
30	H	5.521862	5.892428	7.346651	7.329504	7.681540
31	C	3.920080	4.465323	5.457132	5.277158	5.558751
32	O	3.206994	4.139741	5.373853	4.926783	5.397475
33	O	3.959964	4.259254	4.678837	4.666887	4.747297
34	H	3.166236	3.514303	3.767027	3.720775	3.866532

		26	27	28	29	30
26	H	0.000000				
27	H	1.773578	0.000000			
28	C	7.773338	6.348410	0.000000		
29	H	8.243399	6.722190	1.090212	0.000000	
30	H	8.271697	6.829434	1.082832	1.748897	0.000000
31	C	6.270531	4.820943	1.531174	2.125466	2.138875
32	O	5.819438	4.308153	2.450515	3.024253	2.600076
33	O	5.724669	4.423772	2.364880	2.758518	3.260897
34	H	4.768303	3.541906	3.192727	3.664275	3.958763

		31	32	33	34
31	C	0.000000			
32	O	1.211715	0.000000		
33	O	1.340878	2.243695	0.000000	
34	H	1.889202	2.324006	0.971731	0.000000

Stoichiometry C11H17BrN2O3
Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.490631	1.051975	1.227976
2	6	0	-1.538789	0.184551	1.156603
3	7	0	-2.511938	0.808495	0.381416
4	6	0	-2.024003	1.978997	-0.058558
5	7	0	-0.800099	2.155583	0.444459
6	6	0	0.021428	3.376106	0.299561
7	1	0	0.475121	0.944914	1.686040
8	1	0	-1.649796	-0.791979	1.599382

9	1	0	-0.655855	4.221829	0.184344
10	1	0	0.568025	3.508935	1.233702
11	35	0	-1.483851	-2.344838	-0.672401
12	1	0	-2.560534	2.687150	-0.669966
13	6	0	-3.814604	0.331773	0.056603
14	6	0	-4.484338	-0.535421	0.803024
15	1	0	-4.191761	0.732707	-0.877057
16	1	0	-5.456916	-0.875905	0.474872
17	1	0	-4.089602	-0.960212	1.716802
18	6	0	2.345081	-1.849748	-0.180444
19	6	0	3.366563	-2.019642	0.864298
20	8	0	2.695313	-0.751940	0.696963
21	1	0	2.666005	-1.707994	-1.209902
22	1	0	1.331863	-2.221925	-0.039275
23	1	0	3.054259	-2.529002	1.774216
24	6	0	4.840045	-2.050282	0.568441
25	1	0	5.413417	-1.599283	1.382534
26	1	0	5.173511	-3.086356	0.456929
27	1	0	5.063940	-1.513648	-0.355575
28	6	0	0.987031	3.323157	-0.890782
29	1	0	1.598676	4.224896	-0.854473
30	1	0	0.476418	3.321169	-1.845662
31	6	0	1.942349	2.127419	-0.845266
32	8	0	2.249149	1.420240	-1.780159
33	8	0	2.344891	1.890460	0.411620
34	1	0	2.686658	0.982093	0.459845

Rotational constants (GHZ): 0.3547240 0.2549784 0.1678192

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 538 symmetry adapted cartesian basis functions of A symmetry.

There are 519 symmetry adapted basis functions of A symmetry.

519 basis functions, 823 primitive gaussians, 538 cartesian basis functions

78 alpha electrons 78 beta electrons

nuclear repulsion energy 1591.4062598086 Hartrees.

NAtoms= 34 NActive= 34 NUniq= 34 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 519 RedAO= T EigKep= 3.11D-06 NBF= 519

NBsUse= 519 1.00D-06 EigRej= -1.00D+00 NBFU= 519

Initial guess from the checkpoint file: "./coohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.998723 -0.005587 0.000605 0.050214 Ang= -5.79 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3338.89024787 A.U. after 14 cycles
NFock= 14 Conv=0.27D-08 -V/T= 2.0019
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.001119958	-0.001369232	-0.000907048
2	6	-0.002922736	0.005119584	0.003070362
3	7	0.002275555	-0.000908073	0.000386240
4	6	-0.001815909	0.000546543	0.000262861
5	7	-0.001154105	0.003037269	0.003026493
6	6	0.001651050	-0.002476335	-0.002800762
7	1	-0.000364016	-0.000167467	0.000732398
8	1	-0.002756791	-0.000476595	-0.005087067
9	1	-0.001562580	-0.000332651	0.000219937
10	1	-0.000320654	-0.001780426	-0.001008933
11	35	0.001762542	-0.000426247	0.000676279
12	1	0.001100729	-0.001053294	0.000823909
13	6	-0.001122108	-0.001244722	0.001151320
14	6	0.000747042	0.000842813	-0.001828119
15	1	0.000221914	-0.000385897	0.001621320
16	1	0.000331771	-0.000088630	-0.000144017
17	1	0.000293800	0.000257972	-0.000653615
18	6	-0.000222358	-0.002782831	-0.000377954

19	6	-0.001090157	-0.001294187	-0.001025679
20	8	-0.001247402	0.005711538	0.003079716
21	1	-0.000578744	0.000008329	0.001072140
22	1	0.000779390	-0.000499082	-0.002177864
23	1	0.000504273	0.000058815	0.000005221
24	6	0.000050448	-0.000633027	-0.000296023
25	1	0.000094418	0.000433122	0.000389899
26	1	0.000230308	-0.000049039	-0.000028318
27	1	-0.000098963	0.000051202	-0.000234851
28	6	0.010035039	-0.000621968	0.002364249
29	1	-0.000041864	0.003956356	-0.000948585
30	1	-0.002529378	-0.003328691	-0.003193340
31	6	0.000932432	-0.015729269	-0.003652338
32	8	-0.009806471	0.013964461	0.002467078
33	8	-0.008468697	0.012431705	-0.000110379
34	1	0.013972264	-0.010772046	0.003125467

Cartesian Forces: Max 0.015729269 RMS 0.003803521

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.015828470 RMS 0.002732600
Search for a local minimum.
Step number 7 out of a maximum of 175
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 6 7
DE= -1.60D-03 DEPred=-4.83D-03 R= 3.32D-01
Trust test= 3.32D-01 RLast= 6.43D-01 DXMaxT set to 4.24D-01
ITU= 0 1 0 -1 0 1 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00225	0.00242	0.00288	0.00698	0.00784
Eigenvalues ---	0.00955	0.01294	0.01425	0.01554	0.01587
Eigenvalues ---	0.01704	0.01754	0.01960	0.02112	0.02248
Eigenvalues ---	0.02261	0.02378	0.02477	0.02553	0.02972
Eigenvalues ---	0.03050	0.03069	0.03235	0.03738	0.03816
Eigenvalues ---	0.04183	0.04852	0.05091	0.05464	0.05540
Eigenvalues ---	0.05741	0.05901	0.07767	0.09438	0.09670
Eigenvalues ---	0.11924	0.12613	0.12619	0.13235	0.13704
Eigenvalues ---	0.15363	0.15805	0.15867	0.15958	0.15999
Eigenvalues ---	0.16000	0.16000	0.16001	0.16006	0.16285

Eigenvalues --- 0.16866 0.18098 0.19189 0.21999 0.22512
Eigenvalues --- 0.22913 0.23050 0.23659 0.24485 0.25173
Eigenvalues --- 0.25444 0.27968 0.28640 0.29218 0.30775
Eigenvalues --- 0.31848 0.32484 0.34497 0.34559 0.34617
Eigenvalues --- 0.34765 0.34885 0.34897 0.34966 0.35010
Eigenvalues --- 0.35135 0.35536 0.35714 0.35765 0.36539
Eigenvalues --- 0.36621 0.36680 0.37182 0.37362 0.37888
Eigenvalues --- 0.41078 0.42384 0.45607 0.49008 0.52484
Eigenvalues --- 0.54689 0.55402 0.56095 0.60346 0.86887
Eigenvalues --- 0.97172
RFO step: Lambda=-3.71823157D-03 EMin= 2.24939403D-03
Quartic linear search produced a step of -0.34625.
Iteration 1 RMS(Cart)= 0.16557261 RMS(Int)= 0.00441107
Iteration 2 RMS(Cart)= 0.00783315 RMS(Int)= 0.00019551
Iteration 3 RMS(Cart)= 0.00005000 RMS(Int)= 0.00019353
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00019353

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.57458	-0.00166	0.00204	-0.00588	-0.00384	2.57074
R2	2.62367	-0.00035	-0.00039	-0.00161	-0.00196	2.62171
R3	2.02999	-0.00009	0.00049	-0.00009	0.00040	2.03039
R4	2.63021	-0.00368	-0.00263	-0.00638	-0.00904	2.62117
R5	2.03704	-0.00212	-0.00077	-0.00782	-0.00860	2.02844
R6	2.53655	-0.00078	-0.00203	0.00295	0.00090	2.53745
R7	2.69225	0.00002	0.00066	-0.00174	-0.00108	2.69117
R8	2.52273	0.00113	0.00046	0.00166	0.00213	2.52486
R9	2.03807	-0.00163	-0.00123	-0.00312	-0.00435	2.03372
R10	2.79372	-0.00178	-0.00033	-0.00631	-0.00663	2.78708
R11	2.05905	0.00108	0.00066	0.00219	0.00285	2.06190
R12	2.06061	-0.00174	0.00017	-0.00450	-0.00433	2.05628
R13	2.89820	0.00116	0.00098	-0.00090	0.00009	2.89828
R14	5.20958	0.00025	0.04350	-0.06729	-0.02379	5.18580
R15	2.50538	-0.00292	-0.00076	-0.00359	-0.00434	2.50103
R16	2.04817	-0.00157	-0.00138	-0.00243	-0.00380	2.04436
R17	2.04363	-0.00017	-0.00035	0.00015	-0.00020	2.04343
R18	2.04515	-0.00046	-0.00023	-0.00066	-0.00090	2.04425
R19	2.77975	0.00015	-0.00141	-0.00135	-0.00281	2.77694
R20	2.73696	0.00318	-0.00054	0.00745	0.00693	2.74389
R21	2.05526	-0.00119	-0.00043	-0.00268	-0.00310	2.05216
R22	2.05716	-0.00088	-0.00163	-0.00086	-0.00249	2.05467
R23	2.72910	0.00063	0.00182	0.00017	0.00202	2.73111
R24	2.05705	-0.00008	-0.00034	0.00007	-0.00026	2.05679
R25	2.84064	0.00025	0.00056	0.00007	0.00062	2.84127
R26	3.30738	-0.00124	0.00048	-0.01040	-0.00992	3.29747

R27	2.06569	0.00058	0.00055	0.00086	0.00141	2.06710
R28	2.06757	0.00017	0.00010	0.00043	0.00054	2.06811
R29	2.06310	0.00023	0.00029	0.00042	0.00071	2.06381
R30	2.06020	0.00389	0.00358	0.00534	0.00891	2.06911
R31	2.04626	0.00490	0.00392	0.00879	0.01270	2.05896
R32	2.89350	-0.00425	-0.00210	-0.01551	-0.01762	2.87588
R33	2.28981	-0.01465	-0.00458	-0.01269	-0.01727	2.27254
R34	2.53389	0.00490	0.00083	0.00594	0.00677	2.54066
R35	1.83630	0.01583	0.01017	0.01634	0.02651	1.86281
A1	1.88078	-0.00101	-0.00170	-0.00315	-0.00484	1.87594
A2	2.27909	-0.00009	0.00090	-0.00131	-0.00025	2.27884
A3	2.11794	0.00108	0.00198	0.00276	0.00483	2.12277
A4	1.85633	0.00205	0.00096	0.00722	0.00754	1.86387
A5	2.25814	0.00016	0.00649	0.00376	0.00975	2.26789
A6	2.16866	-0.00220	-0.00801	-0.01014	-0.01853	2.15013
A7	1.89580	-0.00023	-0.00014	-0.00042	-0.00067	1.89513
A8	2.23480	-0.00194	-0.00326	-0.00757	-0.01072	2.22408
A9	2.15249	0.00217	0.00313	0.00806	0.01132	2.16382
A10	1.90192	-0.00033	0.00059	-0.00329	-0.00318	1.89874
A11	2.18653	-0.00017	0.00027	0.00060	0.00055	2.18708
A12	2.19302	0.00059	-0.00073	0.00533	0.00428	2.19730
A13	1.88794	-0.00043	-0.00008	0.00311	0.00288	1.89082
A14	2.19900	-0.00053	0.00656	-0.01392	-0.00745	2.19156
A15	2.19166	0.00099	-0.00608	0.01276	0.00664	2.19830
A16	1.88152	-0.00194	-0.00847	-0.00361	-0.01186	1.86966
A17	1.87042	-0.00292	-0.00544	0.00407	-0.00153	1.86888
A18	1.97952	0.00578	0.01995	-0.01213	0.00778	1.98730
A19	1.88349	0.00105	-0.00105	0.00161	0.00066	1.88415
A20	1.91355	-0.00201	0.00209	-0.00897	-0.00684	1.90671
A21	1.93211	-0.00016	-0.00828	0.01934	0.01096	1.94307
A22	1.73716	0.00537	-0.01603	0.01903	0.00300	1.74016
A23	2.15605	-0.00074	-0.00054	-0.00291	-0.00351	2.15254
A24	1.97229	0.00097	0.00242	0.00259	0.00495	1.97724
A25	2.15456	-0.00024	-0.00196	-0.00004	-0.00205	2.15250
A26	2.08221	0.00028	0.00063	0.00095	0.00158	2.08379
A27	2.15059	-0.00072	-0.00107	-0.00303	-0.00409	2.14650
A28	2.04952	0.00042	0.00026	0.00204	0.00231	2.05183
A29	2.07421	-0.00009	-0.00012	-0.00144	-0.00148	2.07273
A30	2.11151	0.00117	0.00142	0.00403	0.00537	2.11688
A31	1.98588	-0.00036	0.00073	-0.00285	-0.00213	1.98376
A32	1.98849	0.00138	0.00161	0.00492	0.00653	1.99502
A33	2.02857	-0.00113	-0.00233	-0.00250	-0.00483	2.02373
A34	2.03588	0.00127	0.00251	0.00226	0.00480	2.04068
A35	2.14511	-0.00148	-0.00235	-0.00109	-0.00347	2.14165

A36	1.95439	0.00065	0.00078	-0.00005	0.00074	1.95513
A37	2.03834	-0.00114	0.00045	-0.00177	-0.00135	2.03699
A38	2.02218	0.00002	-0.00054	-0.00114	-0.00168	2.02050
A39	2.30192	-0.00048	0.00744	-0.02399	-0.01658	2.28534
A40	2.66311	0.00076	-0.00355	0.00613	0.00233	2.66544
A41	1.93817	-0.00020	0.00031	-0.00174	-0.00143	1.93674
A42	1.91571	0.00031	0.00054	0.00151	0.00205	1.91776
A43	1.93648	-0.00018	-0.00002	-0.00112	-0.00114	1.93534
A44	1.88256	-0.00002	-0.00016	0.00026	0.00010	1.88266
A45	1.89648	0.00013	-0.00042	0.00073	0.00031	1.89679
A46	1.89304	-0.00003	-0.00028	0.00045	0.00017	1.89321
A47	1.87426	-0.00250	-0.01346	0.01084	-0.00267	1.87159
A48	1.96883	-0.00297	-0.00598	-0.00422	-0.01012	1.95870
A49	1.97873	0.00852	0.01175	0.01258	0.02424	2.00296
A50	1.87072	0.00151	0.00764	-0.01062	-0.00289	1.86783
A51	1.87015	-0.00062	0.00452	-0.00298	0.00130	1.87145
A52	1.89546	-0.00411	-0.00406	-0.00661	-0.01067	1.88479
A53	2.20285	-0.01310	-0.01057	-0.03436	-0.04450	2.15835
A54	1.93176	0.00788	-0.00314	0.02528	0.02258	1.95433
A55	2.14607	0.00544	0.01343	0.01057	0.02442	2.17050
A56	1.89368	-0.00117	0.01494	-0.00905	0.00589	1.89957
A57	2.77800	-0.00466	-0.00695	-0.00728	-0.01423	2.76377
D1	-0.05485	0.00035	-0.00292	0.03799	0.03508	-0.01977
D2	3.09816	-0.00045	0.01464	-0.04460	-0.03092	3.06723
D3	-3.08382	0.00044	-0.01829	0.05556	0.03754	-3.04628
D4	0.06919	-0.00036	-0.00073	-0.02704	-0.02847	0.04072
D5	0.03073	0.00049	-0.00059	-0.00686	-0.00739	0.02335
D6	3.07386	0.00094	0.00359	0.01499	0.01852	3.09238
D7	3.07221	0.00034	0.01304	-0.02275	-0.00989	3.06232
D8	-0.16784	0.00079	0.01722	-0.00089	0.01601	-0.15183
D9	0.06018	-0.00112	0.00541	-0.05615	-0.05075	0.00944
D10	-3.09597	-0.00090	-0.00477	-0.05047	-0.05516	3.13206
D11	-3.09208	-0.00036	-0.01039	0.02120	0.00994	-3.08214
D12	0.03495	-0.00014	-0.02057	0.02688	0.00553	0.04048
D13	-1.90555	0.00465	0.04144	0.12747	0.16875	-1.73680
D14	1.24930	0.00370	0.06142	0.03146	0.09304	1.34233
D15	-0.04206	0.00154	-0.00586	0.05330	0.04719	0.00513
D16	-3.12362	-0.00011	-0.00831	0.00685	-0.00148	-3.12510
D17	3.11326	0.00138	0.00393	0.04810	0.05164	-3.11829
D18	0.03170	-0.00027	0.00148	0.00165	0.00296	0.03466
D19	0.43969	-0.00116	0.01686	-0.07083	-0.05405	0.38564
D20	-2.67699	-0.00056	0.02014	-0.05477	-0.03468	-2.71168
D21	-2.71842	-0.00094	0.00520	-0.06448	-0.05922	-2.77764
D22	0.44808	-0.00034	0.00848	-0.04842	-0.03986	0.40823

D23	0.00736	-0.00128	0.00396	-0.02898	-0.02489	-0.01753
D24	-3.03629	-0.00162	-0.00097	-0.04883	-0.04992	-3.08621
D25	3.08864	0.00034	0.00646	0.01748	0.02398	3.11263
D26	0.04499	0.00000	0.00153	-0.00237	-0.00105	0.04395
D27	-2.54095	0.00158	0.00359	0.01228	0.01594	-2.52501
D28	-0.51749	0.00035	-0.00429	0.01441	0.01008	-0.50741
D29	1.62019	0.00177	-0.00595	0.03398	0.02797	1.64816
D30	0.48556	0.00201	0.00890	0.03692	0.04591	0.53147
D31	2.50901	0.00078	0.00103	0.03905	0.04006	2.54907
D32	-1.63650	0.00220	-0.00063	0.05862	0.05795	-1.57854
D33	-3.05739	-0.00095	0.02136	-0.08796	-0.06681	-3.12420
D34	1.16852	0.00051	0.02367	-0.07942	-0.05584	1.11268
D35	-0.99507	0.00165	0.02470	-0.07713	-0.05249	-1.04756
D36	1.12176	-0.00091	0.01688	-0.06881	-0.05196	1.06980
D37	-0.93551	0.00055	0.01918	-0.06027	-0.04100	-0.97651
D38	-3.09911	0.00169	0.02022	-0.05798	-0.03764	-3.13675
D39	-0.95428	-0.00083	0.02193	-0.07708	-0.05519	-1.00946
D40	-3.01155	0.00062	0.02423	-0.06855	-0.04422	-3.05577
D41	1.10804	0.00176	0.02527	-0.06626	-0.04087	1.06717
D42	-3.10722	0.00062	0.00537	0.00843	0.01379	-3.09343
D43	-0.01163	0.00011	0.00119	0.00762	0.00880	-0.00284
D44	0.00690	-0.00003	0.00183	-0.00926	-0.00741	-0.00052
D45	3.10248	-0.00054	-0.00234	-0.01007	-0.01240	3.09008
D46	-2.73962	0.00005	0.00105	-0.00319	-0.00214	-2.74177
D47	-0.03505	-0.00040	0.00001	-0.00333	-0.00333	-0.03837
D48	-0.00290	-0.00035	-0.00236	-0.00354	-0.00592	-0.00881
D49	2.70168	-0.00079	-0.00340	-0.00368	-0.00710	2.69458
D50	0.69046	0.00025	-0.00211	-0.00344	-0.00547	0.68498
D51	-1.68988	0.00087	-0.00107	-0.00183	-0.00281	-1.69270
D52	2.17685	0.00062	-0.01508	0.05147	0.03642	2.21327
D53	-0.21330	0.00112	-0.01564	0.05534	0.03974	-0.17356
D54	2.55008	0.00013	-0.00005	-0.00080	-0.00085	2.54923
D55	-1.65309	0.00018	0.00030	-0.00061	-0.00031	-1.65340
D56	0.43890	0.00023	0.00029	0.00021	0.00049	0.43939
D57	1.33584	-0.00029	0.00080	-0.00373	-0.00293	1.33291
D58	-2.86732	-0.00025	0.00114	-0.00354	-0.00240	-2.86972
D59	-0.77534	-0.00020	0.00113	-0.00272	-0.00159	-0.77693
D60	-1.02539	-0.00002	-0.00037	-0.00016	-0.00052	-1.02591
D61	1.05463	0.00003	-0.00002	0.00003	0.00002	1.05465
D62	-3.13657	0.00008	-0.00003	0.00086	0.00082	-3.13574
D63	1.45488	0.00121	0.03622	-0.01530	0.02087	1.47575
D64	-2.93094	-0.00078	0.04545	-0.06761	-0.02210	-2.95304
D65	2.39580	0.00148	-0.02522	0.11033	0.08497	2.48077
D66	-0.67116	-0.00228	-0.08005	0.08730	0.00738	-0.66378

D67	-1.82268	0.00296	-0.03197	0.12911	0.09698	-1.72570
D68	1.39354	-0.00080	-0.08680	0.10607	0.01939	1.41294
D69	0.19273	0.00234	-0.02273	0.11182	0.08897	0.28170
D70	-2.87423	-0.00142	-0.07756	0.08879	0.01138	-2.86284
D71	2.80991	0.00205	0.04760	0.04356	0.09157	2.90148
D72	-0.25992	-0.00062	-0.00649	0.02372	0.01683	-0.24309
D73	-1.59158	0.00176	0.06552	-0.08290	-0.01738	-1.60896

Item	Value	Threshold	Converged?
Maximum Force	0.015828	0.000450	NO
RMS Force	0.002733	0.000300	NO
Maximum Displacement	0.596837	0.001800	NO
RMS Displacement	0.165510	0.001200	NO

Predicted change in Energy=-2.911811D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.816720	1.390725	1.417195
2	6	0	-1.605991	0.295785	1.586856
3	7	0	-2.645751	0.406206	0.675457
4	6	0	-2.476605	1.534879	-0.031998
5	7	0	-1.365006	2.144570	0.389654
6	6	0	-0.858690	3.446422	-0.083671
7	1	0	0.124716	1.649733	1.865559
8	1	0	-1.481893	-0.549061	2.237267
9	1	0	-1.725908	4.043812	-0.369299
10	1	0	-0.382001	3.931836	0.765554
11	35	0	-0.454502	-2.361157	0.450806
12	1	0	-3.137664	1.890650	-0.803122
13	6	0	-3.718256	-0.508114	0.470931
14	6	0	-4.116305	-1.378408	1.385137
15	1	0	-4.146380	-0.450225	-0.520894
16	1	0	-4.908826	-2.074139	1.146053
17	1	0	-3.653350	-1.462560	2.359210
18	6	0	3.195041	-0.806853	0.383309
19	6	0	4.216731	-0.389126	1.353392
20	8	0	3.133050	0.502493	1.007878
21	1	0	3.435165	-0.773845	-0.675252
22	1	0	2.387181	-1.476863	0.667280
23	1	0	4.120861	-0.774418	2.366796
24	6	0	5.599291	0.037277	0.944346

25	1	0	5.979715	0.819855	1.607207
26	1	0	6.283990	-0.814468	1.002834
27	1	0	5.603130	0.414612	-0.080511
28	6	0	0.099165	3.342971	-1.277011
29	1	0	0.419478	4.360202	-1.525021
30	1	0	-0.388432	2.937271	-2.162892
31	6	0	1.356148	2.525581	-1.016429
32	8	0	1.858645	1.797488	-1.831025
33	8	0	1.833673	2.719113	0.225377
34	1	0	2.499373	2.019469	0.423015

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.360378	0.000000			
3	N	2.205631	1.387062	0.000000		
4	C	2.208202	2.216757	1.342761	0.000000	
5	N	1.387350	2.215711	2.178050	1.336101	0.000000
6	C	2.545634	3.643574	3.607322	2.504858	1.474860
7	H	1.074438	2.214994	3.261623	3.221922	2.154630
8	H	2.208561	1.073405	2.169412	3.237564	3.268483
9	H	3.325215	4.229495	3.894843	2.640466	2.076868
10	H	2.659109	3.923462	4.190793	3.281594	2.074107
11	Br	3.891237	3.110607	3.536996	4.416004	4.597209
12	H	3.250617	3.256011	2.152150	1.076199	2.151629
13	C	3.594429	2.520556	1.424107	2.443043	3.546988
14	C	4.307712	3.024117	2.418889	3.630996	4.579521
15	H	4.269886	3.384186	2.101576	2.639661	3.911279
16	H	5.368811	4.088956	3.390440	4.508716	5.561323
17	H	4.132202	2.807131	2.709717	4.010891	4.703940
18	C	4.689616	5.070922	5.972580	6.150102	5.431847
19	C	5.339248	5.867512	6.941599	7.100834	6.205174
20	O	4.069052	4.778750	5.789155	5.797878	4.828159
21	H	5.209821	5.628010	6.339912	6.379107	5.717763
22	H	4.364678	4.464675	5.373678	5.763331	5.222141
23	H	5.474422	5.877965	7.074004	7.390103	6.521067
24	C	6.574239	7.238491	8.257671	8.271406	7.297246
25	H	6.823015	7.603816	8.685501	8.643356	7.561894
26	H	7.446789	7.989090	9.018730	9.128983	8.224295
27	H	6.664112	7.400382	8.283453	8.157172	7.195048
28	C	3.450921	4.516042	4.468924	3.384353	2.521454
29	H	4.359198	5.505069	5.465511	4.312640	3.429196
30	H	3.923297	4.745578	4.422443	3.296646	2.845622
31	C	3.454241	4.530271	4.834194	4.079288	3.086571

32	O	4.227762	5.093204	5.339260	4.701047	3.929860
33	O	3.195251	4.422379	5.061359	4.477404	3.254018
34	H	3.518549	4.602133	5.398022	5.020181	3.866547

		6	7	8	9	10
6	C	0.000000				
7	H	2.827486	0.000000			
8	H	4.662512	2.748464	0.000000		
9	H	1.091112	3.761784	5.286607	0.000000	
10	H	1.088138	2.583557	4.842947	1.762532	0.000000
11	Br	5.846110	4.292348	2.744206	6.581237	6.301276
12	H	2.851624	4.221732	4.235296	2.611008	3.771057
13	C	4.911523	4.622740	2.850077	5.039392	5.561525
14	C	6.004035	5.233230	2.890340	6.180009	6.521319
15	H	5.117024	5.324213	3.836237	5.106666	5.918443
16	H	6.956466	6.302496	3.906467	7.060920	7.530516
17	H	6.154339	4.919739	2.358935	6.440491	6.506994
18	C	5.894163	4.202235	5.037592	6.950620	5.949497
19	C	6.521999	4.600418	5.768980	7.611410	6.337554
20	O	5.078601	3.331944	4.890282	6.168228	4.916777
21	H	6.049613	4.825819	5.719332	7.066832	6.228171
22	H	5.944606	4.041067	4.277313	6.962029	6.077174
23	H	6.972533	4.700736	5.608780	8.055201	6.707352
24	C	7.374593	5.780971	7.222092	8.452014	7.139707
25	H	7.518093	5.919161	7.612260	8.583538	7.131917
26	H	8.387703	6.689786	7.867859	9.468057	8.186522
27	H	7.137717	5.943545	7.516536	8.183477	6.993459
28	C	1.533705	3.569798	5.477025	2.155462	2.179532
29	H	2.132181	4.350811	6.470771	2.457332	2.464265
30	H	2.191698	4.260223	5.719403	2.496047	3.092734
31	C	2.573615	3.254135	5.300419	3.496123	2.859053
32	O	3.627139	4.085717	5.763375	4.475672	4.039574
33	O	2.805942	2.598905	5.071651	3.844358	2.582964
34	H	3.683682	2.802969	5.073394	4.751708	3.475168

		11	12	13	14	15
11	Br	0.000000				
12	H	5.181656	0.000000			
13	C	3.753167	2.777475	0.000000		
14	C	3.904813	4.053758	1.323491	0.000000	
15	H	4.269172	2.564539	1.081831	2.120231	0.000000
16	H	4.517383	4.759816	2.079827	1.081338	2.448904
17	H	3.831724	4.637919	2.116785	1.081770	3.092393
18	C	3.967314	6.984790	6.920304	7.401764	7.405487
19	C	5.150144	7.995940	7.984793	8.391613	8.570782
20	O	4.623997	6.672972	6.946225	7.498883	7.498995

21	H	4.349377	7.093516	7.249537	7.850822	7.590019
22	H	2.983957	6.635219	6.184933	6.543725	6.719610
23	H	5.207945	8.356862	8.069509	8.317413	8.763055
24	C	6.530274	9.100716	9.345495	9.828086	9.867254
25	H	7.270162	9.491201	9.854201	10.334955	10.424957
26	H	6.935723	9.967282	10.021063	10.422587	10.547372
27	H	6.684466	8.893949	9.383163	9.991519	9.797695
28	C	5.985730	3.579228	5.697268	6.866487	5.743231
29	H	7.060056	4.390112	6.693666	7.872356	6.707872
30	H	5.908394	3.240782	5.467672	6.716445	5.319160
31	C	5.414004	4.543455	6.096321	7.138375	6.275253
32	O	5.277474	5.101800	6.458841	7.491998	6.544386
33	O	5.576352	5.143769	6.426447	7.316896	6.809014
34	H	5.283562	5.770285	6.711921	7.499229	7.152369

		16	17	18	19	20
16	H	0.000000				
17	H	1.849864	0.000000			
18	C	8.237745	7.157834	0.000000		
19	C	9.282136	8.006379	1.469493	0.000000	
20	O	8.445702	7.193243	1.452004	1.445243	0.000000
21	H	8.638872	7.741404	1.085956	2.207771	2.133832
22	H	7.336053	6.273025	1.087286	2.236331	2.142469
23	H	9.204060	7.804611	2.189158	1.088406	2.110196
24	C	10.720042	9.479595	2.609164	1.503533	2.510540
25	H	11.276001	9.928286	3.449423	2.152712	2.926332
26	H	11.264387	10.050398	3.150473	2.139479	3.415089
27	H	10.871962	9.754918	2.739708	2.150389	2.700668
28	C	7.765069	7.099056	5.437108	6.148326	4.742730
29	H	8.770758	8.098131	6.167976	6.727592	5.353594
30	H	7.516470	7.104056	5.774330	6.681070	5.327548
31	C	8.067444	7.238458	4.055356	4.721705	3.368692
32	O	8.345727	7.652978	3.670399	4.525745	3.370534
33	O	8.323714	7.221292	3.782949	4.075847	2.685906
34	H	8.494811	7.330032	2.910950	3.101007	1.744944

		21	22	23	24	25
21	H	0.000000				
22	H	1.842525	0.000000			
23	H	3.118370	2.527336	0.000000		
24	C	2.822137	3.561887	2.206348	0.000000	
25	H	3.771503	4.366312	2.563986	1.093863	0.000000
26	H	3.306573	3.966924	2.557562	1.094396	1.768859
27	H	2.542876	3.805154	3.098423	1.092121	1.776072
28	C	5.332840	5.678563	6.812067	6.790687	7.018953
29	H	6.014558	6.538299	7.430396	7.184421	7.298023

30	H	5.532211	5.932831	7.391105	7.342869	7.697429
31	C	3.914707	4.462898	5.475385	5.295334	5.583041
32	O	3.230013	4.152380	5.417936	4.979304	5.455313
33	O	3.946729	4.255333	4.692724	4.678572	4.765113
34	H	3.143963	3.506649	3.770055	3.716230	3.867062

		26	27	28	29	30
26	H	0.000000				
27	H	1.774217	0.000000			
28	C	7.793205	6.348269	0.000000		
29	H	8.219474	6.672670	1.094928	0.000000	
30	H	8.283634	6.826341	1.089554	1.756226	0.000000
31	C	6.286253	4.834148	1.521852	2.121756	2.127775
32	O	5.868284	4.358648	2.406494	2.955053	2.541377
33	O	5.735499	4.428667	2.378001	2.785141	3.269431
34	H	4.763477	3.530214	3.225328	3.687795	3.983553

		31	32	33	34
31	C	0.000000			
32	O	1.202576	0.000000		
33	O	1.344458	2.253621	0.000000	
34	H	1.906597	2.353828	0.985758	0.000000

Stoichiometry C11H17BrN2O3
Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.817280	0.979896	1.284492
2	6	0	-1.803546	0.048845	1.179357
3	7	0	-2.759731	0.573048	0.322116
4	6	0	-2.349994	1.784786	-0.086311
5	7	0	-1.165957	2.049864	0.473114
6	6	0	-0.404358	3.305234	0.334467
7	1	0	0.133289	0.937574	1.783535
8	1	0	-1.869996	-0.935420	1.602447
9	1	0	-1.130698	4.108866	0.203579
10	1	0	0.112972	3.470968	1.277306
11	35	0	-1.112892	-2.426310	-0.573491
12	1	0	-2.895641	2.435918	-0.746992
13	6	0	-3.972442	-0.041654	-0.101621

14	6	0	-4.568708	-1.013436	0.570490
15	1	0	-4.334276	0.334524	-1.049209
16	1	0	-5.464352	-1.465604	0.167179
17	1	0	-4.176722	-1.417012	1.494449
18	6	0	2.760934	-1.631942	-0.254074
19	6	0	3.794749	-1.664342	0.789758
20	8	0	2.913538	-0.524808	0.672901
21	1	0	3.053494	-1.391645	-1.271899
22	1	0	1.829934	-2.182690	-0.144048
23	1	0	3.580439	-2.256610	1.677405
24	6	0	5.250474	-1.425556	0.499142
25	1	0	5.737506	-0.913734	1.334231
26	1	0	5.761301	-2.381421	0.347221
27	1	0	5.373533	-0.820432	-0.401640
28	6	0	0.573680	3.310386	-0.846917
29	1	0	1.089022	4.276407	-0.837214
30	1	0	0.062221	3.231415	-1.805719
31	6	0	1.642841	2.228660	-0.794011
32	8	0	2.039711	1.635726	-1.762057
33	8	0	2.087906	2.021977	0.457694
34	1	0	2.601687	1.180945	0.478002

Rotational constants (GHZ): 0.3659357 0.2435028 0.1633775

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 538 symmetry adapted cartesian basis functions of A symmetry.

There are 519 symmetry adapted basis functions of A symmetry.

519 basis functions, 823 primitive gaussians, 538 cartesian basis functions

78 alpha electrons 78 beta electrons

nuclear repulsion energy 1581.5145582394 Hartrees.

NAtoms= 34 NActive= 34 NUniq= 34 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 519 RedAO= T EigKep= 2.93D-06 NBF= 519

NBsUse= 519 1.00D-06 EigRej= -1.00D+00 NBFU= 519

Initial guess from the checkpoint file: "./coohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.998178 -0.000469 0.004229 -0.060186 Ang= -6.92 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3338.89326358 A.U. after 14 cycles
NFock= 14 Conv=0.25D-08 -V/T= 2.0019
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000184043	0.000528782	-0.000908210
2	6	0.000215503	0.000661331	-0.000198249
3	7	-0.001375432	0.001719466	0.002584955
4	6	0.002402636	-0.001336182	-0.002928077
5	7	-0.000372646	0.001493581	0.003948799
6	6	-0.001951199	-0.000526418	-0.004607297
7	1	-0.000181364	0.000645276	0.000598906
8	1	-0.000440428	-0.001754711	-0.002012571
9	1	-0.000455094	0.000470191	0.000645885
10	1	0.000898656	-0.000798139	-0.000211149
11	35	0.001215999	-0.000566535	0.000705851
12	1	0.000161917	-0.000117675	-0.000081028
13	6	0.000425040	0.000847734	0.000551920
14	6	0.000049167	-0.001355200	-0.000170103
15	1	-0.000414588	0.000526728	0.000346398
16	1	0.000202751	-0.000055436	0.000054213
17	1	-0.000150416	-0.000045211	-0.000119445
18	6	-0.000623072	-0.001140278	0.000190284
19	6	-0.000523434	-0.000256630	-0.000957128
20	8	-0.000570288	0.002335090	0.001851193
21	1	-0.000111665	0.000144971	-0.000060766
22	1	-0.000417985	0.000593359	-0.000698558
23	1	0.000131550	-0.000054506	-0.000025781

24	6	0.000342533	-0.000223334	-0.000095270
25	1	0.000000089	0.000098863	0.000039251
26	1	0.000056884	0.000052379	-0.000021118
27	1	-0.000037606	0.000046572	-0.000009029
28	6	0.002128692	0.001476074	0.002591462
29	1	-0.000273688	0.000924640	-0.000244962
30	1	-0.000567535	-0.001291033	0.000291055
31	6	0.000673116	-0.001731605	0.001170530
32	8	-0.000154762	0.000621262	-0.001940200
33	8	-0.004427261	0.001215790	-0.001098863
34	1	0.004327978	-0.003149198	0.000817099

Cartesian Forces: Max 0.004607297 RMS 0.001327238

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.006826413 RMS 0.001222576
Search for a local minimum.
Step number 8 out of a maximum of 175
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 7 8
DE= -3.02D-03 DEPred=-2.91D-03 R= 1.04D+00
TightC=F SS= 1.41D+00 RLast= 3.79D-01 DXNew= 7.1352D-01 1.1384D+00
Trust test= 1.04D+00 RLast= 3.79D-01 DXMaxT set to 7.14D-01
ITU= 1 0 1 0 -1 0 1 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00211	0.00240	0.00314	0.00698	0.00763
Eigenvalues ---	0.00953	0.01195	0.01428	0.01485	0.01618
Eigenvalues ---	0.01736	0.01850	0.02031	0.02181	0.02260
Eigenvalues ---	0.02270	0.02387	0.02470	0.02607	0.02976
Eigenvalues ---	0.03050	0.03070	0.03202	0.03680	0.03823
Eigenvalues ---	0.04456	0.04697	0.04986	0.05300	0.05516
Eigenvalues ---	0.05757	0.05893	0.07937	0.09588	0.09754
Eigenvalues ---	0.11924	0.12593	0.12708	0.13213	0.13750
Eigenvalues ---	0.15350	0.15796	0.15877	0.15995	0.15999
Eigenvalues ---	0.16000	0.16000	0.16003	0.16008	0.16244
Eigenvalues ---	0.16863	0.18109	0.18993	0.21987	0.22280
Eigenvalues ---	0.22783	0.23503	0.23710	0.24517	0.25110
Eigenvalues ---	0.25740	0.26868	0.28641	0.29229	0.30021
Eigenvalues ---	0.31850	0.32418	0.34497	0.34553	0.34612

Eigenvalues --- 0.34764 0.34881 0.34889 0.34949 0.35008
Eigenvalues --- 0.35107 0.35531 0.35699 0.35763 0.36532
Eigenvalues --- 0.36609 0.36890 0.36970 0.37292 0.37771
Eigenvalues --- 0.41079 0.42325 0.45589 0.48982 0.51949
Eigenvalues --- 0.53034 0.55522 0.56097 0.60433 0.89819
Eigenvalues --- 0.97769
RFO step: Lambda=-2.64072606D-03 EMin= 2.11441292D-03
Quartic linear search produced a step of 0.12539.
Iteration 1 RMS(Cart)= 0.13476242 RMS(Int)= 0.00573287
Iteration 2 RMS(Cart)= 0.01269231 RMS(Int)= 0.00014202
Iteration 3 RMS(Cart)= 0.00004121 RMS(Int)= 0.00014115
Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00014115

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.57074	-0.00003	-0.00048	0.00437	0.00388	2.57463
R2	2.62171	-0.00066	-0.00025	0.00173	0.00151	2.62323
R3	2.03039	0.00025	0.00005	0.00015	0.00020	2.03060
R4	2.62117	-0.00049	-0.00113	-0.00455	-0.00572	2.61545
R5	2.02844	0.00112	-0.00108	0.00368	0.00260	2.03104
R6	2.53745	0.00076	0.00011	-0.00085	-0.00076	2.53669
R7	2.69117	-0.00012	-0.00014	-0.00146	-0.00159	2.68958
R8	2.52486	-0.00056	0.00027	-0.00088	-0.00059	2.52428
R9	2.03372	-0.00008	-0.00055	-0.00035	-0.00090	2.03282
R10	2.78708	-0.00083	-0.00083	0.00326	0.00243	2.78951
R11	2.06190	0.00045	0.00036	0.00150	0.00186	2.06376
R12	2.05628	-0.00012	-0.00054	-0.00201	-0.00255	2.05373
R13	2.89828	-0.00144	0.00001	-0.00105	-0.00104	2.89724
R14	5.18580	0.00037	-0.00298	-0.00581	-0.00880	5.17700
R15	2.50103	0.00075	-0.00054	0.00100	0.00046	2.50149
R16	2.04436	-0.00012	-0.00048	-0.00029	-0.00076	2.04360
R17	2.04343	-0.00012	-0.00002	-0.00020	-0.00022	2.04321
R18	2.04425	-0.00018	-0.00011	-0.00071	-0.00082	2.04343
R19	2.77694	0.00067	-0.00035	-0.00031	-0.00066	2.77628
R20	2.74389	0.00003	0.00087	0.00427	0.00514	2.74904
R21	2.05216	0.00004	-0.00039	0.00018	-0.00021	2.05195
R22	2.05467	-0.00024	-0.00031	-0.00132	-0.00163	2.05304
R23	2.73111	-0.00022	0.00025	-0.00057	-0.00033	2.73078
R24	2.05679	-0.00001	-0.00003	0.00028	0.00025	2.05704
R25	2.84127	0.00034	0.00008	0.00098	0.00106	2.84233
R26	3.29747	-0.00194	-0.00124	-0.02348	-0.02472	3.27275
R27	2.06710	0.00010	0.00018	0.00064	0.00082	2.06792
R28	2.06811	-0.00001	0.00007	0.00012	0.00019	2.06830
R29	2.06381	0.00002	0.00009	0.00003	0.00012	2.06393
R30	2.06911	0.00084	0.00112	0.00320	0.00432	2.07344

R31	2.05896	0.00049	0.00159	0.00161	0.00321	2.06217
R32	2.87588	-0.00046	-0.00221	0.00237	0.00016	2.87605
R33	2.27254	0.00087	-0.00217	0.00082	-0.00135	2.27119
R34	2.54066	-0.00074	0.00085	0.00352	0.00437	2.54502
R35	1.86281	0.00305	0.00332	0.00613	0.00945	1.87227
A1	1.87594	0.00033	-0.00061	-0.00180	-0.00236	1.87358
A2	2.27884	-0.00004	-0.00003	0.00170	0.00163	2.28047
A3	2.12277	-0.00033	0.00061	0.00025	0.00084	2.12362
A4	1.86387	-0.00039	0.00095	0.00120	0.00205	1.86592
A5	2.26789	-0.00003	0.00122	0.00836	0.00950	2.27739
A6	2.15013	0.00045	-0.00232	-0.00933	-0.01172	2.13840
A7	1.89513	0.00025	-0.00008	-0.00038	-0.00066	1.89447
A8	2.22408	-0.00034	-0.00134	-0.00075	-0.00225	2.22183
A9	2.16382	0.00008	0.00142	0.00056	0.00183	2.16564
A10	1.89874	-0.00045	-0.00040	0.00248	0.00206	1.90080
A11	2.18708	0.00024	0.00007	-0.00191	-0.00191	2.18518
A12	2.19730	0.00020	0.00054	-0.00064	-0.00016	2.19714
A13	1.89082	0.00025	0.00036	-0.00125	-0.00114	1.88968
A14	2.19156	-0.00212	-0.00093	0.01676	0.01549	2.20705
A15	2.19830	0.00194	0.00083	-0.01270	-0.01223	2.18607
A16	1.86966	0.00218	-0.00149	-0.00838	-0.00999	1.85967
A17	1.86888	-0.00081	-0.00019	-0.01051	-0.01065	1.85824
A18	1.98730	-0.00236	0.00098	0.02498	0.02597	2.01327
A19	1.88415	-0.00015	0.00008	0.00448	0.00450	1.88865
A20	1.90671	0.00064	-0.00086	0.00279	0.00192	1.90863
A21	1.94307	0.00062	0.00137	-0.01406	-0.01261	1.93046
A22	1.74016	0.00499	0.00038	0.05458	0.05495	1.79511
A23	2.15254	0.00102	-0.00044	0.00502	0.00452	2.15706
A24	1.97724	-0.00055	0.00062	-0.00308	-0.00252	1.97472
A25	2.15250	-0.00049	-0.00026	-0.00260	-0.00292	2.14958
A26	2.08379	0.00003	0.00020	0.00005	0.00025	2.08404
A27	2.14650	0.00009	-0.00051	0.00038	-0.00013	2.14637
A28	2.05183	-0.00012	0.00029	-0.00049	-0.00021	2.05162
A29	2.07273	0.00024	-0.00019	-0.00394	-0.00391	2.06881
A30	2.11688	0.00035	0.00067	0.01259	0.01299	2.12987
A31	1.98376	0.00013	-0.00027	-0.00511	-0.00538	1.97838
A32	1.99502	-0.00021	0.00082	-0.00439	-0.00358	1.99144
A33	2.02373	-0.00035	-0.00061	-0.00233	-0.00301	2.02072
A34	2.04068	0.00056	0.00060	0.00402	0.00471	2.04540
A35	2.14165	-0.00048	-0.00043	-0.00277	-0.00329	2.13836
A36	1.95513	0.00003	0.00009	-0.00114	-0.00100	1.95413
A37	2.03699	0.00014	-0.00017	0.00064	0.00042	2.03741
A38	2.02050	-0.00010	-0.00021	-0.00133	-0.00155	2.01895
A39	2.28534	-0.00093	-0.00208	-0.02725	-0.02901	2.25633

A40	2.66544	0.00055	0.00029	0.00868	0.00840	2.67383
A41	1.93674	-0.00005	-0.00018	0.00000	-0.00018	1.93656
A42	1.91776	0.00014	0.00026	0.00102	0.00128	1.91903
A43	1.93534	-0.00006	-0.00014	-0.00108	-0.00122	1.93411
A44	1.88266	-0.00002	0.00001	0.00002	0.00004	1.88269
A45	1.89679	0.00001	0.00004	-0.00033	-0.00030	1.89650
A46	1.89321	-0.00001	0.00002	0.00040	0.00042	1.89362
A47	1.87159	-0.00047	-0.00033	0.00623	0.00559	1.87718
A48	1.95870	0.00009	-0.00127	-0.02067	-0.02171	1.93700
A49	2.00296	-0.00043	0.00304	0.03779	0.04076	2.04372
A50	1.86783	0.00032	-0.00036	-0.00153	-0.00198	1.86585
A51	1.87145	0.00221	0.00016	-0.00606	-0.00641	1.86504
A52	1.88479	-0.00153	-0.00134	-0.01714	-0.01825	1.86654
A53	2.15835	-0.00222	-0.00558	-0.00020	-0.00610	2.15225
A54	1.95433	0.00097	0.00283	-0.01478	-0.01228	1.94205
A55	2.17050	0.00125	0.00306	0.01490	0.01763	2.18813
A56	1.89957	-0.00299	0.00074	0.04261	0.04334	1.94291
A57	2.76377	-0.00683	-0.00178	0.02777	0.02599	2.78976
D1	-0.01977	-0.00084	0.00440	-0.00582	-0.00139	-0.02115
D2	3.06723	-0.00026	-0.00388	-0.00132	-0.00532	3.06191
D3	-3.04628	-0.00039	0.00471	-0.00740	-0.00253	-3.04881
D4	0.04072	0.00019	-0.00357	-0.00290	-0.00646	0.03426
D5	0.02335	0.00052	-0.00093	-0.01252	-0.01345	0.00990
D6	3.09238	0.00151	0.00232	0.02729	0.03003	3.12241
D7	3.06232	0.00013	-0.00124	-0.01099	-0.01234	3.04998
D8	-0.15183	0.00113	0.00201	0.02883	0.03114	-0.12070
D9	0.00944	0.00088	-0.00636	0.02208	0.01565	0.02509
D10	3.13206	0.00023	-0.00692	-0.01066	-0.01753	3.11453
D11	-3.08214	0.00036	0.00125	0.01730	0.01842	-3.06372
D12	0.04048	-0.00029	0.00069	-0.01544	-0.01476	0.02572
D13	-1.73680	0.00251	0.02116	0.01236	0.03353	-1.70327
D14	1.34233	0.00315	0.01167	0.01792	0.02957	1.37191
D15	0.00513	-0.00057	0.00592	-0.03026	-0.02435	-0.01922
D16	-3.12510	-0.00070	-0.00019	-0.02353	-0.02359	3.13449
D17	-3.11829	0.00005	0.00647	0.00110	0.00757	-3.11072
D18	0.03466	-0.00007	0.00037	0.00784	0.00833	0.04299
D19	0.38564	-0.00070	-0.00678	-0.07929	-0.08611	0.29953
D20	-2.71168	-0.00042	-0.00435	-0.06292	-0.06729	-2.77897
D21	-2.77764	-0.00144	-0.00743	-0.11673	-0.12413	-2.90177
D22	0.40823	-0.00116	-0.00500	-0.10035	-0.10531	0.30291
D23	-0.01753	0.00004	-0.00312	0.02649	0.02337	0.00585
D24	-3.08621	-0.00074	-0.00626	-0.01508	-0.02089	-3.10710
D25	3.11263	0.00017	0.00301	0.01969	0.02259	3.13522
D26	0.04395	-0.00061	-0.00013	-0.02187	-0.02167	0.02227

D27	-2.52501	0.00060	0.00200	0.04033	0.04225	-2.48276
D28	-0.50741	0.00109	0.00126	0.03627	0.03755	-0.46986
D29	1.64816	-0.00027	0.00351	0.02710	0.03060	1.67876
D30	0.53147	0.00165	0.00576	0.08782	0.09354	0.62501
D31	2.54907	0.00215	0.00502	0.08375	0.08884	2.63791
D32	-1.57854	0.00078	0.00727	0.07459	0.08189	-1.49666
D33	-3.12420	0.00180	-0.00838	0.04280	0.03435	-3.08985
D34	1.11268	0.00164	-0.00700	0.05236	0.04536	1.15804
D35	-1.04756	0.00399	-0.00658	0.06258	0.05621	-0.99135
D36	1.06980	0.00010	-0.00652	0.03516	0.02848	1.09828
D37	-0.97651	-0.00005	-0.00514	0.04472	0.03950	-0.93701
D38	-3.13675	0.00229	-0.00472	0.05494	0.05034	-3.08641
D39	-1.00946	-0.00050	-0.00692	0.03651	0.02946	-0.98001
D40	-3.05577	-0.00066	-0.00555	0.04607	0.04047	-3.01530
D41	1.06717	0.00169	-0.00512	0.05629	0.05132	1.11849
D42	-3.09343	0.00029	0.00173	0.01182	0.01354	-3.07989
D43	-0.00284	0.00017	0.00110	0.01045	0.01155	0.00871
D44	-0.00052	-0.00001	-0.00093	-0.00617	-0.00709	-0.00760
D45	3.09008	-0.00013	-0.00155	-0.00753	-0.00908	3.08100
D46	-2.74177	-0.00033	-0.00027	-0.00746	-0.00779	-2.74955
D47	-0.03837	-0.00040	-0.00042	-0.00790	-0.00838	-0.04676
D48	-0.00881	0.00028	-0.00074	0.00955	0.00878	-0.00003
D49	2.69458	0.00020	-0.00089	0.00911	0.00819	2.70277
D50	0.68498	0.00048	-0.00069	0.00326	0.00286	0.68784
D51	-1.69270	0.00110	-0.00035	0.01742	0.01727	-1.67542
D52	2.21327	0.00051	0.00457	0.05251	0.05719	2.27046
D53	-0.17356	0.00047	0.00498	0.05524	0.06034	-0.11322
D54	2.54923	-0.00012	-0.00011	-0.00039	-0.00051	2.54871
D55	-1.65340	-0.00009	-0.00004	0.00030	0.00024	-1.65316
D56	0.43939	-0.00005	0.00006	0.00076	0.00080	0.44020
D57	1.33291	0.00006	-0.00037	-0.00229	-0.00263	1.33028
D58	-2.86972	0.00009	-0.00030	-0.00160	-0.00188	-2.87160
D59	-0.77693	0.00013	-0.00020	-0.00114	-0.00131	-0.77824
D60	-1.02591	-0.00004	-0.00007	0.00042	0.00036	-1.02555
D61	1.05465	-0.00001	0.00000	0.00111	0.00111	1.05576
D62	-3.13574	0.00003	0.00010	0.00157	0.00168	-3.13407
D63	1.47575	-0.00108	0.00262	-0.11158	-0.10899	1.36676
D64	-2.95304	-0.00154	-0.00277	-0.16322	-0.16596	-3.11900
D65	2.48077	-0.00079	0.01065	0.10990	0.12036	2.60114
D66	-0.66378	0.00081	0.00093	0.08259	0.08361	-0.58017
D67	-1.72570	-0.00009	0.01216	0.13655	0.14855	-1.57715
D68	1.41294	0.00150	0.00243	0.10925	0.11179	1.52473
D69	0.28170	0.00064	0.01116	0.12327	0.13437	0.41607
D70	-2.86284	0.00223	0.00143	0.09596	0.09761	-2.76524

D71	2.90148	-0.00378	0.01148	-0.00737	0.00450	2.90598
D72	-0.24309	-0.00218	0.00211	-0.03494	-0.03322	-0.27631
D73	-1.60896	-0.00100	-0.00218	-0.08271	-0.08489	-1.69385

Item	Value	Threshold	Converged?
Maximum Force	0.006826	0.000450	NO
RMS Force	0.001223	0.000300	NO
Maximum Displacement	0.771793	0.001800	NO
RMS Displacement	0.138096	0.001200	NO

Predicted change in Energy=-1.682598D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.909398	1.511614	1.522639
2	6	0	-1.675980	0.394637	1.667342
3	7	0	-2.636941	0.434197	0.672083
4	6	0	-2.434151	1.531667	-0.073815
5	7	0	-1.394073	2.206672	0.423117
6	6	0	-0.885316	3.491291	-0.096425
7	1	0	-0.018995	1.821350	2.038288
8	1	0	-1.586668	-0.429115	2.351894
9	1	0	-1.756968	4.060603	-0.426238
10	1	0	-0.440149	4.010591	0.748124
11	35	0	-0.287743	-2.323808	0.859222
12	1	0	-3.024974	1.820806	-0.924995
13	6	0	-3.643692	-0.536064	0.406141
14	6	0	-4.012571	-1.465376	1.273652
15	1	0	-4.035086	-0.477576	-0.600275
16	1	0	-4.744520	-2.205054	0.980114
17	1	0	-3.579711	-1.554307	2.260572
18	6	0	3.120462	-0.849881	0.463609
19	6	0	4.223143	-0.431369	1.339579
20	8	0	3.123616	0.468956	1.077521
21	1	0	3.273593	-0.824751	-0.611092
22	1	0	2.322459	-1.499542	0.812093
23	1	0	4.212249	-0.800037	2.363725
24	6	0	5.570363	-0.027224	0.806693
25	1	0	6.014523	0.760791	1.422515
26	1	0	6.249433	-0.885507	0.818374
27	1	0	5.488604	0.335972	-0.220085
28	6	0	0.116781	3.381588	-1.251558

29	1	0	0.448747	4.397611	-1.499299
30	1	0	-0.360313	2.976781	-2.145618
31	6	0	1.370878	2.555238	-1.005228
32	8	0	1.939839	1.945056	-1.870351
33	8	0	1.770451	2.644244	0.277817
34	1	0	2.445180	1.951658	0.493852

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.362433	0.000000			
3	N	2.206507	1.384034	0.000000		
4	C	2.207700	2.213434	1.342359	0.000000	
5	N	1.388151	2.216086	2.179076	1.335791	0.000000
6	C	2.557551	3.650382	3.606192	2.497905	1.476145
7	H	1.074546	2.217817	3.262568	3.221471	2.155943
8	H	2.216481	1.074782	2.161052	3.232176	3.271796
9	H	3.318711	4.222433	3.889921	2.641647	2.071270
10	H	2.657998	3.930313	4.197889	3.285833	2.066331
11	Br	3.941706	3.157564	3.627719	4.510246	4.683952
12	H	3.249949	3.251761	2.150329	1.075723	2.150845
13	C	3.593871	2.515695	1.423263	2.443124	3.547347
14	C	4.307452	3.012357	2.421285	3.645455	4.589540
15	H	4.270077	3.386476	2.098818	2.622443	3.902238
16	H	5.368064	4.080026	3.391522	4.517926	5.567681
17	H	4.132189	2.788278	2.714085	4.035456	4.722098
18	C	4.789361	5.099378	5.902543	6.067482	5.452081
19	C	5.491054	5.965683	6.946619	7.083133	6.273140
20	O	4.189328	4.836273	5.774911	5.774401	4.884405
21	H	5.244886	5.583587	6.177856	6.198364	5.660939
22	H	4.474018	4.506315	5.324903	5.709501	5.263073
23	H	5.681763	6.048425	7.162150	7.453395	6.651099
24	C	6.698352	7.309458	8.221367	8.202298	7.323988
25	H	6.965231	7.703107	8.690089	8.614718	7.614241
26	H	7.582285	8.072899	8.985024	9.057780	8.254756
27	H	6.734512	7.409257	8.174967	8.013809	7.161318
28	C	3.499431	4.544870	4.468836	3.364007	2.543157
29	H	4.393819	5.528642	5.472204	4.307754	3.448461
30	H	3.988022	4.789271	4.425744	3.268261	2.874044
31	C	3.560747	4.592839	4.834749	4.048886	3.131553
32	O	4.451787	5.290861	5.449181	4.746601	4.055047
33	O	3.164494	4.343892	4.946196	4.363502	3.197936
34	H	3.536275	4.559096	5.306826	4.930164	3.848364

	6	7	8	9	10

6	C	0.000000				
7	H	2.845384	0.000000			
8	H	4.675013	2.760533	0.000000		
9	H	1.092095	3.756154	5.282480	0.000000	
10	H	1.086789	2.575785	4.857734	1.765118	0.000000
11	Br	5.923321	4.317958	2.739551	6.676207	6.337207
12	H	2.838166	4.221013	4.227159	2.621696	3.778334
13	C	4.907219	4.621659	2.833503	5.038048	5.572406
14	C	6.018752	5.228373	2.849815	6.205950	6.559313
15	H	5.091838	5.326918	3.835675	5.080864	5.906386
16	H	6.964247	6.297797	3.873986	7.082496	7.564104
17	H	6.186538	4.911534	2.290549	6.486027	6.566006
18	C	5.933437	4.412627	5.089179	6.978110	6.031840
19	C	6.598918	4.853728	5.897347	7.684898	6.467389
20	O	5.155985	3.553596	4.961586	6.243502	5.035087
21	H	6.015781	4.986201	5.705958	7.014799	6.246590
22	H	6.001970	4.244324	4.335675	7.006454	6.164225
23	H	7.103028	4.988086	5.810780	8.187874	6.884557
24	C	7.407521	6.014564	7.332958	8.480580	7.241108
25	H	7.574337	6.156891	7.749693	8.643074	7.258016
26	H	8.420087	6.936026	7.997779	9.492920	8.290189
27	H	7.113240	6.135164	7.567028	8.149459	7.042043
28	C	1.533155	3.643606	5.514351	2.157116	2.168997
29	H	2.137567	4.401184	6.501684	2.475927	2.447617
30	H	2.177049	4.353916	5.773361	2.466086	3.073903
31	C	2.606248	3.425394	5.378077	3.519201	2.910690
32	O	3.676840	4.373761	5.991686	4.497486	4.097218
33	O	2.812586	2.641690	5.001758	3.865805	2.640993
34	H	3.716329	2.911086	5.037480	4.790852	3.553728

		11	12	13	14	15
11	Br	0.000000				
12	H	5.277659	0.000000			
13	C	3.829322	2.776611	0.000000		
14	C	3.844867	4.075339	1.323733	0.000000	
15	H	4.425074	2.531467	1.081427	2.118457	0.000000
16	H	4.459998	4.774288	2.080095	1.081221	2.446448
17	H	3.659640	4.674073	2.116560	1.081336	3.090496
18	C	3.734278	6.843039	6.771674	7.205218	7.243779
19	C	4.915300	7.920593	7.922712	8.300633	8.483131
20	O	4.414132	6.606264	6.874392	7.396301	7.413361
21	H	4.134261	6.838820	6.997638	7.553201	7.316928
22	H	2.737661	6.529718	6.057065	6.351913	6.592235
23	H	4.983507	8.370298	8.100471	8.323377	8.769710
24	C	6.292414	8.960680	9.236784	9.701493	9.718386

25	H	7.039220	9.399305	9.797753	10.272322	10.325690
26	H	6.693658	9.817234	9.907874	10.288453	10.389913
27	H	6.450234	8.670792	9.195185	9.785113	9.565933
28	C	6.096768	3.523252	5.677774	6.849912	5.705726
29	H	7.161181	4.363082	6.687294	7.871927	6.684343
30	H	6.093487	3.150653	5.443540	6.690527	5.274905
31	C	5.480172	4.457504	6.057559	7.095079	6.211794
32	O	5.534969	5.055541	6.520290	7.546322	6.571298
33	O	5.408857	5.012075	6.280427	7.164077	6.649891
34	H	5.087433	5.652683	6.578055	7.347568	7.006578

		16	17	18	19	20
16	H	0.000000				
17	H	1.849277	0.000000			
18	C	7.997576	6.972633	0.000000		
19	C	9.148452	7.936860	1.469143	0.000000	
20	O	8.310679	7.101252	1.454727	1.445068	0.000000
21	H	8.290194	7.466357	1.085847	2.204884	2.132507
22	H	7.104095	6.077556	1.086421	2.243176	2.141797
23	H	9.171269	7.829061	2.192014	1.088536	2.109452
24	C	10.543711	9.389867	2.607007	1.504095	2.511198
25	H	11.169108	9.905117	3.448094	2.153407	2.926010
26	H	11.074041	9.956872	3.149220	2.140969	3.416499
27	H	10.611980	9.589637	2.735284	2.150059	2.700858
28	C	7.734544	7.096630	5.465276	6.173722	4.790521
29	H	8.758579	8.111130	6.207032	6.754579	5.406408
30	H	7.472810	7.092939	5.793722	6.691050	5.368014
31	C	8.000004	7.215409	4.100410	4.749037	3.429651
32	O	8.368346	7.731461	3.827913	4.600492	3.502877
33	O	8.151917	7.084022	3.750461	4.074608	2.683739
34	H	8.319044	7.191133	2.881934	3.091152	1.731863

		21	22	23	24	25
21	H	0.000000				
22	H	1.839961	0.000000			
23	H	3.119491	2.543261	0.000000		
24	C	2.814483	3.566039	2.205916	0.000000	
25	H	3.763269	4.371849	2.563250	1.094295	0.000000
26	H	3.301922	3.974696	2.558425	1.094497	1.769313
27	H	2.531094	3.802497	3.097689	1.092186	1.776287
28	C	5.298014	5.740131	6.879617	6.752627	6.985887
29	H	6.003476	6.605281	7.490157	7.150365	7.262322
30	H	5.478293	5.998566	7.450292	7.274140	7.634181
31	C	3.898717	4.544161	5.539053	5.252413	5.538720
32	O	3.322117	4.382597	5.534147	4.923125	5.371081
33	O	3.883751	4.214395	4.709189	4.675018	4.782247

34	H	3.100905	3.468014	3.767066	3.712225	3.875667
		26	27	28	29	30
26	H	0.000000				
27	H	1.774618	0.000000			
28	C	7.752558	6.260687	0.000000		
29	H	8.181131	6.597989	1.097215	0.000000	
30	H	8.209218	6.700103	1.091251	1.758142	0.000000
31	C	6.242159	4.743127	1.521938	2.118672	2.115469
32	O	5.814975	4.231579	2.402097	2.894143	2.535927
33	O	5.728231	4.404621	2.370082	2.824772	3.244036
34	H	4.756802	3.518888	3.242314	3.733775	3.986034
		31	32	33	34	
31	C	0.000000				
32	O	1.201864	0.000000			
33	O	1.346768	2.265432	0.000000		
34	H	1.940534	2.417616	0.990760	0.000000	

Stoichiometry C11H17BrN2O3
Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.978138	1.005198	1.360692
2	6	0	-1.917172	0.039760	1.154859
3	7	0	-2.797518	0.530206	0.206174
4	6	0	-2.380596	1.748264	-0.173878
5	7	0	-1.280186	2.063475	0.514655
6	6	0	-0.546231	3.339956	0.410203
7	1	0	-0.083480	0.996198	1.955801
8	1	0	-1.999628	-0.951553	1.561868
9	1	0	-1.296455	4.118491	0.256190
10	1	0	-0.077869	3.506041	1.376724
11	35	0	-0.923831	-2.513422	-0.415091
12	1	0	-2.865869	2.369324	-0.905981
13	6	0	-3.925307	-0.136317	-0.350170
14	6	0	-4.487132	-1.204062	0.194386
15	1	0	-4.240517	0.279919	-1.297204
16	1	0	-5.306310	-1.691456	-0.315941
17	1	0	-4.134607	-1.650158	1.114175

18	6	0	2.690493	-1.580343	-0.310867
19	6	0	3.789391	-1.628360	0.663041
20	8	0	2.862084	-0.520088	0.670277
21	1	0	2.911056	-1.266550	-1.326716
22	1	0	1.781022	-2.160606	-0.182539
23	1	0	3.658479	-2.274404	1.529297
24	6	0	5.213218	-1.316870	0.291566
25	1	0	5.736538	-0.830526	1.120473
26	1	0	5.747892	-2.241660	0.053215
27	1	0	5.252095	-0.659700	-0.579918
28	6	0	0.495125	3.408438	-0.712940
29	1	0	0.996230	4.381864	-0.640719
30	1	0	0.016198	3.369993	-1.692726
31	6	0	1.587329	2.348540	-0.711200
32	8	0	2.105789	1.933284	-1.712817
33	8	0	1.916734	1.988465	0.544039
34	1	0	2.460523	1.160297	0.550262

Rotational constants (GHZ): 0.3547222 0.2527239 0.1627992

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 538 symmetry adapted cartesian basis functions of A symmetry.

There are 519 symmetry adapted basis functions of A symmetry.

519 basis functions, 823 primitive gaussians, 538 cartesian basis functions

78 alpha electrons 78 beta electrons

nuclear repulsion energy 1580.8946754281 Hartrees.

NAtoms= 34 NActive= 34 NUniq= 34 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 519 RedAO= T EigKep= 2.63D-06 NBF= 519

NBsUse= 519 1.00D-06 EigRej= -1.00D+00 NBFU= 519

Initial guess from the checkpoint file: "./coohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999821 -0.005495 0.006928 -0.016736 Ang= -2.17 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid=

0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3338.89450256 A.U. after 14 cycles

NFock= 14 Conv=0.35D-08 -V/T= 2.0019

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.001073801	0.000050672	-0.001401655
2	6	0.001212483	0.001494131	0.002462624
3	7	-0.000696773	-0.000067786	-0.000375792
4	6	0.000158582	-0.000040692	-0.001884100
5	7	0.001919275	-0.001297396	-0.000302938
6	6	0.000768131	0.000452626	0.000415070
7	1	-0.000326466	0.000554652	0.000363782
8	1	0.001113242	-0.000693080	-0.001633339
9	1	0.000929672	0.001109941	0.000510203
10	1	0.000254150	0.000424221	0.001057992
11	35	-0.000818985	-0.000297118	0.000920570
12	1	-0.000304334	0.000351811	-0.000067986
13	6	0.000398000	0.000294635	-0.000360888
14	6	0.000647714	-0.000931802	0.000226306
15	1	-0.000834315	0.000827736	0.000100128
16	1	-0.000064366	0.000159760	0.000087448
17	1	-0.000163414	-0.000437606	-0.000088132
18	6	-0.000376133	0.000132443	0.000149111
19	6	-0.000250379	-0.000150633	-0.000964750
20	8	-0.000353092	0.002955714	0.001373138
21	1	0.000438423	0.000000309	-0.000488272
22	1	-0.000144801	-0.000203377	0.000205249
23	1	-0.000218243	-0.000298051	-0.000281304
24	6	0.000240194	0.000256173	0.000042290
25	1	-0.000035009	-0.000078783	-0.000087561
26	1	-0.000058504	0.000026478	0.000021433
27	1	0.000047142	0.000058422	0.000028073

28	6	-0.002378666	-0.001928244	-0.003042905
29	1	-0.001372163	-0.000500555	0.000274340
30	1	0.000307602	0.000254702	-0.000595301
31	6	0.002801740	0.002395113	0.008267609
32	8	-0.000331041	-0.001522982	-0.000461423
33	8	-0.003793827	-0.001502207	-0.002201364
34	1	0.002357964	-0.001849227	-0.002267658

Cartesian Forces: Max 0.008267609 RMS 0.001371184

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.004906671 RMS 0.000970221

Search for a local minimum.

Step number 9 out of a maximum of 175

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 8 9

DE= -1.24D-03 DEPred=-1.68D-03 R= 7.36D-01

TightC=F SS= 1.41D+00 RLast= 4.93D-01 DXNew= 1.2000D+00 1.4783D+00

Trust test= 7.36D-01 RLast= 4.93D-01 DXMaxT set to 1.20D+00

ITU= 1 1 0 1 0 -1 0 1 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00218	0.00239	0.00403	0.00661	0.00698
Eigenvalues ---	0.00921	0.00996	0.01425	0.01496	0.01650
Eigenvalues ---	0.01756	0.01825	0.02137	0.02228	0.02280
Eigenvalues ---	0.02327	0.02432	0.02552	0.02645	0.02955
Eigenvalues ---	0.03045	0.03068	0.03091	0.03627	0.03798
Eigenvalues ---	0.04366	0.04654	0.05197	0.05372	0.05757
Eigenvalues ---	0.05886	0.06690	0.07643	0.09887	0.09986
Eigenvalues ---	0.11929	0.12639	0.12869	0.13325	0.13831
Eigenvalues ---	0.15332	0.15808	0.15874	0.15990	0.15999
Eigenvalues ---	0.16000	0.16000	0.16003	0.16020	0.16226
Eigenvalues ---	0.16769	0.18536	0.18761	0.21844	0.22132
Eigenvalues ---	0.22910	0.23102	0.23583	0.24772	0.25147
Eigenvalues ---	0.26023	0.26941	0.28653	0.29230	0.30353
Eigenvalues ---	0.31848	0.32368	0.34497	0.34601	0.34632
Eigenvalues ---	0.34765	0.34881	0.34898	0.34962	0.35026
Eigenvalues ---	0.35135	0.35530	0.35711	0.35763	0.36527
Eigenvalues ---	0.36600	0.36857	0.37096	0.37322	0.37783
Eigenvalues ---	0.41080	0.42617	0.45581	0.48976	0.51692

Eigenvalues --- 0.54425 0.55514 0.56117 0.60444 0.89537
Eigenvalues --- 0.95469
RFO step: Lambda=-1.89245962D-03 EMin= 2.18336053D-03
Quartic linear search produced a step of -0.05605.
Iteration 1 RMS(Cart)= 0.07816721 RMS(Int)= 0.00193838
Iteration 2 RMS(Cart)= 0.00327446 RMS(Int)= 0.00007129
Iteration 3 RMS(Cart)= 0.00000398 RMS(Int)= 0.00007124
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00007124

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.57463	-0.00051	-0.00022	-0.00319	-0.00343	2.57120
R2	2.62323	-0.00123	-0.00008	-0.00350	-0.00359	2.61964
R3	2.03060	0.00006	-0.00001	0.00042	0.00041	2.03100
R4	2.61545	0.00158	0.00032	0.00028	0.00061	2.61605
R5	2.03104	0.00033	-0.00015	0.00150	0.00135	2.03239
R6	2.53669	0.00042	0.00004	0.00307	0.00313	2.53982
R7	2.68958	0.00009	0.00009	-0.00040	-0.00031	2.68926
R8	2.52428	0.00017	0.00003	0.00016	0.00021	2.52448
R9	2.03282	0.00032	0.00005	-0.00020	-0.00015	2.03267
R10	2.78951	-0.00106	-0.00014	-0.00641	-0.00654	2.78297
R11	2.06376	-0.00032	-0.00010	0.00105	0.00094	2.06470
R12	2.05373	0.00113	0.00014	0.00063	0.00077	2.05450
R13	2.89724	-0.00191	0.00006	-0.00765	-0.00759	2.88965
R14	5.17700	-0.00068	0.00049	-0.01865	-0.01816	5.15884
R15	2.50149	0.00087	-0.00003	0.00100	0.00097	2.50247
R16	2.04360	0.00026	0.00004	-0.00024	-0.00019	2.04341
R17	2.04321	-0.00009	0.00001	-0.00038	-0.00037	2.04284
R18	2.04343	-0.00012	0.00005	-0.00094	-0.00089	2.04253
R19	2.77628	0.00004	0.00004	-0.00073	-0.00076	2.77552
R20	2.74904	0.00009	-0.00029	0.00524	0.00499	2.75402
R21	2.05195	0.00054	0.00001	0.00043	0.00045	2.05240
R22	2.05304	0.00029	0.00009	-0.00015	-0.00006	2.05298
R23	2.73078	-0.00033	0.00002	-0.00045	-0.00041	2.73038
R24	2.05704	-0.00016	-0.00001	-0.00020	-0.00021	2.05682
R25	2.84233	0.00024	-0.00006	0.00150	0.00144	2.84377
R26	3.27275	-0.00259	0.00139	-0.05222	-0.05083	3.22191
R27	2.06792	-0.00012	-0.00005	0.00010	0.00005	2.06797
R28	2.06830	-0.00006	-0.00001	-0.00008	-0.00009	2.06821
R29	2.06393	-0.00001	-0.00001	0.00002	0.00001	2.06394
R30	2.07344	-0.00094	-0.00024	0.00013	-0.00011	2.07332
R31	2.06217	0.00025	-0.00018	0.00353	0.00335	2.06551
R32	2.87605	0.00069	-0.00001	-0.00357	-0.00358	2.87247
R33	2.27119	0.00095	0.00008	-0.00072	-0.00065	2.27054
R34	2.54502	-0.00491	-0.00024	-0.00527	-0.00552	2.53951

R35	1.87227	0.00003	-0.00053	0.00993	0.00940	1.88167
A1	1.87358	0.00043	0.00013	0.00061	0.00071	1.87428
A2	2.28047	0.00002	-0.00009	0.00090	0.00083	2.28130
A3	2.12362	-0.00039	-0.00005	-0.00138	-0.00141	2.12220
A4	1.86592	-0.00049	-0.00011	-0.00053	-0.00075	1.86516
A5	2.27739	0.00072	-0.00053	0.00438	0.00379	2.28118
A6	2.13840	-0.00021	0.00066	-0.00273	-0.00213	2.13627
A7	1.89447	-0.00001	0.00004	0.00060	0.00055	1.89503
A8	2.22183	0.00065	0.00013	-0.00071	-0.00065	2.22118
A9	2.16564	-0.00064	-0.00010	-0.00109	-0.00126	2.16438
A10	1.90080	-0.00072	-0.00012	-0.00398	-0.00410	1.89670
A11	2.18518	0.00048	0.00011	0.00145	0.00156	2.18673
A12	2.19714	0.00023	0.00001	0.00255	0.00256	2.19970
A13	1.88968	0.00079	0.00006	0.00264	0.00265	1.89232
A14	2.20705	0.00005	-0.00087	-0.00788	-0.00878	2.19826
A15	2.18607	-0.00084	0.00069	0.00583	0.00649	2.19256
A16	1.85967	0.00130	0.00056	0.01797	0.01858	1.87825
A17	1.85824	0.00128	0.00060	-0.00405	-0.00350	1.85473
A18	2.01327	-0.00340	-0.00146	-0.02163	-0.02309	1.99018
A19	1.88865	-0.00080	-0.00025	-0.00079	-0.00106	1.88758
A20	1.90863	0.00067	-0.00011	0.00326	0.00324	1.91187
A21	1.93046	0.00104	0.00071	0.00635	0.00693	1.93738
A22	1.79511	0.00475	-0.00308	0.04577	0.04269	1.83780
A23	2.15706	0.00069	-0.00025	0.00534	0.00508	2.16213
A24	1.97472	-0.00044	0.00014	-0.00448	-0.00435	1.97038
A25	2.14958	-0.00025	0.00016	-0.00143	-0.00127	2.14831
A26	2.08404	-0.00029	-0.00001	-0.00126	-0.00128	2.08276
A27	2.14637	0.00058	0.00001	0.00257	0.00257	2.14895
A28	2.05162	-0.00029	0.00001	-0.00150	-0.00149	2.05013
A29	2.06881	-0.00030	0.00022	-0.00426	-0.00382	2.06500
A30	2.12987	0.00006	-0.00073	0.00896	0.00800	2.13787
A31	1.97838	-0.00002	0.00030	-0.00203	-0.00173	1.97665
A32	1.99144	0.00012	0.00020	-0.00072	-0.00053	1.99092
A33	2.02072	0.00019	0.00017	-0.00222	-0.00205	2.01867
A34	2.04540	-0.00005	-0.00026	0.00150	0.00129	2.04668
A35	2.13836	-0.00006	0.00018	-0.00144	-0.00131	2.13704
A36	1.95413	0.00000	0.00006	0.00088	0.00099	1.95512
A37	2.03741	-0.00010	-0.00002	-0.00119	-0.00128	2.03614
A38	2.01895	0.00010	0.00009	-0.00067	-0.00059	2.01836
A39	2.25633	-0.00030	0.00163	-0.03154	-0.02983	2.22650
A40	2.67383	-0.00009	-0.00047	0.00409	0.00299	2.67683
A41	1.93656	0.00001	0.00001	-0.00130	-0.00129	1.93528
A42	1.91903	-0.00006	-0.00007	0.00122	0.00115	1.92019
A43	1.93411	0.00009	0.00007	-0.00063	-0.00056	1.93355

A44	1.88269	0.00001	0.00000	0.00025	0.00025	1.88294
A45	1.89650	-0.00006	0.00002	-0.00023	-0.00021	1.89628
A46	1.89362	0.00001	-0.00002	0.00073	0.00071	1.89433
A47	1.87718	-0.00027	-0.00031	-0.00001	-0.00029	1.87689
A48	1.93700	0.00154	0.00122	0.00062	0.00180	1.93880
A49	2.04372	-0.00302	-0.00228	-0.00405	-0.00634	2.03739
A50	1.86585	-0.00058	0.00011	-0.00402	-0.00389	1.86196
A51	1.86504	0.00113	0.00036	0.01291	0.01331	1.87835
A52	1.86654	0.00133	0.00102	-0.00509	-0.00409	1.86245
A53	2.15225	-0.00108	0.00034	-0.01939	-0.01904	2.13321
A54	1.94205	0.00191	0.00069	0.01835	0.01905	1.96110
A55	2.18813	-0.00083	-0.00099	0.00116	0.00018	2.18831
A56	1.94291	-0.00348	-0.00243	-0.02768	-0.03011	1.91280
A57	2.78976	0.00092	-0.00146	-0.02440	-0.02586	2.76390
D1	-0.02115	0.00002	0.00008	-0.02250	-0.02242	-0.04358
D2	3.06191	0.00052	0.00030	-0.00058	-0.00023	3.06169
D3	-3.04881	-0.00051	0.00014	-0.02370	-0.02360	-3.07241
D4	0.03426	0.00000	0.00036	-0.00178	-0.00140	0.03285
D5	0.00990	-0.00005	0.00075	0.01330	0.01406	0.02396
D6	3.12241	-0.00025	-0.00168	0.03536	0.03357	-3.12721
D7	3.04998	0.00044	0.00069	0.01454	0.01527	3.06525
D8	-0.12070	0.00024	-0.00175	0.03660	0.03478	-0.08592
D9	0.02509	0.00003	-0.00088	0.02394	0.02307	0.04816
D10	3.11453	0.00001	0.00098	-0.00124	-0.00027	3.11426
D11	-3.06372	-0.00046	-0.00103	0.00388	0.00291	-3.06081
D12	0.02572	-0.00048	0.00083	-0.02129	-0.02044	0.00528
D13	-1.70327	-0.00165	-0.00188	0.00699	0.00509	-1.69817
D14	1.37191	-0.00108	-0.00166	0.03198	0.03033	1.40224
D15	-0.01922	-0.00007	0.00136	-0.01587	-0.01451	-0.03373
D16	3.13449	0.00019	0.00132	-0.01794	-0.01665	3.11784
D17	-3.11072	-0.00009	-0.00042	0.00829	0.00788	-3.10284
D18	0.04299	0.00017	-0.00047	0.00623	0.00574	0.04873
D19	0.29953	-0.00109	0.00483	-0.11753	-0.11269	0.18684
D20	-2.77897	-0.00119	0.00377	-0.10754	-0.10377	-2.88273
D21	-2.90177	-0.00109	0.00696	-0.14630	-0.13934	-3.04111
D22	0.30291	-0.00119	0.00590	-0.13631	-0.13042	0.17250
D23	0.00585	0.00008	-0.00131	0.00168	0.00038	0.00622
D24	-3.10710	0.00026	0.00117	-0.01977	-0.01873	-3.12583
D25	3.13522	-0.00018	-0.00127	0.00375	0.00253	3.13775
D26	0.02227	0.00000	0.00121	-0.01769	-0.01658	0.00570
D27	-2.48276	-0.00013	-0.00237	0.03192	0.02952	-2.45323
D28	-0.46986	0.00016	-0.00210	0.03753	0.03539	-0.43447
D29	1.67876	0.00022	-0.00172	0.02833	0.02672	1.70548
D30	0.62501	-0.00034	-0.00524	0.05747	0.05217	0.67718

D31	2.63791	-0.00005	-0.00498	0.06308	0.05803	2.69594
D32	-1.49666	0.00001	-0.00459	0.05387	0.04936	-1.44730
D33	-3.08985	-0.00038	-0.00193	-0.05254	-0.05445	3.13889
D34	1.15804	-0.00037	-0.00254	-0.04805	-0.05058	1.10746
D35	-0.99135	-0.00113	-0.00315	-0.03838	-0.04153	-1.03289
D36	1.09828	-0.00027	-0.00160	-0.06362	-0.06520	1.03308
D37	-0.93701	-0.00026	-0.00221	-0.05913	-0.06133	-0.99835
D38	-3.08641	-0.00102	-0.00282	-0.04946	-0.05229	-3.13869
D39	-0.98001	-0.00034	-0.00165	-0.06856	-0.07022	-1.05022
D40	-3.01530	-0.00033	-0.00227	-0.06407	-0.06635	-3.08165
D41	1.11849	-0.00108	-0.00288	-0.05440	-0.05730	1.06119
D42	-3.07989	-0.00021	-0.00076	0.00553	0.00477	-3.07512
D43	0.00871	-0.00021	-0.00065	0.00118	0.00054	0.00925
D44	-0.00760	-0.00010	0.00040	-0.00551	-0.00512	-0.01272
D45	3.08100	-0.00010	0.00051	-0.00986	-0.00935	3.07165
D46	-2.74955	0.00012	0.00044	0.00047	0.00087	-2.74869
D47	-0.04676	0.00011	0.00047	-0.00126	-0.00083	-0.04759
D48	-0.00003	0.00003	-0.00049	0.00720	0.00666	0.00663
D49	2.70277	0.00002	-0.00046	0.00547	0.00497	2.70773
D50	0.68784	0.00022	-0.00016	-0.00051	-0.00045	0.68739
D51	-1.67542	-0.00019	-0.00097	0.00582	0.00508	-1.67034
D52	2.27046	0.00065	-0.00321	0.07046	0.06734	2.33780
D53	-0.11322	0.00061	-0.00338	0.07184	0.06855	-0.04467
D54	2.54871	0.00005	0.00003	0.00098	0.00100	2.54972
D55	-1.65316	0.00002	-0.00001	0.00126	0.00124	-1.65192
D56	0.44020	0.00005	-0.00005	0.00257	0.00251	0.44271
D57	1.33028	-0.00001	0.00015	-0.00099	-0.00083	1.32945
D58	-2.87160	-0.00003	0.00011	-0.00071	-0.00059	-2.87219
D59	-0.77824	0.00000	0.00007	0.00060	0.00068	-0.77756
D60	-1.02555	0.00000	-0.00002	-0.00021	-0.00023	-1.02578
D61	1.05576	-0.00002	-0.00006	0.00007	0.00001	1.05577
D62	-3.13407	0.00001	-0.00009	0.00137	0.00128	-3.13279
D63	1.36676	0.00037	0.00611	0.00215	0.00817	1.37494
D64	-3.11900	-0.00025	0.00930	-0.06604	-0.05664	3.10755
D65	2.60114	0.00082	-0.00675	0.04663	0.03992	2.64105
D66	-0.58017	0.00085	-0.00469	0.05013	0.04545	-0.53472
D67	-1.57715	-0.00064	-0.00833	0.05397	0.04566	-1.53150
D68	1.52473	-0.00061	-0.00627	0.05747	0.05119	1.57591
D69	0.41607	-0.00015	-0.00753	0.05305	0.04551	0.46158
D70	-2.76524	-0.00012	-0.00547	0.05655	0.05104	-2.71419
D71	2.90598	0.00249	-0.00025	0.06134	0.06105	2.96703
D72	-0.27631	0.00251	0.00186	0.06438	0.06628	-0.21003
D73	-1.69385	0.00018	0.00476	-0.04275	-0.03799	-1.73184

Item	Value	Threshold	Converged?

Maximum Force	0.004907	0.000450	NO
RMS Force	0.000970	0.000300	NO
Maximum Displacement	0.425936	0.001800	NO
RMS Displacement	0.078386	0.001200	NO

Predicted change in Energy=-1.113940D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.975618	1.576777	1.560227
2	6	0	-1.731101	0.452802	1.691422
3	7	0	-2.669237	0.478370	0.673737
4	6	0	-2.443713	1.561491	-0.089390
5	7	0	-1.422538	2.246997	0.432059
6	6	0	-0.876116	3.507723	-0.097832
7	1	0	-0.112050	1.908729	2.107191
8	1	0	-1.661966	-0.361019	2.391143
9	1	0	-1.717317	4.113354	-0.443307
10	1	0	-0.415006	4.017636	0.744405
11	35	0	-0.278897	-2.318743	1.084617
12	1	0	-3.003642	1.830479	-0.967534
13	6	0	-3.657860	-0.504649	0.388247
14	6	0	-3.953075	-1.511213	1.196522
15	1	0	-4.097215	-0.386879	-0.592751
16	1	0	-4.673943	-2.251548	0.878926
17	1	0	-3.468617	-1.664316	2.150527
18	6	0	3.122773	-0.835725	0.455070
19	6	0	4.246996	-0.439097	1.312982
20	8	0	3.142389	0.468686	1.104721
21	1	0	3.252049	-0.780381	-0.621870
22	1	0	2.327932	-1.490848	0.800445
23	1	0	4.264422	-0.834834	2.326765
24	6	0	5.580031	-0.019942	0.754480
25	1	0	6.039658	0.751751	1.379603
26	1	0	6.259882	-0.877095	0.724362
27	1	0	5.469760	0.371573	-0.259145
28	6	0	0.123451	3.321778	-1.240002
29	1	0	0.457555	4.318984	-1.552579
30	1	0	-0.354266	2.863917	-2.109973
31	6	0	1.362641	2.495458	-0.936451
32	8	0	1.936435	1.866045	-1.783947

33	8	0	1.741058	2.594692	0.349194
34	1	0	2.448219	1.920758	0.542126

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.360620	0.000000			
3	N	2.204701	1.384354	0.000000		
4	C	2.208342	2.215469	1.344014	0.000000	
5	N	1.386252	2.213672	2.177316	1.335899	0.000000
6	C	2.547080	3.642112	3.603829	2.499051	1.472682
7	H	1.074761	2.216735	3.261889	3.222141	2.153571
8	H	2.217329	1.075497	2.160707	3.234226	3.270639
9	H	3.316397	4.237559	3.920083	2.676736	2.082415
10	H	2.633941	3.916247	4.196779	3.292950	2.061030
11	Br	3.985812	3.187251	3.702214	4.595752	4.751813
12	H	3.250665	3.253830	2.152626	1.075645	2.152263
13	C	3.591697	2.515428	1.423097	2.443608	3.545439
14	C	4.305022	3.006568	2.424868	3.656946	4.594797
15	H	4.270319	3.394262	2.095655	2.604531	3.891200
16	H	5.366362	4.078477	3.393140	4.522258	5.568503
17	H	4.131366	2.777036	2.722319	4.058754	4.736870
18	C	4.882453	5.171939	5.943235	6.085133	5.492136
19	C	5.603621	6.056099	7.006044	7.122822	6.335198
20	O	4.288745	4.908704	5.827593	5.815898	4.945040
21	H	5.309511	5.630616	6.190693	6.181392	5.668116
22	H	4.571765	4.587741	5.372669	5.733862	5.307845
23	H	5.819061	6.165060	7.247940	7.521919	6.740112
24	C	6.795239	7.386068	8.264700	8.221528	7.367425
25	H	7.065932	7.782756	8.741729	8.647613	7.669288
26	H	7.685871	8.158409	9.031556	9.075321	8.298492
27	H	6.804816	7.460811	8.192982	8.004235	7.176263
28	C	3.477681	4.501515	4.421139	3.318561	2.518139
29	H	4.388991	5.501011	5.429883	4.261696	3.430258
30	H	3.938677	4.707415	4.335778	3.185099	2.825548
31	C	3.541868	4.544161	4.787211	4.009755	3.113162
32	O	4.443785	5.246548	5.401672	4.706376	4.042092
33	O	3.143737	4.294783	4.902535	4.332686	3.183724
34	H	3.588525	4.576297	5.318474	4.945593	3.886040

		6	7	8	9	10
6	C	0.000000				
7	H	2.828905	0.000000			
8	H	4.666875	2.763082	0.000000		
9	H	1.092594	3.733938	5.296904	0.000000	

10	H	1.087196	2.529122	4.841413	1.765173	0.000000
11	Br	5.975163	4.352587	2.729940	6.765758	6.346966
12	H	2.845328	4.221535	4.228886	2.672258	3.796765
13	C	4.906476	4.620814	2.831221	5.077710	5.576200
14	C	6.027666	5.222910	2.828294	6.270838	6.579553
15	H	5.078223	5.333014	3.851589	5.092970	5.894608
16	H	6.967550	6.295030	3.864312	7.141562	7.580191
17	H	6.206945	4.902558	2.240640	6.570883	6.601992
18	C	5.929786	4.552539	5.183382	6.980469	6.012878
19	C	6.619219	5.014413	6.007025	7.705997	6.474567
20	O	5.179794	3.697303	5.042333	6.268712	5.037850
21	H	5.975299	5.098652	5.779417	6.976756	6.191523
22	H	6.004876	4.383859	4.441410	7.022681	6.153880
23	H	7.152735	5.169997	5.945648	8.242516	6.924405
24	C	7.406261	6.160308	7.432464	8.471725	7.227905
25	H	7.589870	6.301706	7.847068	8.648355	7.261692
26	H	8.415765	7.090455	8.111730	9.481758	8.277253
27	H	7.080367	6.254518	7.643444	8.104870	6.995095
28	C	1.529138	3.640861	5.471373	2.156327	2.170720
29	H	2.133802	4.419015	6.476708	2.450069	2.475542
30	H	2.176126	4.330765	5.689494	2.489333	3.079323
31	C	2.596150	3.432597	5.327344	3.513818	2.881376
32	O	3.667224	4.397621	5.944719	4.494176	4.068314
33	O	2.807678	2.644827	4.948369	3.859372	2.613345
34	H	3.738878	3.000759	5.051633	4.809392	3.554697

		11	12	13	14	15
11	Br	0.000000				
12	H	5.371369	0.000000			
13	C	3.897853	2.778303	0.000000		
14	C	3.763537	4.092857	1.324248	0.000000	
15	H	4.596218	2.500608	1.081324	2.118114	0.000000
16	H	4.400369	4.781450	2.079626	1.081024	2.444471
17	H	3.426186	4.706602	2.118082	1.080863	3.090721
18	C	3.763912	6.831208	6.789039	7.146584	7.309420
19	C	4.906009	7.932432	7.959031	8.270680	8.559229
20	O	4.413090	6.627399	6.906815	7.367091	7.485003
21	H	4.212628	6.787469	6.988791	7.466892	7.359849
22	H	2.749859	6.525538	6.080477	6.293516	6.666503
23	H	4.938286	8.413148	8.162685	8.322391	8.867989
24	C	6.302421	8.948119	9.257845	9.659161	9.777463
25	H	7.031293	9.404997	9.828691	10.247401	10.389555
26	H	6.705502	9.798282	9.930422	10.243511	10.452012
27	H	6.487724	8.627210	9.192406	9.718728	9.602789
28	C	6.114018	3.475186	5.620591	6.775877	5.655713

29	H	7.180292	4.302885	6.631055	7.810404	6.619090
30	H	6.088600	3.064694	5.338733	6.559428	5.184525
31	C	5.473198	4.416739	5.996740	6.989980	6.183528
32	O	5.536136	5.007210	6.452499	7.414539	6.549774
33	O	5.363107	4.982967	6.225412	7.071037	6.622874
34	H	5.069993	5.657739	6.571946	7.292683	7.032485

		16	17	18	19	20
16	H	0.000000				
17	H	1.847869	0.000000			
18	C	7.935552	6.856206	0.000000		
19	C	9.113535	7.857056	1.468742	0.000000	
20	O	8.279233	7.024871	1.457367	1.444852	0.000000
21	H	8.199882	7.323584	1.086083	2.202283	2.133849
22	H	7.043513	5.954225	1.086389	2.247594	2.143757
23	H	9.165025	7.779396	2.192397	1.088424	2.109861
24	C	10.494738	9.302201	2.606389	1.504859	2.510682
25	H	11.137851	9.840681	3.447181	2.153183	2.924013
26	H	11.020958	9.863942	3.148917	2.142435	3.416805
27	H	10.539007	9.478710	2.734231	2.150331	2.699299
28	C	7.652895	7.018531	5.399447	6.137225	4.769890
29	H	8.684260	8.057773	6.140445	6.723886	5.393920
30	H	7.332196	6.953843	5.688286	6.618016	5.319586
31	C	7.891134	7.083375	4.016364	4.689464	3.382558
32	O	8.230586	7.560299	3.704073	4.499260	3.428023
33	O	8.057226	6.965965	3.699745	4.051234	2.656023
34	H	8.261160	7.102722	2.839155	3.065735	1.704963

		21	22	23	24	25
21	H	0.000000				
22	H	1.838949	0.000000			
23	H	3.118063	2.551470	0.000000		
24	C	2.809290	3.569569	2.206117	0.000000	
25	H	3.758203	4.375109	2.562387	1.094324	0.000000
26	H	3.296779	3.980289	2.559558	1.094447	1.769457
27	H	2.525235	3.802949	3.097610	1.092190	1.776179
28	C	5.195952	5.673141	6.866360	6.702188	6.961959
29	H	5.888882	6.541344	7.490219	7.098490	7.244495
30	H	5.338620	5.884615	7.395789	7.192887	7.584237
31	C	3.794726	4.454125	5.491791	5.193541	5.502646
32	O	3.175662	4.254536	5.441712	4.824557	5.299636
33	O	3.823242	4.152070	4.694658	4.662434	4.789169
34	H	3.049128	3.423485	3.751909	3.690482	3.868640

		26	27	28	29	30
26	H	0.000000				
27	H	1.775035	0.000000			

28	C	7.690581	6.184562	0.000000		
29	H	8.114844	6.509779	1.097156	0.000000	
30	H	8.110214	6.599744	1.093023	1.756975	0.000000
31	C	6.173766	4.673121	1.520046	2.126979	2.112033
32	O	5.701633	4.128299	2.387874	2.873591	2.519792
33	O	5.710852	4.383555	2.381354	2.870069	3.241969
34	H	4.731803	3.488799	3.247058	3.755265	3.972040

		31	32	33	34
31	C	0.000000			
32	O	1.201520	0.000000		
33	O	1.343848	2.262606	0.000000	
34	H	1.922225	2.382337	0.995735	0.000000

Stoichiometry C11H17BrN2O3
Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.055985	1.037633	1.376643
2	6	0	-1.966192	0.056460	1.131477
3	7	0	-2.827520	0.540769	0.161944
4	6	0	-2.408024	1.761569	-0.212281
5	7	0	-1.335857	2.087019	0.515159
6	6	0	-0.588925	3.352889	0.423197
7	1	0	-0.190049	1.047336	2.013175
8	1	0	-2.053303	-0.936344	1.535763
9	1	0	-1.315525	4.155689	0.277161
10	1	0	-0.114347	3.497464	1.390601
11	35	0	-0.876535	-2.570453	-0.307462
12	1	0	-2.870415	2.373401	-0.966514
13	6	0	-3.923120	-0.142500	-0.436396
14	6	0	-4.403695	-1.295185	0.004053
15	1	0	-4.280913	0.341648	-1.334643
16	1	0	-5.199104	-1.781173	-0.543445
17	1	0	-4.004546	-1.810787	0.866085
18	6	0	2.729644	-1.494858	-0.382292
19	6	0	3.843084	-1.561258	0.573241
20	8	0	2.889450	-0.478530	0.649919
21	1	0	2.931202	-1.124780	-1.383288

22	1	0	1.832188	-2.097679	-0.275420
23	1	0	3.743368	-2.252764	1.407833
24	6	0	5.253012	-1.193889	0.196754
25	1	0	5.775638	-0.735583	1.041953
26	1	0	5.808411	-2.090451	-0.095693
27	1	0	5.260359	-0.492411	-0.640357
28	6	0	0.443566	3.386149	-0.704242
29	1	0	0.930856	4.368788	-0.677406
30	1	0	-0.038530	3.301572	-1.681549
31	6	0	1.535646	2.329657	-0.662709
32	8	0	2.067871	1.918859	-1.658516
33	8	0	1.844492	1.962624	0.592612
34	1	0	2.438519	1.163796	0.570392

Rotational constants (GHZ): 0.3540677 0.2539715 0.1620816

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 538 symmetry adapted cartesian basis functions of A symmetry.

There are 519 symmetry adapted basis functions of A symmetry.

519 basis functions, 823 primitive gaussians, 538 cartesian basis functions

78 alpha electrons 78 beta electrons

nuclear repulsion energy 1581.0162057999 Hartrees.

NAtoms= 34 NActive= 34 NUniq= 34 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 519 RedAO= T EigKep= 2.48D-06 NBF= 519

NBsUse= 519 1.00D-06 EigRej= -1.00D+00 NBFU= 519

Initial guess from the checkpoint file: "./coohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999962 0.002377 0.000791 -0.008299 Ang= 0.99 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3338.89589060 A.U. after 14 cycles
NFock= 14 Conv=0.19D-08 -V/T= 2.0019
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.001181488	-0.000432019	-0.001704287
2	6	-0.002095599	0.001123969	0.004272128
3	7	0.000382809	-0.001769989	-0.002290904
4	6	-0.000211632	-0.000543300	0.000015247
5	7	-0.000283789	-0.000248336	0.000867097
6	6	0.000417033	0.000800743	0.000198112
7	1	-0.000063346	0.000051206	-0.000072737
8	1	0.001464363	-0.000219622	-0.001576098
9	1	0.000230910	-0.000170210	0.000942745
10	1	0.000591046	0.000845420	0.000333438
11	35	-0.001047849	0.000238155	0.000992717
12	1	-0.000318768	0.000406823	-0.000019212
13	6	0.000696549	0.000474098	-0.001254295
14	6	0.001086879	-0.000723342	0.000577034
15	1	-0.001119839	0.000811627	0.000087143
16	1	-0.000389600	0.000198604	0.000015228
17	1	0.000126238	-0.000632319	-0.000139361
18	6	-0.000678765	0.001133129	-0.000700390
19	6	0.000093255	-0.000333541	-0.000742563
20	8	0.000091885	0.001277783	0.001031458
21	1	0.000415182	0.000299887	-0.000418903
22	1	0.000087820	-0.000407179	0.001326347
23	1	-0.000383309	-0.000188329	-0.000197605
24	6	-0.000045082	0.000238301	0.000122799
25	1	-0.000031310	-0.000132730	-0.000092840
26	1	-0.000102635	-0.000003724	0.000037880
27	1	0.000068149	0.000008777	0.000009319
28	6	-0.002965106	0.000020101	-0.002369664
29	1	-0.000004940	-0.000950464	0.000267474
30	1	0.000464999	0.000805304	0.000343797
31	6	0.000921440	0.004263039	0.006087885

32	8	0.002504146	-0.003351442	-0.001804884
33	8	-0.000518937	-0.002510188	-0.004485521
34	1	-0.000563685	-0.000380233	0.000341416

Cartesian Forces: Max 0.006087885 RMS 0.001342814

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.004224530 RMS 0.000942122
Search for a local minimum.
Step number 10 out of a maximum of 175
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 9 10
DE= -1.39D-03 DEPred=-1.11D-03 R= 1.25D+00
TightC=F SS= 1.41D+00 RLast= 3.92D-01 DXNew= 2.0182D+00 1.1771D+00
Trust test= 1.25D+00 RLast= 3.92D-01 DXMaxT set to 1.20D+00
ITU= 1 1 1 0 1 0 -1 0 1 0

Eigenvalues ---	0.00140	0.00270	0.00351	0.00445	0.00698
Eigenvalues ---	0.00873	0.01082	0.01437	0.01510	0.01684
Eigenvalues ---	0.01780	0.01829	0.02207	0.02285	0.02291
Eigenvalues ---	0.02418	0.02467	0.02592	0.02905	0.03000
Eigenvalues ---	0.03052	0.03095	0.03299	0.03777	0.03897
Eigenvalues ---	0.04352	0.04647	0.05221	0.05233	0.05764
Eigenvalues ---	0.05880	0.06377	0.07801	0.09740	0.09896
Eigenvalues ---	0.11931	0.12627	0.12770	0.13395	0.13965
Eigenvalues ---	0.15318	0.15802	0.15881	0.15953	0.15997
Eigenvalues ---	0.16000	0.16000	0.16001	0.16004	0.16247
Eigenvalues ---	0.16722	0.18144	0.19371	0.21766	0.22233
Eigenvalues ---	0.22534	0.23027	0.23757	0.24534	0.25074
Eigenvalues ---	0.25702	0.28299	0.28852	0.29700	0.31272
Eigenvalues ---	0.31873	0.32397	0.34497	0.34535	0.34613
Eigenvalues ---	0.34764	0.34884	0.34904	0.34965	0.35002
Eigenvalues ---	0.35122	0.35533	0.35699	0.35767	0.36534
Eigenvalues ---	0.36840	0.37014	0.37079	0.37501	0.38149
Eigenvalues ---	0.41107	0.42324	0.45770	0.48985	0.51727
Eigenvalues ---	0.53280	0.55515	0.56139	0.60397	0.90042
Eigenvalues ---	0.96686				

En-DIIS/RFO-DIIS IScMMF= 0 using points: 10 9
RFO step: Lambda=-5.30251245D-04.
DidBck=F Rises=F RFO-DIIS coefs: 1.75793 -0.75793

Iteration 1 RMS(Cart)= 0.31892978 RMS(Int)= 0.09433149
Iteration 2 RMS(Cart)= 0.24665531 RMS(Int)= 0.05080583
Iteration 3 RMS(Cart)= 0.18301726 RMS(Int)= 0.01227179
Iteration 4 RMS(Cart)= 0.02670118 RMS(Int)= 0.00124361
Iteration 5 RMS(Cart)= 0.00064009 RMS(Int)= 0.00119016
Iteration 6 RMS(Cart)= 0.00000049 RMS(Int)= 0.00119016

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.57120	0.00098	-0.00260	-0.00208	-0.00462	2.56658
R2	2.61964	-0.00028	-0.00272	-0.00776	-0.01029	2.60935
R3	2.03100	-0.00007	0.00031	-0.00035	-0.00004	2.03096
R4	2.61605	0.00153	0.00046	0.00581	0.00613	2.62218
R5	2.03239	-0.00037	0.00102	0.00406	0.00508	2.03748
R6	2.53982	-0.00007	0.00237	0.00569	0.00790	2.54772
R7	2.68926	-0.00021	-0.00024	-0.00316	-0.00340	2.68586
R8	2.52448	0.00056	0.00016	0.00146	0.00166	2.52614
R9	2.03267	0.00029	-0.00011	-0.00001	-0.00012	2.03255
R10	2.78297	0.00123	-0.00496	-0.00395	-0.00891	2.77406
R11	2.06470	-0.00057	0.00071	0.00028	0.00100	2.06570
R12	2.05450	0.00090	0.00058	0.00401	0.00459	2.05910
R13	2.88965	0.00050	-0.00575	-0.01358	-0.01933	2.87032
R14	5.15884	-0.00118	-0.01377	-0.26688	-0.28064	4.87820
R15	2.50247	0.00097	0.00074	0.00463	0.00536	2.50783
R16	2.04341	0.00047	-0.00015	0.00073	0.00058	2.04399
R17	2.04284	0.00012	-0.00028	-0.00050	-0.00078	2.04206
R18	2.04253	0.00002	-0.00068	-0.00295	-0.00362	2.03891
R19	2.77552	-0.00007	-0.00057	-0.00367	-0.00540	2.77012
R20	2.75402	-0.00080	0.00378	0.01301	0.01749	2.77151
R21	2.05240	0.00048	0.00034	0.00305	0.00339	2.05578
R22	2.05298	0.00060	-0.00005	0.00251	0.00247	2.05544
R23	2.73038	-0.00033	-0.00031	-0.00235	-0.00221	2.72817
R24	2.05682	-0.00012	-0.00016	-0.00098	-0.00114	2.05568
R25	2.84377	-0.00010	0.00109	0.00265	0.00375	2.84752
R26	3.22191	-0.00169	-0.03853	-0.12778	-0.16631	3.05561
R27	2.06797	-0.00015	0.00004	-0.00004	0.00000	2.06797
R28	2.06821	-0.00006	-0.00007	-0.00022	-0.00029	2.06791
R29	2.06394	-0.00002	0.00001	0.00013	0.00014	2.06408
R30	2.07332	-0.00094	-0.00008	0.00086	0.00078	2.07410
R31	2.06551	-0.00081	0.00254	0.00747	0.01001	2.07553
R32	2.87247	0.00166	-0.00271	0.00246	-0.00025	2.87222
R33	2.27054	0.00422	-0.00049	0.00387	0.00338	2.27393
R34	2.53951	-0.00408	-0.00418	-0.02554	-0.02972	2.50979
R35	1.88167	-0.00164	0.00712	0.02045	0.02757	1.90924
A1	1.87428	0.00032	0.00054	0.00599	0.00648	1.88076

A2	2.28130	-0.00007	0.00063	0.00296	0.00299	2.28428
A3	2.12220	-0.00018	-0.00107	-0.00377	-0.00547	2.11673
A4	1.86516	-0.00041	-0.00057	-0.00324	-0.00404	1.86113
A5	2.28118	0.00017	0.00287	0.00446	0.00701	2.28820
A6	2.13627	0.00023	-0.00161	-0.00048	-0.00242	2.13385
A7	1.89503	-0.00024	0.00042	0.00043	0.00063	1.89566
A8	2.22118	0.00095	-0.00049	0.00812	0.00760	2.22878
A9	2.16438	-0.00068	-0.00096	-0.00819	-0.00916	2.15523
A10	1.89670	0.00044	-0.00311	-0.00232	-0.00554	1.89116
A11	2.18673	-0.00007	0.00118	0.00107	0.00208	2.18882
A12	2.19970	-0.00037	0.00194	0.00152	0.00331	2.20301
A13	1.89232	-0.00005	0.00201	0.00135	0.00300	1.89532
A14	2.19826	0.00105	-0.00666	-0.00614	-0.01361	2.18465
A15	2.19256	-0.00100	0.00492	0.00524	0.00926	2.20182
A16	1.87825	-0.00026	0.01408	0.02452	0.03911	1.91736
A17	1.85473	0.00144	-0.00266	0.00082	-0.00223	1.85251
A18	1.99018	-0.00174	-0.01750	-0.05327	-0.07070	1.91949
A19	1.88758	-0.00047	-0.00081	-0.00384	-0.00508	1.88251
A20	1.91187	0.00127	0.00246	0.02031	0.02332	1.93519
A21	1.93738	-0.00021	0.00525	0.01302	0.01726	1.95465
A22	1.83780	0.00379	0.03235	0.19016	0.22251	2.06031
A23	2.16213	-0.00004	0.00385	0.01414	0.01793	2.18006
A24	1.97038	0.00007	-0.00329	-0.00848	-0.01183	1.95854
A25	2.14831	-0.00002	-0.00097	-0.00649	-0.00752	2.14079
A26	2.08276	-0.00047	-0.00097	-0.00880	-0.00988	2.07288
A27	2.14895	0.00067	0.00195	0.01354	0.01538	2.16433
A28	2.05013	-0.00020	-0.00113	-0.00596	-0.00720	2.04293
A29	2.06500	0.00002	-0.00289	-0.01056	-0.00913	2.05586
A30	2.13787	-0.00092	0.00607	0.00651	0.00814	2.14601
A31	1.97665	-0.00005	-0.00131	-0.00707	-0.00859	1.96807
A32	1.99092	-0.00027	-0.00040	0.00278	0.00237	1.99329
A33	2.01867	0.00082	-0.00155	0.00565	0.00412	2.02279
A34	2.04668	-0.00033	0.00097	-0.00177	-0.00040	2.04629
A35	2.13704	0.00028	-0.00100	-0.00189	-0.00331	2.13374
A36	1.95512	-0.00005	0.00075	0.00145	0.00344	1.95856
A37	2.03614	0.00010	-0.00097	-0.00179	-0.00424	2.03190
A38	2.01836	0.00009	-0.00045	0.00071	0.00023	2.01859
A39	2.22650	-0.00022	-0.02261	-0.10663	-0.12795	2.09855
A40	2.67683	0.00009	0.00227	0.01107	0.00198	2.67881
A41	1.93528	0.00004	-0.00098	-0.00231	-0.00329	1.93199
A42	1.92019	-0.00016	0.00087	0.00079	0.00166	1.92185
A43	1.93355	0.00013	-0.00043	0.00016	-0.00028	1.93327
A44	1.88294	0.00003	0.00019	0.00010	0.00029	1.88323
A45	1.89628	-0.00005	-0.00016	-0.00040	-0.00056	1.89572

A46	1.89433	0.00002	0.00054	0.00173	0.00227	1.89660
A47	1.87689	0.00122	-0.00022	0.00871	0.00849	1.88538
A48	1.93880	0.00098	0.00136	0.00805	0.00934	1.94814
A49	2.03739	-0.00352	-0.00480	-0.00724	-0.01205	2.02533
A50	1.86196	-0.00060	-0.00295	-0.01756	-0.02046	1.84151
A51	1.87835	0.00031	0.01009	0.01107	0.02121	1.89956
A52	1.86245	0.00175	-0.00310	-0.00433	-0.00741	1.85504
A53	2.13321	0.00281	-0.01443	-0.03749	-0.05192	2.08129
A54	1.96110	-0.00225	0.01444	0.02858	0.04301	2.00411
A55	2.18831	-0.00054	0.00014	0.00869	0.00882	2.19713
A56	1.91280	0.00214	-0.02282	-0.03446	-0.05728	1.85551
A57	2.76390	0.00013	-0.01960	-0.00925	-0.02885	2.73505
D1	-0.04358	0.00105	-0.01700	0.02692	0.00993	-0.03365
D2	3.06169	0.00075	-0.00017	0.05040	0.05042	3.11210
D3	-3.07241	0.00029	-0.01789	-0.02669	-0.04487	-3.11728
D4	0.03285	-0.00001	-0.00106	-0.00320	-0.00438	0.02847
D5	0.02396	-0.00057	0.01066	0.00228	0.01302	0.03698
D6	-3.12721	-0.00042	0.02544	0.05148	0.07645	-3.05076
D7	3.06525	0.00011	0.01157	0.05041	0.06205	3.12730
D8	-0.08592	0.00026	0.02636	0.09961	0.12548	0.03956
D9	0.04816	-0.00117	0.01749	-0.04680	-0.02932	0.01884
D10	3.11426	-0.00072	-0.00021	-0.04195	-0.04231	3.07194
D11	-3.06081	-0.00090	0.00220	-0.06803	-0.06565	-3.12646
D12	0.00528	-0.00046	-0.01549	-0.06317	-0.07864	-0.07336
D13	-1.69817	-0.00098	0.00386	0.08353	0.08730	-1.61087
D14	1.40224	-0.00133	0.02299	0.11013	0.13320	1.53544
D15	-0.03373	0.00080	-0.01100	0.04873	0.03769	0.00396
D16	3.11784	0.00058	-0.01262	0.02028	0.00749	3.12533
D17	-3.10284	0.00029	0.00598	0.04322	0.04914	-3.05369
D18	0.04873	0.00007	0.00435	0.01477	0.01895	0.06767
D19	0.18684	-0.00156	-0.08541	-0.53512	-0.62049	-0.43365
D20	-2.88273	-0.00179	-0.07865	-0.52215	-0.60076	2.79969
D21	-3.04111	-0.00102	-0.10561	-0.52907	-0.63472	2.60736
D22	0.17250	-0.00125	-0.09885	-0.51610	-0.61499	-0.44249
D23	0.00622	-0.00013	0.00029	-0.03160	-0.03131	-0.02509
D24	-3.12583	-0.00031	-0.01420	-0.08052	-0.09537	3.06199
D25	3.13775	0.00008	0.00192	-0.00289	-0.00081	3.13694
D26	0.00570	-0.00009	-0.01257	-0.05180	-0.06487	-0.05917
D27	-2.45323	-0.00014	0.02238	0.15396	0.17613	-2.27711
D28	-0.43447	-0.00010	0.02682	0.16161	0.18819	-0.24628
D29	1.70548	-0.00043	0.02025	0.14501	0.16593	1.87141
D30	0.67718	0.00005	0.03954	0.21134	0.25053	0.92771
D31	2.69594	0.00009	0.04399	0.21900	0.26259	2.95854
D32	-1.44730	-0.00024	0.03741	0.20239	0.24034	-1.20696

D33	3.13889	-0.00019	-0.04127	-0.17236	-0.21366	2.92522
D34	1.10746	-0.00073	-0.03834	-0.16075	-0.19914	0.90832
D35	-1.03289	-0.00120	-0.03148	-0.15600	-0.18750	-1.22039
D36	1.03308	0.00040	-0.04942	-0.18267	-0.23193	0.80115
D37	-0.99835	-0.00013	-0.04649	-0.17106	-0.21741	-1.21576
D38	-3.13869	-0.00061	-0.03963	-0.16631	-0.20578	2.93872
D39	-1.05022	0.00031	-0.05322	-0.19903	-0.25235	-1.30257
D40	-3.08165	-0.00023	-0.05029	-0.18741	-0.23783	2.96371
D41	1.06119	-0.00070	-0.04343	-0.18266	-0.22619	0.83500
D42	-3.07512	-0.00048	0.00362	-0.01196	-0.00835	-3.08347
D43	0.00925	-0.00055	0.00041	-0.03797	-0.03756	-0.02831
D44	-0.01272	-0.00023	-0.00388	-0.02618	-0.03007	-0.04279
D45	3.07165	-0.00030	-0.00709	-0.05219	-0.05927	3.01237
D46	-2.74869	-0.00006	0.00066	0.00069	0.00062	-2.74806
D47	-0.04759	0.00006	-0.00063	-0.00671	-0.00811	-0.05570
D48	0.00663	-0.00012	0.00505	0.00657	0.01086	0.01749
D49	2.70773	0.00001	0.00376	-0.00083	0.00213	2.70986
D50	0.68739	0.00013	-0.00034	-0.00016	0.00375	0.69114
D51	-1.67034	-0.00077	0.00385	-0.00417	0.00410	-1.66624
D52	2.33780	0.00046	0.05104	0.24582	0.29769	2.63549
D53	-0.04467	0.00026	0.05195	0.24503	0.29810	0.25343
D54	2.54972	-0.00003	0.00076	0.00603	0.00667	2.55639
D55	-1.65192	-0.00008	0.00094	0.00520	0.00602	-1.64590
D56	0.44271	-0.00008	0.00190	0.00797	0.00975	0.45246
D57	1.32945	0.00015	-0.00063	-0.00075	-0.00120	1.32825
D58	-2.87219	0.00010	-0.00045	-0.00158	-0.00185	-2.87404
D59	-0.77756	0.00010	0.00052	0.00119	0.00188	-0.77568
D60	-1.02578	0.00000	-0.00018	-0.00183	-0.00206	-1.02784
D61	1.05577	-0.00005	0.00001	-0.00266	-0.00271	1.05305
D62	-3.13279	-0.00005	0.00097	0.00011	0.00102	-3.13177
D63	1.37494	-0.00076	0.00619	-0.45077	-0.44673	0.92820
D64	3.10755	-0.00059	-0.04293	-0.67705	-0.71783	2.38972
D65	2.64105	-0.00023	0.03025	0.01918	0.04948	2.69053
D66	-0.53472	0.00024	0.03445	0.01266	0.04715	-0.48758
D67	-1.53150	-0.00077	0.03460	0.03430	0.06893	-1.46257
D68	1.57591	-0.00029	0.03880	0.02777	0.06659	1.64251
D69	0.46158	-0.00046	0.03449	0.01723	0.05165	0.51323
D70	-2.71419	0.00001	0.03869	0.01070	0.04932	-2.66487
D71	2.96703	-0.00039	0.04627	0.09941	0.14568	3.11272
D72	-0.21003	0.00018	0.05024	0.09159	0.14183	-0.06820
D73	-1.73184	-0.00144	-0.02880	-0.26303	-0.29182	-2.02366

Item	Value	Threshold	Converged?
Maximum Force	0.004225	0.000450	NO
RMS Force	0.000942	0.000300	NO

Maximum Displacement 2.810710 0.001800 NO
RMS Displacement 0.658112 0.001200 NO
Predicted change in Energy=-3.329092D-03
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.224266	1.709076	1.705729
2	6	0	-1.940689	0.555382	1.725084
3	7	0	-2.662602	0.516173	0.540716
4	6	0	-2.363545	1.614251	-0.182072
5	7	0	-1.475100	2.340502	0.503641
6	6	0	-0.813502	3.565264	0.037622
7	1	0	-0.525212	2.114917	2.414022
8	1	0	-2.004050	-0.227340	2.463878
9	1	0	-1.562466	4.286632	-0.299415
10	1	0	-0.310437	3.987419	0.907104
11	35	0	-0.407414	-2.243008	2.236669
12	1	0	-2.761282	1.848232	-1.153633
13	6	0	-3.498763	-0.530858	0.066749
14	6	0	-3.387273	-1.807277	0.412407
15	1	0	-4.193521	-0.189250	-0.688592
16	1	0	-4.043022	-2.530648	-0.050682
17	1	0	-2.626952	-2.188489	1.076270
18	6	0	2.953939	-0.501359	1.365522
19	6	0	4.395064	-0.244174	1.289097
20	8	0	3.477981	0.868439	1.361751
21	1	0	2.434539	-0.755842	0.444147
22	1	0	2.451417	-0.784089	2.287809
23	1	0	4.971274	-0.362696	2.204131
24	6	0	5.171129	-0.390640	0.005805
25	1	0	5.981684	0.343031	-0.041844
26	1	0	5.616690	-1.388399	-0.052730
27	1	0	4.519792	-0.247324	-0.859217
28	6	0	0.161603	3.235548	-1.079312
29	1	0	0.467853	4.177640	-1.551887
30	1	0	-0.317787	2.649935	-1.875272
31	6	0	1.405952	2.463381	-0.672500
32	8	0	1.964538	1.776772	-1.487672
33	8	0	1.798949	2.659374	0.580914
34	1	0	2.608551	2.071137	0.719754

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.358177	0.000000			
3	N	2.202063	1.387597	0.000000		
4	C	2.206975	2.221993	1.348195	0.000000	
5	N	1.380809	2.212544	2.177088	1.336778	0.000000
6	C	2.529178	3.630078	3.601282	2.501470	1.467967
7	H	1.074738	2.215933	3.260935	3.220223	2.145398
8	H	2.220937	1.078186	2.164499	3.243724	3.273550
9	H	3.283105	4.261910	4.016526	2.792332	2.107120
10	H	2.581421	3.886604	4.209094	3.321669	2.057076
11	Br	4.070395	3.231662	3.946545	4.955320	5.015167
12	H	3.249267	3.260652	2.157530	1.075581	2.154797
13	C	3.588439	2.521426	1.421297	2.439697	3.539886
14	C	4.326201	3.065597	2.437218	3.620536	4.568238
15	H	4.260621	3.384607	2.086272	2.618777	3.900112
16	H	5.385687	4.134820	3.396827	4.474158	5.534401
17	H	4.189840	2.901852	2.757406	4.014179	4.708123
18	C	4.739111	5.020296	5.767254	5.928447	5.332486
19	C	5.963694	6.400870	7.137847	7.162183	6.461913
20	O	4.789167	5.439853	6.205236	6.087943	5.237971
21	H	4.588493	4.743703	5.254350	5.388051	4.987601
22	H	4.479434	4.626168	5.558436	5.919138	5.325773
23	H	6.551746	6.989105	7.862279	7.962528	7.194073
24	C	6.942595	7.377590	7.904163	7.799115	7.202731
25	H	7.539616	8.119798	8.665624	8.442660	7.738932
26	H	7.712666	8.003305	8.516235	8.527414	8.031671
27	H	6.587917	7.004339	7.357277	7.162703	6.670304
28	C	3.465142	4.412206	4.242125	3.132095	2.446558
29	H	4.423702	5.446133	5.252150	4.057607	3.372735
30	H	3.811888	4.470294	3.985988	2.850385	2.663522
31	C	3.625327	4.537497	4.670829	3.894952	3.114301
32	O	4.513409	5.202344	5.207100	4.523638	4.014253
33	O	3.362753	4.440810	4.949784	4.358989	3.290448
34	H	3.974132	4.899366	5.498639	5.073832	4.098228

		6	7	8	9	10
6	C	0.000000				
7	H	2.798910	0.000000			
8	H	4.657034	2.770490	0.000000		
9	H	1.093121	3.626980	5.311001	0.000000	
10	H	1.089628	2.413130	4.801673	1.764311	0.000000
11	Br	6.223884	4.363122	2.581431	7.099441	6.371450

12	H	2.856770	4.218921	4.238843	2.848270	3.850896
13	C	4.897927	4.620803	2.841218	5.204953	5.593429
14	C	5.969000	5.251805	2.935650	6.400964	6.579525
15	H	5.103753	5.328404	3.838399	5.206480	5.921922
16	H	6.899112	6.327008	3.973116	7.258811	7.571971
17	H	6.121525	4.972544	2.481848	6.704688	6.598235
18	C	5.700382	4.477583	5.085580	6.789315	5.569150
19	C	6.573216	5.571344	6.506077	7.651388	6.339877
20	O	5.238607	4.322793	5.698076	6.312656	4.928170
21	H	5.420976	4.569659	4.905068	6.477305	5.499796
22	H	5.885567	4.156979	4.493567	6.965428	5.683438
23	H	7.320264	6.032742	6.981471	8.400819	6.964356
24	C	7.173980	6.672752	7.586302	8.204348	7.072999
25	H	7.520881	7.177085	8.389035	8.516603	7.332998
26	H	8.117531	7.488728	8.109072	9.154623	8.059252
27	H	6.616960	6.461141	7.321466	7.606839	6.662136
28	C	1.518909	3.732414	5.407018	2.164586	2.175772
29	H	2.131528	4.579240	6.452947	2.388045	2.586224
30	H	2.177779	4.327507	5.472698	2.590623	3.087156
31	C	2.577672	3.657519	5.357701	3.503562	2.786366
32	O	3.639056	4.640734	5.948184	4.488998	3.974597
33	O	2.817925	3.009725	5.132394	3.836933	2.513884
34	H	3.795809	3.562714	5.440685	4.831616	3.496818

		11	12	13	14	15
11	Br	0.000000				
12	H	5.811462	0.000000			
13	C	4.146861	2.773676	0.000000		
14	C	3.520988	4.025804	1.327086	0.000000	
15	H	5.206697	2.533556	1.081631	2.116660	0.000000
16	H	4.304923	4.694033	2.075854	1.080613	2.431404
17	H	2.505165	4.613635	2.127658	1.078945	3.092869
18	C	3.884705	6.673116	6.582177	6.544068	7.443319
19	C	5.287440	7.845915	7.993049	7.986028	8.813516
20	O	5.053996	6.798202	7.232567	7.429160	8.010903
21	H	3.674437	6.027491	5.949548	5.916081	6.747985
22	H	3.209980	6.778264	6.356247	6.217261	7.305340
23	H	5.697975	8.715228	8.737175	8.669625	9.612045
24	C	6.287143	8.323460	8.671240	8.684378	9.392519
25	H	7.259462	8.940982	9.521258	9.623280	10.209623
26	H	6.500887	9.048657	9.156481	9.025695	9.903663
27	H	6.151798	7.582352	8.076821	8.159176	8.715177
28	C	6.429159	3.236268	5.375645	6.344276	5.554189
29	H	7.506262	4.001507	6.365845	7.385099	6.445418
30	H	6.391947	2.670985	4.899745	5.875540	4.948788

31	C	5.822513	4.239780	5.793806	6.510803	6.196032
32	O	5.971223	4.738149	6.130990	6.715474	6.513483
33	O	5.625203	4.945939	6.205457	6.846624	6.755442
34	H	5.478040	5.691606	6.670539	7.147480	7.304860

		16	17	18	19	20
16	H	0.000000				
17	H	1.841832	0.000000			
18	C	7.421665	5.837502	0.000000		
19	C	8.844448	7.289332	1.465887	0.000000	
20	O	8.373425	6.833485	1.466622	1.443685	0.000000
21	H	6.734507	5.298183	1.087874	2.195314	2.137535
22	H	7.120164	5.406477	1.087694	2.250932	2.154591
23	H	9.541579	7.895482	2.189094	1.087820	2.110739
24	C	9.459567	8.073923	2.603271	1.506841	2.508111
25	H	10.428463	9.042532	3.443967	2.152575	2.917989
26	H	9.727013	8.358973	3.144602	2.145256	3.415868
27	H	8.898825	7.654423	2.732378	2.151934	2.694994
28	C	7.210130	6.468598	5.266767	5.969926	4.749774
29	H	8.222089	7.550671	6.048548	6.560992	5.338630
30	H	6.636637	6.119983	5.580107	6.371818	5.297160
31	C	7.417432	6.400188	3.916565	4.484809	3.312902
32	O	7.530577	6.586264	3.782792	4.207390	3.351834
33	O	7.839890	6.582990	3.455409	3.958779	2.576103
34	H	8.124865	6.758847	2.674704	2.979336	1.616957

		21	22	23	24	25
21	H	0.000000				
22	H	1.843956	0.000000			
23	H	3.112416	2.556219	0.000000		
24	C	2.795433	3.572000	2.207569	0.000000	
25	H	3.745123	4.377267	2.561909	1.094323	0.000000
26	H	3.282241	3.982747	2.561650	1.094292	1.769517
27	H	2.511101	3.803954	3.098588	1.092265	1.775879
28	C	4.839252	5.721733	6.845531	6.278699	6.581514
29	H	5.673733	6.580011	7.416409	6.739168	6.883806
30	H	4.955231	6.065662	7.327458	6.550705	6.954610
31	C	3.559254	4.516911	5.382679	4.773058	5.082414
32	O	3.219776	4.587953	5.219884	4.148539	4.503720
33	O	3.476548	3.898287	4.672407	4.583114	4.821675
34	H	2.845707	3.261257	3.702617	3.624482	3.865799

		26	27	28	29	30
26	H	0.000000				
27	H	1.776418	0.000000			
28	C	7.224454	5.583247	0.000000		
29	H	7.729087	6.039727	1.097567	0.000000	

30	H	7.405931	5.729629	1.098321	1.748053	0.000000
31	C	5.740265	4.132648	1.519915	2.142904	2.110151
32	O	5.041387	3.319826	2.354858	2.829904	2.474197
33	O	5.600101	4.233894	2.401922	2.936969	3.242454
34	H	4.649088	3.394297	3.252699	3.765674	3.953811

		31	32	33	34
31	C	0.000000			
32	O	1.203309	0.000000		
33	O	1.328122	2.255095	0.000000	
34	H	1.881083	2.318217	1.010325	0.000000

Stoichiometry C11H17BrN2O3
Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.166486	1.155232	1.416049
2	6	0	-2.120584	0.312971	0.941771
3	7	0	-2.709172	0.949312	-0.141770
4	6	0	-2.100818	2.138420	-0.324957
5	7	0	-1.146846	2.270476	0.602122
6	6	0	-0.184759	3.374563	0.703643
7	1	0	-0.469949	1.043849	2.226908
8	1	0	-2.431649	-0.664561	1.273663
9	1	0	-0.715639	4.330080	0.711879
10	1	0	0.309077	3.258323	1.667958
11	35	0	-1.310762	-2.725603	0.196859
12	1	0	-2.335699	2.845706	-1.100490
13	6	0	-3.705538	0.435399	-1.015401
14	6	0	-3.917471	-0.853266	-1.251166
15	1	0	-4.226259	1.219581	-1.548161
16	1	0	-4.667772	-1.132643	-1.976922
17	1	0	-3.332760	-1.650056	-0.818314
18	6	0	2.425131	-1.662086	0.142401
19	6	0	3.887430	-1.758422	0.177419
20	8	0	3.239392	-0.590002	0.724291
21	1	0	1.958154	-1.373446	-0.796795
22	1	0	1.781345	-2.170794	0.856428
23	1	0	4.326845	-2.384837	0.950640

24	6	0	4.737172	-1.541973	-1.048003
25	1	0	5.691619	-1.078644	-0.779861
26	1	0	4.952295	-2.500148	-1.530804
27	1	0	4.225391	-0.896283	-1.765085
28	6	0	0.800171	3.312473	-0.450974
29	1	0	1.355310	4.258989	-0.475081
30	1	0	0.285341	3.249189	-1.419093
31	6	0	1.792900	2.161960	-0.420125
32	8	0	2.263757	1.763813	-1.453433
33	8	0	2.090618	1.714711	0.794469
34	1	0	2.730099	0.943472	0.664041

Rotational constants (GHZ): 0.3272633 0.2553274 0.1598728

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 538 symmetry adapted cartesian basis functions of A symmetry.

There are 519 symmetry adapted basis functions of A symmetry.

519 basis functions, 823 primitive gaussians, 538 cartesian basis functions

78 alpha electrons 78 beta electrons

nuclear repulsion energy 1570.1564698773 Hartrees.

NAtoms= 34 NActive= 34 NUniq= 34 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 519 RedAO= T EigKep= 4.77D-06 NBF= 519

NBsUse= 519 1.00D-06 EigRej= -1.00D+00 NBFU= 519

Initial guess from the checkpoint file: "./coohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.998743 -0.001600 0.000331 0.050091 Ang= -5.75 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3338.89556271 A.U. after 18 cycles
NFock= 18 Conv=0.35D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.003993475	0.000277978	0.000167332
2	6	-0.008053162	-0.000258919	0.001554864
3	7	0.005901816	0.004712769	0.002003735
4	6	0.000933990	-0.003802195	0.002325124
5	7	-0.006945906	0.001746236	0.004164872
6	6	-0.002059879	0.000226031	0.000809047
7	1	0.000575290	-0.000891819	0.000450103
8	1	0.002627999	-0.001601541	-0.001430046
9	1	-0.001623139	-0.002495114	0.000613402
10	1	0.001123501	0.000596789	-0.001980979
11	35	0.003202439	-0.000722032	0.001466581
12	1	0.000416388	-0.000366911	-0.000460684
13	6	-0.004343656	-0.005364277	-0.007310539
14	6	-0.002646044	0.002093231	-0.003648706
15	1	-0.002383973	0.001260075	0.000319440
16	1	-0.003103326	0.000587985	-0.001108907
17	1	0.005774584	0.000231331	0.007152887
18	6	-0.003054260	0.004122336	-0.002330962
19	6	0.002608053	-0.001232644	-0.002221940
20	8	0.000735563	-0.002593074	0.004700101
21	1	-0.000459409	-0.001093023	0.002847650
22	1	0.002340555	-0.001542789	-0.002651155
23	1	0.000007371	0.000608527	0.000486518
24	6	-0.000470225	0.000021826	0.000348799
25	1	-0.000350616	-0.000189912	0.000182520
26	1	-0.000234155	-0.000027828	0.000408782
27	1	0.000177526	0.000141219	0.000393172
28	6	-0.001479472	0.005729689	-0.004218590
29	1	0.003407729	-0.001680815	0.001556505
30	1	0.000944067	0.002881997	0.003425846
31	6	-0.006601019	0.007748071	-0.007336511
32	8	0.008552574	-0.007887460	-0.002105655
33	8	0.007556962	-0.004570243	-0.004453472

34 1 -0.007071641 0.003334507 0.005880864

Cartesian Forces: Max 0.008552574 RMS 0.003416346

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.013098926 RMS 0.002832105

Search for a local minimum.

Step number 11 out of a maximum of 175

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 9 11 10

DE= 3.28D-04 DEPred=-3.33D-03 R=-9.85D-02

Trust test=-9.85D-02 RLast= 1.89D+00 DXMaxT set to 6.00D-01

ITU= -1 1 1 1 0 1 0 -1 0 1 0

Use linear search instead of GDIIS.

Energy rises -- skip Quadratic/GDIIS search.

Quartic linear search produced a step of -0.45803.

Iteration 1 RMS(Cart)= 0.22268845 RMS(Int)= 0.02649352

Iteration 2 RMS(Cart)= 0.09741319 RMS(Int)= 0.00280764

Iteration 3 RMS(Cart)= 0.00587512 RMS(Int)= 0.00027544

Iteration 4 RMS(Cart)= 0.00002254 RMS(Int)= 0.00027521

Iteration 5 RMS(Cart)= 0.00000001 RMS(Int)= 0.00027521

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56658	0.00194	0.00211	0.00000	0.00210	2.56868
R2	2.60935	0.00120	0.00471	0.00000	0.00466	2.61401
R3	2.03096	0.00033	0.00002	0.00000	0.00002	2.03098
R4	2.62218	0.00182	-0.00281	0.00000	-0.00277	2.61941
R5	2.03748	0.00137	-0.00233	0.00000	-0.00233	2.03515
R6	2.54772	-0.00159	-0.00362	0.00000	-0.00358	2.54414
R7	2.68586	0.00634	0.00156	0.00000	0.00156	2.68742
R8	2.52614	0.00010	-0.00076	0.00000	-0.00077	2.52538
R9	2.03255	0.00018	0.00006	0.00000	0.00006	2.03261
R10	2.77406	0.00534	0.00408	0.00000	0.00408	2.77814
R11	2.06570	-0.00072	-0.00046	0.00000	-0.00046	2.06524
R12	2.05910	-0.00083	-0.00210	0.00000	-0.00210	2.05699
R13	2.87032	0.00717	0.00885	0.00000	0.00885	2.87918
R14	4.87820	0.00241	0.12854	0.00000	0.12854	5.00674
R15	2.50783	-0.00218	-0.00246	0.00000	-0.00246	2.50537
R16	2.04399	0.00171	-0.00027	0.00000	-0.00027	2.04372

R17	2.04206	0.00196	0.00036	0.00000	0.00036	2.04242
R18	2.03891	0.00839	0.00166	0.00000	0.00166	2.04057
R19	2.77012	0.00108	0.00247	0.00000	0.00281	2.77293
R20	2.77151	-0.00058	-0.00801	0.00000	-0.00820	2.76331
R21	2.05578	-0.00194	-0.00155	0.00000	-0.00155	2.05423
R22	2.05544	-0.00293	-0.00113	0.00000	-0.00113	2.05431
R23	2.72817	0.00016	0.00101	0.00000	0.00086	2.72903
R24	2.05568	0.00035	0.00052	0.00000	0.00052	2.05620
R25	2.84752	-0.00159	-0.00172	0.00000	-0.00172	2.84580
R26	3.05561	0.00291	0.07617	0.00000	0.07617	3.13178
R27	2.06797	-0.00040	0.00000	0.00000	0.00000	2.06797
R28	2.06791	-0.00009	0.00013	0.00000	0.00013	2.06805
R29	2.06408	-0.00040	-0.00006	0.00000	-0.00006	2.06402
R30	2.07410	-0.00116	-0.00036	0.00000	-0.00036	2.07374
R31	2.07553	-0.00443	-0.00459	0.00000	-0.00459	2.07094
R32	2.87222	0.00312	0.00011	0.00000	0.00011	2.87234
R33	2.27393	0.00990	-0.00155	0.00000	-0.00155	2.27238
R34	2.50979	0.00348	0.01361	0.00000	0.01361	2.52340
R35	1.90924	-0.00441	-0.01263	0.00000	-0.01263	1.89661
A1	1.88076	0.00033	-0.00297	0.00000	-0.00296	1.87780
A2	2.28428	-0.00104	-0.00137	0.00000	-0.00122	2.28306
A3	2.11673	0.00067	0.00251	0.00000	0.00267	2.11940
A4	1.86113	-0.00092	0.00185	0.00000	0.00188	1.86301
A5	2.28820	-0.00532	-0.00321	0.00000	-0.00314	2.28505
A6	2.13385	0.00624	0.00111	0.00000	0.00118	2.13503
A7	1.89566	-0.00008	-0.00029	0.00000	-0.00025	1.89541
A8	2.22878	0.00189	-0.00348	0.00000	-0.00349	2.22529
A9	2.15523	-0.00175	0.00419	0.00000	0.00418	2.15941
A10	1.89116	0.00173	0.00254	0.00000	0.00257	1.89373
A11	2.18882	-0.00095	-0.00095	0.00000	-0.00091	2.18790
A12	2.20301	-0.00077	-0.00152	0.00000	-0.00148	2.20153
A13	1.89532	-0.00106	-0.00137	0.00000	-0.00130	1.89402
A14	2.18465	-0.00182	0.00623	0.00000	0.00643	2.19109
A15	2.20182	0.00284	-0.00424	0.00000	-0.00404	2.19778
A16	1.91736	-0.00316	-0.01791	0.00000	-0.01803	1.89933
A17	1.85251	-0.00254	0.00102	0.00000	0.00111	1.85362
A18	1.91949	0.00827	0.03238	0.00000	0.03236	1.95185
A19	1.88251	0.00159	0.00233	0.00000	0.00243	1.88493
A20	1.93519	-0.00027	-0.01068	0.00000	-0.01080	1.92439
A21	1.95465	-0.00417	-0.00791	0.00000	-0.00768	1.94696
A22	2.06031	0.00115	-0.10192	0.00000	-0.10192	1.95839
A23	2.18006	-0.00427	-0.00821	0.00000	-0.00820	2.17186
A24	1.95854	0.00175	0.00542	0.00000	0.00543	1.96397
A25	2.14079	0.00271	0.00345	0.00000	0.00346	2.14424

A26	2.07288	-0.00104	0.00453	0.00000	0.00456	2.07743
A27	2.16433	-0.00255	-0.00705	0.00000	-0.00702	2.15731
A28	2.04293	0.00378	0.00330	0.00000	0.00332	2.04626
A29	2.05586	0.00087	0.00418	0.00000	0.00320	2.05906
A30	2.14601	-0.00050	-0.00373	0.00000	-0.00272	2.14329
A31	1.96807	0.00162	0.00393	0.00000	0.00398	1.97204
A32	1.99329	0.00036	-0.00109	0.00000	-0.00107	1.99222
A33	2.02279	-0.00103	-0.00189	0.00000	-0.00190	2.02090
A34	2.04629	0.00011	0.00018	0.00000	0.00007	2.04636
A35	2.13374	-0.00005	0.00152	0.00000	0.00164	2.13537
A36	1.95856	-0.00046	-0.00157	0.00000	-0.00185	1.95670
A37	2.03190	0.00073	0.00194	0.00000	0.00229	2.03418
A38	2.01859	0.00000	-0.00010	0.00000	-0.00010	2.01849
A39	2.09855	-0.00078	0.05860	0.00000	0.05846	2.15701
A40	2.67881	-0.00122	-0.00091	0.00000	0.00176	2.68057
A41	1.93199	-0.00016	0.00150	0.00000	0.00151	1.93350
A42	1.92185	-0.00060	-0.00076	0.00000	-0.00076	1.92109
A43	1.93327	-0.00002	0.00013	0.00000	0.00013	1.93340
A44	1.88323	0.00035	-0.00013	0.00000	-0.00013	1.88310
A45	1.89572	0.00011	0.00026	0.00000	0.00026	1.89598
A46	1.89660	0.00035	-0.00104	0.00000	-0.00104	1.89557
A47	1.88538	0.00258	-0.00389	0.00000	-0.00389	1.88149
A48	1.94814	0.00061	-0.00428	0.00000	-0.00426	1.94387
A49	2.02533	-0.00383	0.00552	0.00000	0.00552	2.03085
A50	1.84151	0.00004	0.00937	0.00000	0.00936	1.85086
A51	1.89956	-0.00008	-0.00971	0.00000	-0.00972	1.88984
A52	1.85504	0.00095	0.00339	0.00000	0.00339	1.85843
A53	2.08129	0.01191	0.02378	0.00000	0.02378	2.10507
A54	2.00411	-0.00901	-0.01970	0.00000	-0.01970	1.98441
A55	2.19713	-0.00278	-0.00404	0.00000	-0.00404	2.19309
A56	1.85551	0.01310	0.02624	0.00000	0.02624	1.88175
A57	2.73505	0.00211	0.01321	0.00000	0.01321	2.74826
D1	-0.03365	-0.00031	-0.00455	0.00000	-0.00455	-0.03820
D2	3.11210	-0.00144	-0.02309	0.00000	-0.02313	3.08897
D3	-3.11728	0.00043	0.02055	0.00000	0.02062	-3.09666
D4	0.02847	-0.00070	0.00200	0.00000	0.00203	0.03051
D5	0.03698	-0.00036	-0.00596	0.00000	-0.00598	0.03100
D6	-3.05076	0.00036	-0.03502	0.00000	-0.03492	-3.08568
D7	3.12730	-0.00108	-0.02842	0.00000	-0.02843	3.09887
D8	0.03956	-0.00037	-0.05747	0.00000	-0.05737	-0.01781
D9	0.01884	0.00086	0.01343	0.00000	0.01343	0.03228
D10	3.07194	0.00153	0.01938	0.00000	0.01942	3.09136
D11	-3.12646	0.00183	0.03007	0.00000	0.03004	-3.09642
D12	-0.07336	0.00251	0.03602	0.00000	0.03602	-0.03734

D13	-1.61087	0.00635	-0.03999	0.00000	-0.03997	-1.65084
D14	1.53544	0.00509	-0.06101	0.00000	-0.06103	1.47441
D15	0.00396	-0.00108	-0.01726	0.00000	-0.01725	-0.01329
D16	3.12533	-0.00040	-0.00343	0.00000	-0.00339	3.12193
D17	-3.05369	-0.00194	-0.02251	0.00000	-0.02249	-3.07619
D18	0.06767	-0.00126	-0.00868	0.00000	-0.00864	0.05904
D19	-0.43365	0.00179	0.28420	0.00000	0.28420	-0.14945
D20	2.79969	-0.00060	0.27517	0.00000	0.27516	3.07485
D21	2.60736	0.00267	0.29072	0.00000	0.29073	2.89809
D22	-0.44249	0.00029	0.28169	0.00000	0.28169	-0.16080
D23	-0.02509	0.00089	0.01434	0.00000	0.01434	-0.01075
D24	3.06199	-0.00002	0.04368	0.00000	0.04382	3.10581
D25	3.13694	0.00020	0.00037	0.00000	0.00034	3.13728
D26	-0.05917	-0.00071	0.02971	0.00000	0.02982	-0.02935
D27	-2.27711	0.00068	-0.08067	0.00000	-0.08063	-2.35773
D28	-0.24628	-0.00043	-0.08620	0.00000	-0.08614	-0.33242
D29	1.87141	-0.00233	-0.07600	0.00000	-0.07615	1.79526
D30	0.92771	0.00167	-0.11475	0.00000	-0.11468	0.81303
D31	2.95854	0.00056	-0.12028	0.00000	-0.12019	2.83835
D32	-1.20696	-0.00134	-0.11008	0.00000	-0.11020	-1.31716
D33	2.92522	0.00315	0.09786	0.00000	0.09787	3.02310
D34	0.90832	0.00124	0.09121	0.00000	0.09123	0.99954
D35	-1.22039	0.00241	0.08588	0.00000	0.08589	-1.13450
D36	0.80115	0.00175	0.10623	0.00000	0.10620	0.90734
D37	-1.21576	-0.00016	0.09958	0.00000	0.09955	-1.11621
D38	2.93872	0.00100	0.09425	0.00000	0.09421	3.03293
D39	-1.30257	0.00275	0.11558	0.00000	0.11561	-1.18696
D40	2.96371	0.00083	0.10893	0.00000	0.10897	3.07267
D41	0.83500	0.00200	0.10360	0.00000	0.10363	0.93862
D42	-3.08347	-0.00234	0.00382	0.00000	0.00383	-3.07964
D43	-0.02831	0.00043	0.01720	0.00000	0.01720	-0.01110
D44	-0.04279	0.00018	0.01377	0.00000	0.01377	-0.02902
D45	3.01237	0.00295	0.02715	0.00000	0.02715	3.03952
D46	-2.74806	0.00072	-0.00029	0.00000	-0.00012	-2.74819
D47	-0.05570	0.00087	0.00371	0.00000	0.00389	-0.05181
D48	0.01749	-0.00151	-0.00497	0.00000	-0.00480	0.01270
D49	2.70986	-0.00136	-0.00098	0.00000	-0.00078	2.70908
D50	0.69114	-0.00146	-0.00172	0.00000	-0.00268	0.68846
D51	-1.66624	-0.00198	-0.00188	0.00000	-0.00289	-1.66913
D52	2.63549	0.00018	-0.13635	0.00000	-0.13656	2.49893
D53	0.25343	-0.00011	-0.13654	0.00000	-0.13682	0.11661
D54	2.55639	-0.00009	-0.00306	0.00000	-0.00303	2.55335
D55	-1.64590	-0.00014	-0.00276	0.00000	-0.00273	-1.64864
D56	0.45246	-0.00011	-0.00447	0.00000	-0.00445	0.44801

D57	1.32825	0.00019	0.00055	0.00000	0.00052	1.32876
D58	-2.87404	0.00014	0.00085	0.00000	0.00082	-2.87323
D59	-0.77568	0.00018	-0.00086	0.00000	-0.00089	-0.77657
D60	-1.02784	0.00008	0.00094	0.00000	0.00095	-1.02689
D61	1.05305	0.00003	0.00124	0.00000	0.00125	1.05431
D62	-3.13177	0.00007	-0.00047	0.00000	-0.00046	-3.13223
D63	0.92820	0.00097	0.20462	0.00000	0.20507	1.13327
D64	2.38972	0.00024	0.32879	0.00000	0.32834	2.71806
D65	2.69053	-0.00157	-0.02266	0.00000	-0.02267	2.66786
D66	-0.48758	0.00181	-0.02160	0.00000	-0.02160	-0.50918
D67	-1.46257	-0.00094	-0.03157	0.00000	-0.03157	-1.49415
D68	1.64251	0.00244	-0.03050	0.00000	-0.03051	1.61200
D69	0.51323	-0.00046	-0.02366	0.00000	-0.02364	0.48959
D70	-2.66487	0.00292	-0.02259	0.00000	-0.02258	-2.68745
D71	3.11272	-0.00534	-0.06673	0.00000	-0.06673	3.04598
D72	-0.06820	-0.00136	-0.06496	0.00000	-0.06496	-0.13316
D73	-2.02366	0.00163	0.13366	0.00000	0.13366	-1.89000

Item	Value	Threshold	Converged?
Maximum Force	0.013099	0.000450	NO
RMS Force	0.002832	0.000300	NO
Maximum Displacement	1.215083	0.001800	NO
RMS Displacement	0.305417	0.001200	NO

Predicted change in Energy=-3.089498D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.123489	1.658840	1.649957
2	6	0	-1.864536	0.521191	1.715255
3	7	0	-2.681897	0.512250	0.595792
4	6	0	-2.406193	1.601487	-0.145882
5	7	0	-1.455299	2.306943	0.473811
6	6	0	-0.838031	3.545261	-0.023002
7	1	0	-0.347629	2.029705	2.294616
8	1	0	-1.873269	-0.274363	2.441098
9	1	0	-1.626347	4.216468	-0.372893
10	1	0	-0.356727	4.010371	0.835416
11	35	0	-0.310981	-2.293507	1.732636
12	1	0	-2.872885	1.851397	-1.082194
13	6	0	-3.594010	-0.503709	0.197916
14	6	0	-3.685342	-1.695692	0.771104

15	1	0	-4.158365	-0.231786	-0.683664
16	1	0	-4.370679	-2.423784	0.360830
17	1	0	-3.062841	-2.012036	1.594778
18	6	0	2.970610	-0.704546	0.951316
19	6	0	4.342384	-0.332636	1.316146
20	8	0	3.306630	0.673673	1.306099
21	1	0	2.738904	-0.826940	-0.103681
22	1	0	2.287366	-1.188297	1.644814
23	1	0	4.671615	-0.571448	2.325367
24	6	0	5.436160	-0.183073	0.291880
25	1	0	6.136053	0.605959	0.583636
26	1	0	5.999676	-1.117175	0.205082
27	1	0	5.019234	0.064661	-0.686776
28	6	0	0.157947	3.272081	-1.143153
29	1	0	0.484355	4.239579	-1.545204
30	1	0	-0.314760	2.741323	-1.977317
31	6	0	1.393564	2.470768	-0.767023
32	8	0	1.964637	1.804094	-1.588852
33	8	0	1.768361	2.627731	0.504976
34	1	0	2.528858	1.996922	0.681106

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.359286	0.000000			
3	N	2.203308	1.386130	0.000000		
4	C	2.207635	2.219068	1.346302	0.000000	
5	N	1.383276	2.213045	2.177233	1.336371	0.000000
6	C	2.537491	3.635966	3.603041	2.500497	1.470127
7	H	1.074749	2.216366	3.261515	3.221348	2.149214
8	H	2.219312	1.076954	2.162821	3.239643	3.272316
9	H	3.299432	4.251137	3.971621	2.738215	2.095818
10	H	2.604055	3.901536	4.207218	3.311492	2.058952
11	Br	4.035845	3.215020	3.845247	4.805176	4.904920
12	H	3.249940	3.257597	2.155326	1.075610	2.153654
13	C	3.590058	2.518694	1.422121	2.441507	3.542594
14	C	4.311421	3.020153	2.431592	3.653556	4.591575
15	H	4.269745	3.403445	2.090587	2.592336	3.884773
16	H	5.373445	4.097329	3.395216	4.507635	5.558056
17	H	4.152043	2.804940	2.741370	4.064312	4.742820
18	C	4.778634	5.046253	5.792911	5.952448	5.374546
19	C	5.826935	6.278069	7.111488	7.170889	6.425731
20	O	4.551346	5.189568	6.032665	5.967029	5.102572
21	H	4.916547	5.130072	5.627413	5.689557	5.267452

22	H	4.442988	4.490612	5.355920	5.746214	5.253140
23	H	6.246087	6.654875	7.631512	7.805389	7.018011
24	C	6.947375	7.471421	8.153446	8.054737	7.329766
25	H	7.412595	8.080666	8.818457	8.630947	7.780362
26	H	7.780322	8.173780	8.841798	8.841546	8.208133
27	H	6.762749	7.305097	7.820021	7.602063	6.949414
28	C	3.470748	4.452901	4.324964	3.218734	2.479643
29	H	4.410718	5.474878	5.338726	4.156067	3.402023
30	H	3.870779	4.578851	4.146444	3.004575	2.738164
31	C	3.582817	4.536272	4.722546	3.947102	3.111676
32	O	4.477444	5.217808	5.294507	4.607316	4.025344
33	O	3.257688	4.370380	4.928317	4.347838	3.239731
34	H	3.793760	4.748595	5.418810	5.019463	4.001573

		6	7	8	9	10
6	C	0.000000				
7	H	2.812251	0.000000			
8	H	4.661870	2.767266	0.000000		
9	H	1.092880	3.678676	5.305382	0.000000	
10	H	1.088514	2.460160	4.820483	1.764772	0.000000
11	Br	6.119743	4.359739	2.649453	6.967296	6.367572
12	H	2.851612	4.220374	4.234581	2.765959	3.830071
13	C	4.902895	4.620966	2.836445	5.145639	5.591362
14	C	6.017089	5.228766	2.844761	6.364104	6.606282
15	H	5.072196	5.339119	3.871384	5.127831	5.895418
16	H	6.946685	6.305397	3.896741	7.222373	7.598382
17	H	6.200850	4.919128	2.269548	6.688012	6.645982
18	C	5.789292	4.504586	5.086027	6.863084	5.771919
19	C	6.608184	5.341749	6.316902	7.692396	6.416732
20	O	5.214474	4.021144	5.386868	6.301165	4.977477
21	H	5.649523	4.841378	5.296544	6.675617	5.819314
22	H	5.912384	4.209629	4.333615	6.971354	5.888336
23	H	7.267623	5.653297	6.552645	8.358773	6.963997
24	C	7.305142	6.508422	7.619397	8.347269	7.172025
25	H	7.592454	6.855118	8.268880	8.614267	7.335503
26	H	8.279165	7.386291	8.227597	9.324057	8.191026
27	H	6.845635	6.446186	7.576616	7.842179	6.840077
28	C	1.523594	3.690171	5.435987	2.160758	2.173637
29	H	2.132576	4.507766	6.467199	2.414521	2.535213
30	H	2.177033	4.330923	5.571867	2.543716	3.086050
31	C	2.586139	3.549637	5.338537	3.510366	2.828728
32	O	3.652190	4.525350	5.940538	4.493693	4.016648
33	O	2.813166	2.835112	5.043033	3.849518	2.556732
34	H	3.772143	3.298283	5.256903	4.827321	3.521986

		11	12	13	14	15

11	Br	0.000000				
12	H	5.627330	0.000000			
13	C	4.041908	2.775829	0.000000		
14	C	3.559247	4.083704	1.325786	0.000000	
15	H	4.989144	2.480108	1.081490	2.117338	0.000000
16	H	4.287187	4.754249	2.077605	1.080801	2.437397
17	H	2.769651	4.704081	2.123302	1.079824	3.092048
18	C	3.728820	6.694359	6.610763	6.731756	7.329320
19	C	5.066782	7.910887	8.016611	8.160844	8.733392
20	O	4.698213	6.728847	7.087534	7.401877	7.778506
21	H	3.850283	6.294692	6.348326	6.541476	6.947150
22	H	2.824997	6.580615	6.095306	6.057562	6.919838
23	H	5.305005	8.625610	8.535292	8.574287	9.334784
24	C	6.289621	8.664143	9.036350	9.258481	9.644115
25	H	7.161799	9.245922	9.800729	10.089230	10.405907
26	H	6.598604	9.444143	9.613283	9.718778	10.235212
27	H	6.310760	8.101501	8.677194	8.999661	9.182385
28	C	6.282183	3.347835	5.489284	6.566126	5.578419
29	H	7.352415	4.145944	6.493867	7.614400	6.503091
30	H	6.254061	2.852581	5.100525	6.213030	5.028540
31	C	5.643765	4.322677	5.886809	6.746889	6.175326
32	O	5.744654	4.864212	6.278300	7.052670	6.515774
33	O	5.481733	4.966183	6.217333	6.964603	6.686986
34	H	5.251493	5.684121	6.631452	7.229093	7.179741

		16	17	18	19	20
16	H	0.000000				
17	H	1.844615	0.000000			
18	C	7.563001	6.206940	0.000000		
19	C	9.011271	7.598380	1.467373	0.000000	
20	O	8.332398	6.918565	1.462282	1.444141	0.000000
21	H	7.301497	6.160313	1.087054	2.198043	2.135798
22	H	6.892359	5.413480	1.087096	2.250173	2.149549
23	H	9.436824	7.901321	2.190697	1.088096	2.110076
24	C	10.059803	8.790658	2.604943	1.505933	2.509492
25	H	10.937112	9.617483	3.445671	2.152854	2.920988
26	H	10.453505	9.212017	3.146803	2.143964	3.416412
27	H	9.770379	8.650901	2.733474	2.151201	2.697305
28	C	7.430565	6.766951	5.302021	6.045795	4.760752
29	H	8.461958	7.843773	6.071116	6.631505	5.367574
30	H	6.971065	6.550285	5.589684	6.479592	5.307586
31	C	7.645600	6.747828	3.939846	4.571018	3.344728
32	O	7.862089	7.069220	3.709138	4.319526	3.385193
33	O	7.951504	6.786429	3.570531	4.005916	2.612741
34	H	8.200539	6.940724	2.750652	3.019767	1.657267

		21	22	23	24	25
21	H	0.000000				
22	H	1.841657	0.000000			
23	H	3.114631	2.555054	0.000000		
24	C	2.801111	3.571528	2.206906	0.000000	
25	H	3.750497	4.376969	2.562127	1.094323	0.000000
26	H	3.288192	3.982353	2.560697	1.094363	1.769489
27	H	2.516914	3.803856	3.098141	1.092231	1.776017
28	C	4.954171	5.674694	6.868519	6.469694	6.769620
29	H	5.729799	6.548962	7.460594	6.888766	7.048181
30	H	5.056469	5.944141	7.372347	6.839184	7.261629
31	C	3.622822	4.472650	5.437240	4.950427	5.271907
32	O	3.118903	4.417596	5.319027	4.420120	4.853447
33	O	3.639667	4.016300	4.688013	4.625881	4.813573
34	H	2.938402	3.336566	3.727134	3.654624	3.867316

		26	27	28	29	30
26	H	0.000000				
27	H	1.775785	0.000000			
28	C	7.430282	5.841911	0.000000		
29	H	7.885244	6.223501	1.097378	0.000000	
30	H	7.715114	6.105859	1.095894	1.752163	0.000000
31	C	5.919003	4.352157	1.519975	2.135631	2.111015
32	O	5.294672	3.629040	2.370181	2.850391	2.494986
33	O	5.658470	4.307874	2.392687	2.906882	3.242542
34	H	4.687299	3.436089	3.251949	3.763770	3.963271

		31	32	33	34
31	C	0.000000			
32	O	1.202490	0.000000		
33	O	1.335325	2.258544	0.000000	
34	H	1.900132	2.346964	1.003642	0.000000

Stoichiometry C11H17BrN2O3
Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.151831	1.096654	1.398719
2	6	0	-2.077533	0.172490	1.029050
3	7	0	-2.801479	0.727741	-0.014480

4	6	0	-2.292446	1.942955	-0.291377
5	7	0	-1.283190	2.182054	0.551309
6	6	0	-0.430901	3.379897	0.558526
7	1	0	-0.373067	1.053926	2.138169
8	1	0	-2.273293	-0.818458	1.402588
9	1	0	-1.066808	4.265582	0.483888
10	1	0	0.058838	3.398398	1.530471
11	35	0	-1.028304	-2.684256	-0.007519
12	1	0	-2.641140	2.601931	-1.066683
13	6	0	-3.841226	0.116790	-0.768199
14	6	0	-4.174247	-1.163817	-0.685418
15	1	0	-4.286144	0.793608	-1.484849
16	1	0	-4.941463	-1.549670	-1.341640
17	1	0	-3.675509	-1.870447	-0.038925
18	6	0	2.522708	-1.552409	-0.122981
19	6	0	3.907615	-1.600646	0.359604
20	8	0	3.060654	-0.489480	0.724995
21	1	0	2.350538	-1.232099	-1.147406
22	1	0	1.719091	-2.123199	0.335469
23	1	0	4.117803	-2.251106	1.206172
24	6	0	5.082091	-1.287874	-0.529560
25	1	0	5.882502	-0.805460	0.039793
26	1	0	5.484113	-2.210609	-0.959175
27	1	0	4.785006	-0.624421	-1.344752
28	6	0	0.582815	3.360893	-0.578732
29	1	0	1.096513	4.330580	-0.586501
30	1	0	0.088658	3.272054	-1.552848
31	6	0	1.634452	2.264663	-0.527146
32	8	0	2.142334	1.855322	-1.537333
33	8	0	1.937427	1.869461	0.711852
34	1	0	2.565395	1.089800	0.640563

Rotational constants (GHZ): 0.3413111 0.2567545 0.1602731

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 538 symmetry adapted cartesian basis functions of A symmetry.

There are 519 symmetry adapted basis functions of A symmetry.

519 basis functions, 823 primitive gaussians, 538 cartesian basis functions

78 alpha electrons 78 beta electrons

nuclear repulsion energy 1577.1475450522 Hartrees.

NAtoms= 34 NActive= 34 NUniq= 34 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.
NBasis= 519 RedAO= T EigKep= 3.20D-06 NBF= 519
NBsUse= 519 1.00D-06 EigRej= -1.00D+00 NBFU= 519
Lowest energy guess from the checkpoint file: "./coohpo.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999850 0.001201 -0.000261 0.017295 Ang= 1.99 deg.
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999458 0.003006 -0.000388 -0.032769 Ang= 3.77 deg.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3338.89812759 A.U. after 14 cycles
NFock= 14 Conv=0.18D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.002932562	-0.000136093	-0.001110115
2	6	-0.005525516	0.000566346	0.003156468
3	7	0.002118043	0.000615449	-0.000466770
4	6	0.000391564	-0.002311688	0.001004053
5	7	-0.003591076	0.001112852	0.002758407
6	6	-0.000641418	0.000462399	0.000603332
7	1	0.000364687	-0.000396441	0.000161569
8	1	0.002085095	-0.000159830	-0.001409588
9	1	-0.000725536	-0.001467000	0.000774870
10	1	0.000935734	0.000691811	-0.000937793
11	35	-0.000189006	-0.000647105	0.001253042
12	1	0.000054445	0.000014131	-0.000285997
13	6	-0.001062473	-0.001686608	-0.003963796
14	6	-0.000724480	0.000367965	0.000770536
15	1	-0.001254770	0.001156037	-0.000049682
16	1	-0.001509116	0.000292923	-0.000697862
17	1	0.003168925	-0.000533457	0.001653016
18	6	-0.001234648	0.002480097	-0.000638196
19	6	0.001458708	-0.000523214	-0.001353147
20	8	0.000228285	-0.000283579	0.002332912
21	1	-0.000517946	-0.000701988	0.000999952
22	1	0.001655722	-0.000952261	-0.001408545
23	1	-0.000220071	0.000186394	0.000280285

24	6	-0.000271266	0.000270387	0.000220702
25	1	-0.000153491	-0.000187579	-0.000003436
26	1	-0.000204225	-0.000055956	0.000182115
27	1	0.000053650	-0.000027126	0.000224937
28	6	-0.002461589	0.003095190	-0.003125390
29	1	0.001739640	-0.001366980	0.000965025
30	1	0.000606412	0.001752602	0.002032726
31	6	-0.002854411	0.006685200	-0.000597463
32	8	0.005731917	-0.005933920	-0.002111089
33	8	0.003689091	-0.004237336	-0.004560907
34	1	-0.004073444	0.001858379	0.003345831

Cartesian Forces: Max 0.006685200 RMS 0.002012243

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.007449199 RMS 0.001755183

Search for a local minimum.

Step number 12 out of a maximum of 175

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 10 12

ITU= 0 -1 1 1 1 0 1 0 -1 0 1 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00098	0.00317	0.00330	0.00568	0.00698
Eigenvalues ---	0.00897	0.01083	0.01493	0.01625	0.01753
Eigenvalues ---	0.01812	0.01914	0.02209	0.02277	0.02315
Eigenvalues ---	0.02426	0.02468	0.02764	0.02938	0.03004
Eigenvalues ---	0.03078	0.03158	0.03391	0.03749	0.04107
Eigenvalues ---	0.04339	0.04584	0.05188	0.05270	0.05776
Eigenvalues ---	0.05878	0.06971	0.07853	0.09482	0.09859
Eigenvalues ---	0.11920	0.12640	0.12756	0.13316	0.14220
Eigenvalues ---	0.15341	0.15811	0.15939	0.15967	0.15997
Eigenvalues ---	0.16000	0.16000	0.16004	0.16070	0.16450
Eigenvalues ---	0.16835	0.18163	0.19409	0.21731	0.22389
Eigenvalues ---	0.22533	0.23027	0.23801	0.24953	0.25546
Eigenvalues ---	0.26336	0.28202	0.28895	0.29983	0.31125
Eigenvalues ---	0.31914	0.32307	0.34497	0.34536	0.34612
Eigenvalues ---	0.34765	0.34884	0.34942	0.34959	0.35079
Eigenvalues ---	0.35113	0.35695	0.35739	0.35969	0.36538
Eigenvalues ---	0.36878	0.36996	0.37083	0.37703	0.38262

Eigenvalues --- 0.41288 0.42300 0.45781 0.48994 0.51872
Eigenvalues --- 0.52985 0.55515 0.56117 0.60378 0.89825
Eigenvalues --- 1.00689
RFO step: Lambda=-3.53014033D-03 EMin= 9.81726714D-04
Quartic linear search produced a step of 0.01620.
Iteration 1 RMS(Cart)= 0.17941599 RMS(Int)= 0.01081425
Iteration 2 RMS(Cart)= 0.01521072 RMS(Int)= 0.00018434
Iteration 3 RMS(Cart)= 0.00012120 RMS(Int)= 0.00017311
Iteration 4 RMS(Cart)= 0.00000002 RMS(Int)= 0.00017311

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56868	0.00214	-0.00004	0.00164	0.00158	2.57026
R2	2.61401	0.00082	-0.00009	-0.00154	-0.00155	2.61247
R3	2.03098	0.00022	0.00000	0.00026	0.00026	2.03124
R4	2.61941	0.00103	0.00005	0.00574	0.00571	2.62511
R5	2.03515	0.00047	0.00004	0.00208	0.00212	2.03727
R6	2.54414	-0.00097	0.00007	-0.00042	-0.00039	2.54376
R7	2.68742	0.00183	-0.00003	0.00186	0.00183	2.68925
R8	2.52538	0.00072	0.00001	0.00102	0.00110	2.52647
R9	2.03261	0.00023	0.00000	0.00203	0.00202	2.03463
R10	2.77814	0.00357	-0.00008	0.00416	0.00408	2.78222
R11	2.06524	-0.00063	0.00001	-0.00221	-0.00220	2.06305
R12	2.05699	-0.00002	0.00004	0.00301	0.00305	2.06004
R13	2.87918	0.00406	-0.00017	-0.00065	-0.00082	2.87835
R14	5.00674	0.00005	-0.00246	-0.11102	-0.11348	4.89326
R15	2.50537	0.00056	0.00005	0.00328	0.00333	2.50870
R16	2.04372	0.00099	0.00001	0.00344	0.00345	2.04717
R17	2.04242	0.00103	-0.00001	0.00166	0.00165	2.04407
R18	2.04057	0.00324	-0.00003	0.00502	0.00499	2.04556
R19	2.77293	0.00044	-0.00004	-0.00209	-0.00255	2.77039
R20	2.76331	-0.00014	0.00015	0.00488	0.00521	2.76852
R21	2.05423	-0.00078	0.00003	0.00111	0.00114	2.05537
R22	2.05431	-0.00152	0.00002	-0.00043	-0.00041	2.05390
R23	2.72903	-0.00011	-0.00002	-0.00054	-0.00033	2.72870
R24	2.05620	0.00015	-0.00001	-0.00018	-0.00019	2.05601
R25	2.84580	-0.00083	0.00003	-0.00060	-0.00057	2.84523
R26	3.13178	0.00051	-0.00146	-0.05058	-0.05204	3.07974
R27	2.06797	-0.00023	0.00000	-0.00079	-0.00079	2.06718
R28	2.06805	-0.00007	0.00000	-0.00044	-0.00044	2.06760
R29	2.06402	-0.00022	0.00000	-0.00060	-0.00060	2.06342
R30	2.07374	-0.00104	0.00001	-0.00527	-0.00526	2.06849
R31	2.07094	-0.00266	0.00009	-0.00512	-0.00503	2.06591
R32	2.87234	0.00265	0.00000	0.01444	0.01444	2.88678
R33	2.27238	0.00745	0.00003	0.01045	0.01048	2.28286

R34	2.52340	-0.00053	-0.00026	-0.01132	-0.01158	2.51182
R35	1.89661	-0.00305	0.00024	-0.00374	-0.00350	1.89311
A1	1.87780	0.00009	0.00006	0.00214	0.00171	1.87951
A2	2.28306	-0.00036	0.00003	0.00071	0.00044	2.28350
A3	2.11940	0.00036	-0.00005	0.00067	0.00033	2.11973
A4	1.86301	-0.00047	-0.00003	-0.00188	-0.00219	1.86082
A5	2.28505	-0.00112	0.00006	-0.00252	-0.00232	2.28273
A6	2.13503	0.00159	-0.00002	0.00443	0.00454	2.13957
A7	1.89541	-0.00005	0.00001	0.00069	0.00029	1.89570
A8	2.22529	0.00079	0.00007	0.00778	0.00789	2.23318
A9	2.15941	-0.00068	-0.00008	-0.00643	-0.00648	2.15292
A10	1.89373	0.00126	-0.00005	0.00017	-0.00004	1.89369
A11	2.18790	-0.00056	0.00002	0.00005	0.00014	2.18804
A12	2.20153	-0.00069	0.00003	-0.00027	-0.00017	2.20136
A13	1.89402	-0.00078	0.00003	0.00089	0.00084	1.89486
A14	2.19109	0.00095	-0.00012	0.00485	0.00472	2.19581
A15	2.19778	-0.00016	0.00008	-0.00606	-0.00599	2.19179
A16	1.89933	-0.00357	0.00034	0.00013	0.00048	1.89980
A17	1.85362	-0.00123	-0.00002	0.00465	0.00462	1.85824
A18	1.95185	0.00726	-0.00062	-0.00252	-0.00315	1.94870
A19	1.88493	0.00109	-0.00004	-0.00257	-0.00260	1.88233
A20	1.92439	-0.00074	0.00020	0.00697	0.00718	1.93157
A21	1.94696	-0.00303	0.00016	-0.00673	-0.00657	1.94039
A22	1.95839	0.00704	0.00195	0.08625	0.08821	2.04660
A23	2.17186	-0.00248	0.00016	-0.00122	-0.00113	2.17073
A24	1.96397	0.00088	-0.00010	-0.00175	-0.00192	1.96205
A25	2.14424	0.00168	-0.00007	0.00460	0.00446	2.14871
A26	2.07743	-0.00084	-0.00009	-0.00724	-0.00735	2.07008
A27	2.15731	-0.00060	0.00014	0.00380	0.00390	2.16121
A28	2.04626	0.00141	-0.00006	0.00261	0.00252	2.04877
A29	2.05906	0.00006	-0.00010	-0.00387	-0.00363	2.05543
A30	2.14329	0.00016	0.00009	-0.00433	-0.00471	2.13859
A31	1.97204	0.00050	-0.00007	0.00242	0.00225	1.97429
A32	1.99222	0.00076	0.00002	0.01173	0.01173	2.00395
A33	2.02090	-0.00063	0.00004	0.00111	0.00103	2.02193
A34	2.04636	0.00008	-0.00001	-0.00137	-0.00140	2.04496
A35	2.13537	-0.00007	-0.00003	-0.00022	-0.00025	2.13513
A36	1.95670	-0.00005	0.00003	-0.00022	-0.00009	1.95661
A37	2.03418	0.00007	-0.00003	-0.00118	-0.00140	2.03279
A38	2.01849	0.00002	0.00000	0.00095	0.00097	2.01946
A39	2.15701	-0.00044	-0.00113	-0.03557	-0.03737	2.11964
A40	2.68057	-0.00103	0.00006	-0.01078	-0.01182	2.66875
A41	1.93350	0.00000	-0.00003	-0.00011	-0.00014	1.93336
A42	1.92109	-0.00038	0.00001	-0.00221	-0.00220	1.91889

A43	1.93340	0.00003	0.00000	0.00062	0.00062	1.93402
A44	1.88310	0.00016	0.00000	0.00040	0.00040	1.88350
A45	1.89598	0.00004	0.00000	0.00005	0.00005	1.89603
A46	1.89557	0.00016	0.00002	0.00130	0.00132	1.89688
A47	1.88149	0.00071	0.00007	0.00108	0.00104	1.88253
A48	1.94387	0.00007	0.00008	0.00957	0.00967	1.95355
A49	2.03085	-0.00033	-0.00011	-0.01214	-0.01229	2.01856
A50	1.85086	0.00018	-0.00018	-0.00215	-0.00231	1.84856
A51	1.88984	-0.00143	0.00019	-0.00874	-0.00862	1.88122
A52	1.85843	0.00078	-0.00007	0.01257	0.01255	1.87097
A53	2.10507	0.00713	-0.00046	0.01580	0.01487	2.11994
A54	1.98441	-0.00514	0.00038	-0.00161	-0.00170	1.98271
A55	2.19309	-0.00195	0.00008	-0.01233	-0.01272	2.18037
A56	1.88175	0.00743	-0.00050	0.02131	0.02081	1.90256
A57	2.74826	0.00506	-0.00025	0.02643	0.02618	2.77444
D1	-0.03820	0.00142	0.00009	0.04750	0.04759	0.00939
D2	3.08897	0.00147	0.00044	0.05042	0.05089	3.13987
D3	-3.09666	0.00001	-0.00039	-0.00251	-0.00293	-3.09959
D4	0.03051	0.00006	-0.00004	0.00041	0.00038	0.03088
D5	0.03100	-0.00142	0.00011	-0.02892	-0.02888	0.00212
D6	-3.08568	-0.00155	0.00067	-0.01537	-0.01469	-3.10037
D7	3.09887	-0.00021	0.00054	0.01542	0.01592	3.11479
D8	-0.01781	-0.00034	0.00110	0.02897	0.03011	0.01231
D9	0.03228	-0.00094	-0.00026	-0.04966	-0.04990	-0.01763
D10	3.09136	-0.00012	-0.00037	-0.02277	-0.02299	3.06837
D11	-3.09642	-0.00096	-0.00058	-0.05220	-0.05281	3.13396
D12	-0.03734	-0.00014	-0.00069	-0.02531	-0.02589	-0.06323
D13	-1.65084	0.00038	0.00077	0.02910	0.02984	-1.62100
D14	1.47441	0.00042	0.00117	0.03235	0.03354	1.50795
D15	-0.01329	0.00005	0.00033	0.03213	0.03249	0.01920
D16	3.12193	0.00062	0.00007	0.02474	0.02479	-3.13646
D17	-3.07619	-0.00081	0.00043	0.00568	0.00627	-3.06992
D18	0.05904	-0.00024	0.00017	-0.00171	-0.00143	0.05761
D19	-0.14945	-0.00101	-0.00545	-0.20349	-0.20895	-0.35840
D20	3.07485	-0.00205	-0.00527	-0.22544	-0.23069	2.84416
D21	2.89809	-0.00003	-0.00557	-0.17239	-0.17798	2.72011
D22	-0.16080	-0.00107	-0.00540	-0.19434	-0.19972	-0.36051
D23	-0.01075	0.00083	-0.00027	-0.00222	-0.00250	-0.01325
D24	3.10581	0.00098	-0.00083	-0.01564	-0.01646	3.08935
D25	3.13728	0.00025	-0.00001	0.00524	0.00527	-3.14064
D26	-0.02935	0.00040	-0.00057	-0.00818	-0.00869	-0.03804
D27	-2.35773	0.00097	0.00155	0.06173	0.06326	-2.29447
D28	-0.33242	-0.00014	0.00165	0.06123	0.06288	-0.26955
D29	1.79526	-0.00038	0.00145	0.05450	0.05594	1.85121

D30	0.81303	0.00083	0.00220	0.07746	0.07967	0.89270
D31	2.83835	-0.00029	0.00231	0.07696	0.07928	2.91763
D32	-1.31716	-0.00053	0.00211	0.07024	0.07235	-1.24480
D33	3.02310	0.00053	-0.00188	0.04672	0.04483	3.06793
D34	0.99954	-0.00015	-0.00175	0.04343	0.04167	1.04121
D35	-1.13450	-0.00101	-0.00165	0.02779	0.02615	-1.10835
D36	0.90734	0.00069	-0.00204	0.04342	0.04138	0.94873
D37	-1.11621	0.00001	-0.00191	0.04013	0.03822	-1.07799
D38	3.03293	-0.00085	-0.00181	0.02450	0.02270	3.05563
D39	-1.18696	0.00179	-0.00221	0.04639	0.04418	-1.14278
D40	3.07267	0.00111	-0.00209	0.04310	0.04102	3.11369
D41	0.93862	0.00025	-0.00199	0.02747	0.02550	0.96413
D42	-3.07964	-0.00118	-0.00007	-0.03226	-0.03235	-3.11200
D43	-0.01110	-0.00165	-0.00033	-0.04610	-0.04645	-0.05755
D44	-0.02902	-0.00010	-0.00026	-0.00844	-0.00869	-0.03770
D45	3.03952	-0.00057	-0.00052	-0.02228	-0.02278	3.01674
D46	-2.74819	0.00039	0.00001	0.00609	0.00605	-2.74214
D47	-0.05181	0.00049	-0.00007	0.00469	0.00456	-0.04725
D48	0.01270	-0.00099	0.00010	-0.01533	-0.01527	-0.00257
D49	2.70908	-0.00090	0.00002	-0.01672	-0.01676	2.69232
D50	0.68846	-0.00096	0.00002	-0.00822	-0.00781	0.68065
D51	-1.66913	-0.00134	0.00002	-0.02479	-0.02441	-1.69354
D52	2.49893	0.00047	0.00261	0.08474	0.08734	2.58627
D53	0.11661	0.00041	0.00261	0.08481	0.08747	0.20408
D54	2.55335	-0.00003	0.00006	0.00374	0.00383	2.55718
D55	-1.64864	-0.00007	0.00005	0.00275	0.00284	-1.64580
D56	0.44801	-0.00010	0.00009	0.00333	0.00345	0.45146
D57	1.32876	0.00012	-0.00001	0.00120	0.00116	1.32992
D58	-2.87323	0.00007	-0.00002	0.00021	0.00017	-2.87306
D59	-0.77657	0.00005	0.00002	0.00079	0.00078	-0.77580
D60	-1.02689	0.00008	-0.00002	0.00182	0.00180	-1.02509
D61	1.05431	0.00004	-0.00002	0.00084	0.00081	1.05512
D62	-3.13223	0.00001	0.00001	0.00141	0.00142	-3.13081
D63	1.13327	0.00160	-0.00391	0.04497	0.04064	1.17391
D64	2.71806	0.00057	-0.00631	-0.03874	-0.04463	2.67344
D65	2.66786	0.00033	0.00043	0.06096	0.06121	2.72908
D66	-0.50918	0.00128	0.00041	0.11482	0.11532	-0.39386
D67	-1.49415	-0.00009	0.00060	0.04712	0.04765	-1.44649
D68	1.61200	0.00087	0.00058	0.10099	0.10175	1.71375
D69	0.48959	-0.00017	0.00045	0.04672	0.04703	0.53663
D70	-2.68745	0.00079	0.00043	0.10058	0.10114	-2.58631
D71	3.04598	0.00044	0.00128	0.03503	0.03669	3.08267
D72	-0.13316	0.00166	0.00125	0.09277	0.09364	-0.03952
D73	-1.89000	0.00208	-0.00256	0.01368	0.01112	-1.87888

Item	Value	Threshold	Converged?
Maximum Force	0.007449	0.000450	NO
RMS Force	0.001755	0.000300	NO
Maximum Displacement	1.237278	0.001800	NO
RMS Displacement	0.183155	0.001200	NO

Predicted change in Energy=-2.343257D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.169491	1.761509	1.703007
2	6	0	-1.925054	0.634725	1.800045
3	7	0	-2.663019	0.548947	0.626253
4	6	0	-2.370612	1.613525	-0.143910
5	7	0	-1.457053	2.356791	0.488868
6	6	0	-0.825534	3.575272	-0.044163
7	1	0	-0.438193	2.177167	2.372197
8	1	0	-1.992475	-0.102756	2.583516
9	1	0	-1.606511	4.253497	-0.393351
10	1	0	-0.318658	4.052867	0.794502
11	35	0	-0.465257	-2.184612	2.387376
12	1	0	-2.795000	1.817587	-1.112153
13	6	0	-3.538966	-0.495479	0.217512
14	6	0	-3.507997	-1.731698	0.700403
15	1	0	-4.202867	-0.188792	-0.581706
16	1	0	-4.200750	-2.460766	0.302188
17	1	0	-2.776641	-2.080056	1.418384
18	6	0	2.970215	-0.800195	0.708249
19	6	0	4.282608	-0.426297	1.244023
20	8	0	3.202657	0.531801	1.272244
21	1	0	2.842268	-0.790255	-0.371811
22	1	0	2.265592	-1.414005	1.263268
23	1	0	4.534725	-0.788470	2.238507
24	6	0	5.450947	-0.094594	0.354145
25	1	0	6.082343	0.672142	0.812490
26	1	0	6.065051	-0.986313	0.196566
27	1	0	5.108188	0.270031	-0.616339
28	6	0	0.151566	3.256208	-1.168210
29	1	0	0.525192	4.204422	-1.567502
30	1	0	-0.339011	2.751269	-2.004588
31	6	0	1.359157	2.407772	-0.773884

32	8	0	1.958363	1.746775	-1.588371
33	8	0	1.647022	2.461916	0.522639
34	1	0	2.410268	1.841777	0.713594

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.360123	0.000000			
3	N	2.204616	1.389150	0.000000		
4	C	2.208098	2.221606	1.346098	0.000000	
5	N	1.382457	2.214435	2.177505	1.336952	0.000000
6	C	2.541780	3.640998	3.603394	2.499133	1.472288
7	H	1.074887	2.217486	3.263322	3.222224	2.148783
8	H	2.219929	1.078077	2.169152	3.244605	3.274691
9	H	3.285682	4.243579	3.984908	2.759623	2.097174
10	H	2.607608	3.908366	4.219217	3.322878	2.065437
11	Br	4.066469	3.228718	3.924799	4.946072	5.021188
12	H	3.251239	3.261421	2.156137	1.076681	2.155020
13	C	3.593759	2.527150	1.423088	2.437945	3.541672
14	C	4.321612	3.052029	2.433275	3.632772	4.578959
15	H	4.269070	3.396962	2.091544	2.607139	3.894306
16	H	5.383162	4.123643	3.395292	4.488681	5.547214
17	H	4.173914	2.870696	2.748096	4.030901	4.721326
18	C	4.968807	5.216769	5.793119	5.922555	5.442003
19	C	5.892584	6.322183	7.040914	7.095955	6.423360
20	O	4.562172	5.155831	5.901166	5.851235	5.065291
21	H	5.187541	5.429078	5.753067	5.744930	5.397113
22	H	4.698622	4.695417	5.343236	5.713185	5.355062
23	H	6.271143	6.629214	7.496370	7.689550	6.989658
24	C	7.006764	7.551683	8.143993	8.021379	7.331296
25	H	7.387072	8.068152	8.748212	8.558818	7.732094
26	H	7.884065	8.309073	8.872477	8.833770	8.236737
27	H	6.856611	7.445697	7.874864	7.613187	6.976994
28	C	3.496171	4.471585	4.297820	3.179463	2.478410
29	H	4.419956	5.485146	5.323510	4.138242	3.401719
30	H	3.926268	4.633630	4.143979	2.980602	2.760970
31	C	3.598153	4.533746	4.646882	3.865084	3.086775
32	O	4.540579	5.272471	5.262749	4.565551	4.043774
33	O	3.133142	4.210715	4.716634	4.159980	3.106038
34	H	3.714843	4.629511	5.236151	4.862533	3.907930

		6	7	8	9	10
6	C	0.000000				
7	H	2.818426	0.000000			
8	H	4.668440	2.767399	0.000000		

9	H	1.091717	3.650255	5.290335	0.000000	
10	H	1.090128	2.453907	4.824048	1.763466	0.000000
11	Br	6.262462	4.361890	2.589400	7.105219	6.439323
12	H	2.847605	4.221911	4.241431	2.804075	3.842406
13	C	4.899203	4.626067	2.853742	5.163361	5.602745
14	C	5.992822	5.243837	2.914854	6.374520	6.606204
15	H	5.085618	5.338172	3.861588	5.148832	5.913772
16	H	6.924290	6.320775	3.954889	7.231540	7.598712
17	H	6.158619	4.949954	2.425317	6.690700	6.636539
18	C	5.841109	4.821894	5.350827	6.906501	5.863134
19	C	6.615519	5.507883	6.424609	7.698259	6.437129
20	O	5.217468	4.144022	5.395508	6.305024	5.002580
21	H	5.711213	5.205440	5.708008	6.725439	5.899794
22	H	6.013096	4.629978	4.646888	7.061030	6.065046
23	H	7.279094	5.791614	6.572182	8.370358	7.005642
24	C	7.281537	6.626870	7.770116	8.323002	7.119248
25	H	7.541935	6.871331	8.302993	8.567300	7.238953
26	H	8.267174	7.552031	8.449967	9.308946	8.154913
27	H	6.816235	6.582618	7.797273	7.810564	6.763947
28	C	1.523158	3.747883	5.473117	2.164678	2.169797
29	H	2.130928	4.534215	6.490099	2.434173	2.512791
30	H	2.181502	4.415391	5.650673	2.541521	3.086985
31	C	2.582329	3.630629	5.367339	3.513786	2.825108
32	O	3.671248	4.649174	6.036102	4.518856	4.022558
33	O	2.770263	2.801797	4.906190	3.825477	2.543409
34	H	3.748282	3.313183	5.163523	4.814170	3.513190

		11	12	13	14	15
11	Br	0.000000				
12	H	5.804481	0.000000			
13	C	4.124217	2.769796	0.000000		
14	C	3.508458	4.048599	1.327547	0.000000	
15	H	5.173825	2.507792	1.083314	2.123018	0.000000
16	H	4.286978	4.720254	2.075448	1.081675	2.437855
17	H	2.508460	4.647104	2.129347	1.082466	3.100219
18	C	4.066761	6.588199	6.534762	6.544845	7.313748
19	C	5.190486	7.789681	7.888950	7.917899	8.682913
20	O	4.698512	6.581071	6.900526	7.105161	7.667997
21	H	4.527368	6.255217	6.415165	6.508596	7.073877
22	H	3.052046	6.457199	5.969103	5.809654	6.837107
23	H	5.193380	8.470144	8.327950	8.242623	9.201018
24	C	6.595731	8.590816	8.999884	9.113873	9.699526
25	H	7.315215	9.155519	9.710146	9.887651	10.414919
26	H	6.991458	9.384834	9.616574	9.615233	10.328208
27	H	6.790497	8.068528	8.720928	8.943119	9.322417

28	C	6.528796	3.279486	5.442004	6.462455	5.583288
29	H	7.579037	4.114365	6.464729	7.526456	6.528910
30	H	6.608192	2.774903	5.071372	6.120167	5.059441
31	C	5.866177	4.209485	5.779562	6.557280	6.141270
32	O	6.093955	4.777684	6.205606	6.871634	6.536096
33	O	5.434076	4.776952	5.977772	6.647723	6.516674
34	H	5.223217	5.516227	6.411104	6.913448	7.038080

		16	17	18	19	20
16	H	0.000000				
17	H	1.849032	0.000000			
18	C	7.371914	5.930320	0.000000		
19	C	8.774593	7.252470	1.466025	0.000000	
20	O	8.044060	6.526497	1.465038	1.443968	0.000000
21	H	7.269730	6.036598	1.087657	2.194986	2.140241
22	H	6.620646	5.088398	1.086878	2.245951	2.159707
23	H	9.102441	7.469730	2.188497	1.087995	2.109783
24	C	9.937641	8.530408	2.603323	1.505631	2.508004
25	H	10.761855	9.296413	3.444413	2.152170	2.919531
26	H	10.371684	8.992476	3.142367	2.141935	3.413950
27	H	9.744602	8.475466	2.733284	2.151139	2.695611
28	C	7.334066	6.613666	5.283966	6.036988	4.763126
29	H	8.381826	7.701447	6.016925	6.592906	5.359210
30	H	6.884734	6.403161	5.560878	6.481493	5.311034
31	C	7.468143	6.484710	3.883720	4.544278	3.332327
32	O	7.694952	6.790101	3.575663	4.259907	3.347768
33	O	7.647080	6.403176	3.525148	3.975989	2.589837
34	H	7.898525	6.540759	2.700664	2.988507	1.629727

		21	22	23	24	25
21	H	0.000000				
22	H	1.842581	0.000000			
23	H	3.110976	2.547813	0.000000		
24	C	2.795740	3.565647	2.207204	0.000000	
25	H	3.746900	4.372963	2.561647	1.093904	0.000000
26	H	3.278387	3.969467	2.559407	1.094129	1.769219
27	H	2.513641	3.801217	3.098295	1.091913	1.775450
28	C	4.924225	5.673807	6.868568	6.452044	6.765699
29	H	5.634299	6.527556	7.449231	6.814494	7.001664
30	H	5.032781	5.900199	7.367965	6.869219	7.313855
31	C	3.548050	4.424658	5.419843	4.927172	5.276124
32	O	2.949208	4.268110	5.264038	4.400244	4.891439
33	O	3.578446	3.994237	4.674189	4.586282	4.791595
34	H	2.879639	3.305026	3.709027	3.622770	3.855122

		26	27	28	29	30
26	H	0.000000				

27	H	1.776176	0.000000			
28	C	7.404789	5.812909	0.000000		
29	H	7.793953	6.114573	1.094596	0.000000	
30	H	7.734766	6.144571	1.093232	1.746294	0.000000
31	C	5.882773	4.318563	1.527617	2.133842	2.125181
32	O	5.246013	3.612065	2.391535	2.845074	2.541687
33	O	5.613875	4.252211	2.392960	2.943386	3.227216
34	H	4.650037	3.393800	3.262443	3.786688	3.971677

		31	32	33	34
31	C	0.000000			
32	O	1.208038	0.000000		
33	O	1.329199	2.250494	0.000000	
34	H	1.907295	2.347825	1.001789	0.000000

Stoichiometry C11H17BrN2O3
Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.130511	1.149292	1.411964
2	6	0	-2.103323	0.317204	0.952398
3	7	0	-2.676249	0.944643	-0.146608
4	6	0	-2.073369	2.134974	-0.324454
5	7	0	-1.124032	2.273026	0.606751
6	6	0	-0.193607	3.408440	0.719789
7	1	0	-0.428841	1.032730	2.217851
8	1	0	-2.423981	-0.651429	1.300506
9	1	0	-0.767079	4.337281	0.704609
10	1	0	0.279708	3.323917	1.698159
11	35	0	-1.334602	-2.727307	0.200974
12	1	0	-2.311863	2.844917	-1.097980
13	6	0	-3.680254	0.438054	-1.018686
14	6	0	-3.964788	-0.850268	-1.165818
15	1	0	-4.153497	1.218953	-1.601617
16	1	0	-4.729091	-1.133949	-1.876725
17	1	0	-3.423411	-1.647165	-0.672262
18	6	0	2.505442	-1.615065	-0.544363
19	6	0	3.780583	-1.848470	0.140302
20	8	0	2.921908	-0.774411	0.580889

21	1	0	2.530704	-1.094193	-1.498854
22	1	0	1.622743	-2.221409	-0.358636
23	1	0	3.816586	-2.664802	0.858660
24	6	0	5.102029	-1.448015	-0.459981
25	1	0	5.806189	-1.143851	0.319935
26	1	0	5.539834	-2.294714	-0.997147
27	1	0	4.975321	-0.618381	-1.158498
28	6	0	0.843378	3.398493	-0.395816
29	1	0	1.451028	4.303601	-0.297423
30	1	0	0.380061	3.454491	-1.384430
31	6	0	1.790269	2.199801	-0.407976
32	8	0	2.349669	1.848380	-1.419376
33	8	0	1.903484	1.599073	0.772310
34	1	0	2.493033	0.795111	0.674032

Rotational constants (GHZ): 0.3279702 0.2558542 0.1583981

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 538 symmetry adapted cartesian basis functions of A symmetry.

There are 519 symmetry adapted basis functions of A symmetry.

519 basis functions, 823 primitive gaussians, 538 cartesian basis functions

78 alpha electrons 78 beta electrons

nuclear repulsion energy 1570.5136681816 Hartrees.

NAtoms= 34 NActive= 34 NUniq= 34 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 519 RedAO= T EigKep= 4.62D-06 NBF= 519

NBsUse= 519 1.00D-06 EigRej= -1.00D+00 NBFU= 519

Initial guess from the checkpoint file: "./coohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999362 -0.009710 0.008408 0.033338 Ang= -4.09 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3338.89856457 A.U. after 14 cycles
NFock= 14 Conv=0.37D-08 -V/T= 2.0018
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000455197	0.001510731	0.001122035
2	6	-0.003956443	0.000163814	-0.000478882
3	7	0.002092641	0.004820646	0.002193370
4	6	0.001190457	-0.002975729	0.000765146
5	7	-0.002426843	0.001595247	0.000920780
6	6	-0.000113019	-0.000715333	0.002139895
7	1	0.000200832	-0.000826228	0.000131868
8	1	0.002769638	-0.002023216	-0.002217549
9	1	-0.001102805	-0.001009696	0.000010696
10	1	-0.000136895	-0.000479764	-0.001324561
11	35	0.003543210	-0.001339293	0.000896564
12	1	0.000738711	-0.000503771	0.000185306
13	6	-0.003910737	-0.004425597	-0.003426739
14	6	-0.002495339	0.001315582	-0.003340545
15	1	-0.001068967	0.000851024	0.000843961
16	1	-0.001703302	0.000515728	-0.001115985
17	1	0.003927267	0.000879828	0.004898550
18	6	-0.001196823	0.002114670	-0.001726409
19	6	0.002548829	0.000024467	-0.000764264
20	8	-0.001151644	-0.004877327	0.001261244
21	1	-0.000258328	0.000721846	0.000772001
22	1	0.000545016	0.001150783	0.002027736
23	1	-0.000412855	0.000302754	0.000292163
24	6	-0.000297243	-0.000131599	0.000352766
25	1	-0.000019167	-0.000136202	0.000091304
26	1	0.000066665	-0.000078629	-0.000000396
27	1	-0.000034135	-0.000065340	-0.000066634
28	6	0.003316433	0.002669369	-0.000797534
29	1	0.001587122	0.000294224	-0.000115234
30	1	0.000327112	0.000159588	0.001141035

31	6	-0.003652364	-0.003641933	-0.004617628
32	8	0.001474665	0.001179169	-0.000617122
33	8	0.003398541	0.003717049	-0.001588963
34	1	-0.003335030	-0.000756865	0.002152028

Cartesian Forces: Max 0.004898550 RMS 0.001972900

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.009989576 RMS 0.002398354
Search for a local minimum.
Step number 13 out of a maximum of 175
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 12 13
DE= -4.37D-04 DEPred=-2.34D-03 R= 1.86D-01
Trust test= 1.86D-01 RLast= 5.76D-01 DXMaxT set to 6.00D-01
ITU= 0 0 -1 1 1 1 0 1 0 -1 0 1 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00172	0.00326	0.00375	0.00619	0.00698
Eigenvalues ---	0.00918	0.01077	0.01474	0.01625	0.01798
Eigenvalues ---	0.01832	0.02008	0.02192	0.02327	0.02336
Eigenvalues ---	0.02443	0.02569	0.02847	0.02915	0.03014
Eigenvalues ---	0.03080	0.03302	0.03576	0.03971	0.04196
Eigenvalues ---	0.04393	0.04803	0.05171	0.05347	0.05776
Eigenvalues ---	0.05891	0.06752	0.07894	0.09462	0.09752
Eigenvalues ---	0.11899	0.12601	0.12716	0.13296	0.14368
Eigenvalues ---	0.15343	0.15773	0.15849	0.15989	0.15998
Eigenvalues ---	0.16000	0.16002	0.16004	0.16073	0.16221
Eigenvalues ---	0.16809	0.18117	0.19501	0.20497	0.21850
Eigenvalues ---	0.22395	0.23046	0.23821	0.24896	0.25276
Eigenvalues ---	0.25856	0.28339	0.28707	0.29933	0.31836
Eigenvalues ---	0.32062	0.33264	0.34497	0.34608	0.34635
Eigenvalues ---	0.34764	0.34885	0.34920	0.34987	0.35046
Eigenvalues ---	0.35314	0.35584	0.35734	0.35757	0.36544
Eigenvalues ---	0.36734	0.36932	0.37070	0.37313	0.37966
Eigenvalues ---	0.41165	0.42430	0.45618	0.49018	0.51781
Eigenvalues ---	0.53365	0.55519	0.56088	0.60516	0.88992
Eigenvalues ---	1.00747				

RFO step: Lambda=-3.37445770D-03 EMin= 1.71509654D-03
Quartic linear search produced a step of -0.42051.

Iteration 1 RMS(Cart)= 0.12596368 RMS(Int)= 0.00335617
Iteration 2 RMS(Cart)= 0.00913551 RMS(Int)= 0.00010782
Iteration 3 RMS(Cart)= 0.00003845 RMS(Int)= 0.00010720
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00010720

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.57026	0.00030	-0.00067	0.00441	0.00376	2.57402
R2	2.61247	-0.00017	0.00065	-0.00061	0.00002	2.61248
R3	2.03124	-0.00010	-0.00011	0.00068	0.00057	2.03181
R4	2.62511	0.00065	-0.00240	0.00403	0.00166	2.62677
R5	2.03727	0.00095	-0.00089	0.00122	0.00033	2.03760
R6	2.54376	-0.00106	0.00016	-0.00368	-0.00352	2.54024
R7	2.68925	0.00447	-0.00077	0.01015	0.00938	2.69863
R8	2.52647	0.00022	-0.00046	0.00165	0.00115	2.52763
R9	2.03463	-0.00055	-0.00085	-0.00011	-0.00096	2.03368
R10	2.78222	0.00153	-0.00172	0.01031	0.00859	2.79082
R11	2.06305	0.00016	0.00092	-0.00237	-0.00144	2.06160
R12	2.06004	-0.00130	-0.00128	0.00038	-0.00091	2.05914
R13	2.87835	0.00296	0.00035	0.01058	0.01093	2.88928
R14	4.89326	0.00310	0.04772	-0.00315	0.04457	4.93783
R15	2.50870	-0.00237	-0.00140	-0.00078	-0.00218	2.50652
R16	2.04717	0.00027	-0.00145	0.00325	0.00181	2.04897
R17	2.04407	0.00115	-0.00069	0.00440	0.00371	2.04778
R18	2.04556	0.00562	-0.00210	0.01762	0.01552	2.06108
R19	2.77039	0.00101	0.00107	-0.00024	0.00109	2.77148
R20	2.76852	-0.00392	-0.00219	-0.00515	-0.00746	2.76106
R21	2.05537	-0.00073	-0.00048	-0.00216	-0.00264	2.05274
R22	2.05390	0.00003	0.00017	-0.00393	-0.00375	2.05015
R23	2.72870	0.00044	0.00014	0.00240	0.00239	2.73110
R24	2.05601	0.00007	0.00008	-0.00007	0.00001	2.05602
R25	2.84523	-0.00053	0.00024	-0.00290	-0.00265	2.84257
R26	3.07974	0.00145	0.02189	0.01222	0.03410	3.11384
R27	2.06718	-0.00007	0.00033	-0.00062	-0.00029	2.06689
R28	2.06760	0.00010	0.00019	0.00001	0.00020	2.06780
R29	2.06342	0.00005	0.00025	-0.00039	-0.00014	2.06328
R30	2.06849	0.00084	0.00221	-0.00122	0.00099	2.06948
R31	2.06591	-0.00109	0.00212	-0.00523	-0.00311	2.06279
R32	2.88678	-0.00220	-0.00607	0.00634	0.00026	2.88704
R33	2.28286	0.00051	-0.00441	0.00434	-0.00007	2.28279
R34	2.51182	0.00277	0.00487	-0.00556	-0.00069	2.51113
R35	1.89311	-0.00079	0.00147	-0.00568	-0.00420	1.88890
A1	1.87951	0.00046	-0.00072	0.00080	0.00023	1.87974
A2	2.28350	-0.00095	-0.00018	-0.00447	-0.00457	2.27893
A3	2.11973	0.00040	-0.00014	0.00376	0.00371	2.12344

A4	1.86082	-0.00023	0.00092	-0.00184	-0.00088	1.85994
A5	2.28273	-0.00443	0.00097	-0.01456	-0.01366	2.26908
A6	2.13957	0.00465	-0.00191	0.01627	0.01428	2.15386
A7	1.89570	-0.00044	-0.00012	-0.00039	-0.00045	1.89525
A8	2.23318	0.00151	-0.00332	0.00598	0.00263	2.23582
A9	2.15292	-0.00110	0.00273	-0.00418	-0.00148	2.15144
A10	1.89369	0.00112	0.00002	0.00309	0.00303	1.89671
A11	2.18804	-0.00061	-0.00006	-0.00031	-0.00046	2.18758
A12	2.20136	-0.00051	0.00007	-0.00250	-0.00252	2.19884
A13	1.89486	-0.00087	-0.00035	-0.00143	-0.00178	1.89308
A14	2.19581	-0.00125	-0.00199	0.00675	0.00478	2.20059
A15	2.19179	0.00207	0.00252	-0.00556	-0.00302	2.18877
A16	1.89980	0.00097	-0.00020	-0.01317	-0.01362	1.88618
A17	1.85824	0.00103	-0.00194	-0.00343	-0.00527	1.85297
A18	1.94870	-0.00385	0.00132	0.02204	0.02334	1.97204
A19	1.88233	-0.00019	0.00109	-0.00066	0.00042	1.88275
A20	1.93157	0.00264	-0.00302	0.01509	0.01207	1.94364
A21	1.94039	-0.00054	0.00276	-0.02129	-0.01844	1.92195
A22	2.04660	-0.00039	-0.03709	0.04254	0.00545	2.05205
A23	2.17073	-0.00220	0.00047	-0.01437	-0.01426	2.15648
A24	1.96205	0.00070	0.00081	0.00678	0.00722	1.96927
A25	2.14871	0.00156	-0.00188	0.01092	0.00868	2.15739
A26	2.07008	-0.00055	0.00309	-0.00766	-0.00459	2.06549
A27	2.16121	-0.00223	-0.00164	-0.00936	-0.01103	2.15019
A28	2.04877	0.00289	-0.00106	0.01776	0.01668	2.06545
A29	2.05543	0.00049	0.00153	0.00453	0.00591	2.06134
A30	2.13859	-0.00135	0.00198	-0.01438	-0.01227	2.12632
A31	1.97429	0.00032	-0.00094	0.00535	0.00444	1.97873
A32	2.00395	-0.00199	-0.00493	0.01069	0.00579	2.00974
A33	2.02193	0.00113	-0.00043	0.00032	-0.00014	2.02178
A34	2.04496	-0.00069	0.00059	-0.00261	-0.00198	2.04298
A35	2.13513	0.00128	0.00010	0.00134	0.00142	2.13655
A36	1.95661	-0.00066	0.00004	-0.00262	-0.00264	1.95397
A37	2.03279	0.00180	0.00059	0.00221	0.00291	2.03570
A38	2.01946	-0.00033	-0.00041	0.00194	0.00152	2.02098
A39	2.11964	-0.00050	0.01571	-0.00736	0.00887	2.12851
A40	2.66875	-0.00034	0.00497	-0.02261	-0.01718	2.65157
A41	1.93336	-0.00010	0.00006	0.00064	0.00070	1.93405
A42	1.91889	-0.00001	0.00092	-0.00340	-0.00247	1.91642
A43	1.93402	0.00001	-0.00026	0.00144	0.00118	1.93520
A44	1.88350	0.00000	-0.00017	0.00012	-0.00005	1.88345
A45	1.89603	0.00011	-0.00002	0.00065	0.00063	1.89665
A46	1.89688	-0.00001	-0.00055	0.00056	0.00001	1.89689
A47	1.88253	0.00429	-0.00044	-0.00123	-0.00192	1.88060

A48	1.95355	0.00118	-0.00407	0.01507	0.01106	1.96460
A49	2.01856	-0.00886	0.00517	-0.02791	-0.02283	1.99574
A50	1.84856	-0.00089	0.00097	0.01127	0.01223	1.86079
A51	1.88122	0.00248	0.00363	-0.01261	-0.00919	1.87203
A52	1.87097	0.00242	-0.00528	0.01750	0.01231	1.88329
A53	2.11994	0.00483	-0.00625	0.02699	0.02093	2.14088
A54	1.98271	-0.00960	0.00072	-0.03493	-0.03402	1.94869
A55	2.18037	0.00477	0.00535	0.00748	0.01302	2.19339
A56	1.90256	0.00999	-0.00875	0.06203	0.05328	1.95584
A57	2.77444	-0.00493	-0.01101	0.04940	0.03839	2.81283
D1	0.00939	-0.00276	-0.02001	0.00998	-0.01002	-0.00062
D2	3.13987	-0.00357	-0.02140	-0.00415	-0.02540	3.11446
D3	-3.09959	0.00044	0.00123	0.00648	0.00766	-3.09193
D4	0.03088	-0.00037	-0.00016	-0.00765	-0.00773	0.02316
D5	0.00212	0.00182	0.01214	-0.01942	-0.00720	-0.00508
D6	-3.10037	0.00308	0.00618	-0.01275	-0.00654	-3.10690
D7	3.11479	-0.00104	-0.00670	-0.01649	-0.02315	3.09164
D8	0.01231	0.00022	-0.01266	-0.00982	-0.02249	-0.01018
D9	-0.01763	0.00274	0.02099	0.00277	0.02372	0.00609
D10	3.06837	0.00221	0.00967	0.03089	0.04046	3.10883
D11	3.13396	0.00354	0.02221	0.01570	0.03805	-3.11118
D12	-0.06323	0.00302	0.01089	0.04382	0.05479	-0.00844
D13	-1.62100	0.00562	-0.01255	0.07608	0.06354	-1.55746
D14	1.50795	0.00465	-0.01410	0.05987	0.04575	1.55370
D15	0.01920	-0.00163	-0.01366	-0.01490	-0.02857	-0.00937
D16	-3.13646	-0.00161	-0.01042	0.00639	-0.00402	-3.14048
D17	-3.06992	-0.00123	-0.00264	-0.04182	-0.04448	-3.11440
D18	0.05761	-0.00121	0.00060	-0.02054	-0.01993	0.03767
D19	-0.35840	0.00149	0.08787	-0.04685	0.04100	-0.31740
D20	2.84416	0.00013	0.09701	-0.10704	-0.01000	2.83416
D21	2.72011	0.00092	0.07484	-0.01477	0.06004	2.78015
D22	-0.36051	-0.00043	0.08398	-0.07497	0.00904	-0.35148
D23	-0.01325	-0.00011	0.00105	0.02115	0.02220	0.00895
D24	3.08935	-0.00146	0.00692	0.01485	0.02176	3.11111
D25	-3.14064	-0.00013	-0.00222	-0.00036	-0.00257	3.13998
D26	-0.03804	-0.00148	0.00365	-0.00666	-0.00301	-0.04104
D27	-2.29447	-0.00147	-0.02660	-0.01714	-0.04382	-2.33829
D28	-0.26955	-0.00067	-0.02644	-0.02624	-0.05265	-0.32219
D29	1.85121	-0.00294	-0.02353	-0.04158	-0.06504	1.78616
D30	0.89270	0.00008	-0.03350	-0.00952	-0.04312	0.84959
D31	2.91763	0.00088	-0.03334	-0.01862	-0.05195	2.86568
D32	-1.24480	-0.00139	-0.03043	-0.03397	-0.06434	-1.30915
D33	3.06793	0.00193	-0.01885	0.07120	0.05244	3.12036
D34	1.04121	-0.00025	-0.01752	0.04989	0.03246	1.07367

D35	-1.10835	0.00250	-0.01100	0.03558	0.02474	-1.08361
D36	0.94873	0.00150	-0.01740	0.06242	0.04490	0.99362
D37	-1.07799	-0.00069	-0.01607	0.04111	0.02492	-1.05307
D38	3.05563	0.00207	-0.00955	0.02679	0.01720	3.07284
D39	-1.14278	0.00033	-0.01858	0.06724	0.04861	-1.09417
D40	3.11369	-0.00185	-0.01725	0.04593	0.02864	-3.14086
D41	0.96413	0.00091	-0.01072	0.03162	0.02092	0.98505
D42	-3.11200	-0.00107	0.01361	-0.05954	-0.04596	3.12523
D43	-0.05755	0.00049	0.01953	-0.04850	-0.02900	-0.08655
D44	-0.03770	0.00038	0.00365	0.00663	0.01030	-0.02740
D45	3.01674	0.00194	0.00958	0.01767	0.02727	3.04401
D46	-2.74214	-0.00082	-0.00254	0.00217	-0.00037	-2.74251
D47	-0.04725	-0.00025	-0.00192	0.00432	0.00241	-0.04484
D48	-0.00257	0.00020	0.00642	-0.02479	-0.01832	-0.02089
D49	2.69232	0.00077	0.00705	-0.02264	-0.01554	2.67678
D50	0.68065	-0.00068	0.00328	-0.02912	-0.02595	0.65470
D51	-1.69354	-0.00060	0.01026	-0.04724	-0.03715	-1.73069
D52	2.58627	-0.00022	-0.03673	0.01416	-0.02254	2.56373
D53	0.20408	-0.00095	-0.03678	0.01164	-0.02514	0.17894
D54	2.55718	-0.00047	-0.00161	0.00242	0.00079	2.55797
D55	-1.64580	-0.00054	-0.00119	0.00080	-0.00041	-1.64621
D56	0.45146	-0.00055	-0.00145	0.00022	-0.00125	0.45021
D57	1.32992	0.00064	-0.00049	0.00411	0.00365	1.33357
D58	-2.87306	0.00058	-0.00007	0.00250	0.00245	-2.87061
D59	-0.77580	0.00056	-0.00033	0.00191	0.00161	-0.77419
D60	-1.02509	-0.00001	-0.00076	0.00346	0.00270	-1.02238
D61	1.05512	-0.00008	-0.00034	0.00184	0.00150	1.05662
D62	-3.13081	-0.00009	-0.00060	0.00126	0.00066	-3.13014
D63	1.17391	-0.00332	-0.01709	0.00991	-0.00692	1.16699
D64	2.67344	-0.00179	0.01877	-0.01375	0.00476	2.67819
D65	2.72908	-0.00262	-0.02574	-0.01195	-0.03772	2.69136
D66	-0.39386	-0.00235	-0.04849	0.01429	-0.03434	-0.42820
D67	-1.44649	-0.00106	-0.02004	-0.04139	-0.06130	-1.50779
D68	1.71375	-0.00079	-0.04279	-0.01515	-0.05791	1.65584
D69	0.53663	0.00028	-0.01978	-0.02591	-0.04563	0.49100
D70	-2.58631	0.00054	-0.04253	0.00033	-0.04225	-2.62856
D71	3.08267	-0.00705	-0.01543	-0.04043	-0.05601	3.02666
D72	-0.03952	-0.00677	-0.03938	-0.01335	-0.05258	-0.09210
D73	-1.87888	-0.00592	-0.00468	0.01394	0.00927	-1.86961

Item	Value	Threshold	Converged?
Maximum Force	0.009990	0.000450	NO
RMS Force	0.002398	0.000300	NO
Maximum Displacement	0.617432	0.001800	NO
RMS Displacement	0.130374	0.001200	NO

Predicted change in Energy=-2.478892D-03
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.025548	1.647068	1.620176
2	6	0	-1.790833	0.525244	1.726026
3	7	0	-2.638686	0.518457	0.624536
4	6	0	-2.379140	1.605292	-0.122727
5	7	0	-1.406810	2.308801	0.467803
6	6	0	-0.810035	3.552838	-0.058769
7	1	0	-0.222277	2.006499	2.237913
8	1	0	-1.777995	-0.254994	2.470127
9	1	0	-1.621987	4.224231	-0.341871
10	1	0	-0.274264	4.008322	0.773588
11	35	0	-0.192109	-2.290916	2.060645
12	1	0	-2.881568	1.865827	-1.038063
13	6	0	-3.605666	-0.468196	0.262874
14	6	0	-3.606283	-1.704713	0.742823
15	1	0	-4.333003	-0.101894	-0.452979
16	1	0	-4.390186	-2.380666	0.422113
17	1	0	-2.821999	-2.093019	1.393741
18	6	0	2.929863	-0.784786	0.802780
19	6	0	4.239035	-0.383032	1.327742
20	8	0	3.151624	0.568696	1.306456
21	1	0	2.802029	-0.827934	-0.275071
22	1	0	2.239908	-1.386204	1.385231
23	1	0	4.484189	-0.697981	2.339893
24	6	0	5.410995	-0.088115	0.432070
25	1	0	6.038145	0.699548	0.859347
26	1	0	6.027164	-0.985437	0.320274
27	1	0	5.074661	0.230628	-0.556562
28	6	0	0.144325	3.308956	-1.228117
29	1	0	0.517445	4.282506	-1.563189
30	1	0	-0.352744	2.852969	-2.086344
31	6	0	1.360746	2.452594	-0.880261
32	8	0	1.951381	1.794240	-1.703054
33	8	0	1.647908	2.512285	0.415798
34	1	0	2.374788	1.874599	0.669044

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.362115	0.000000			
3	N	2.206190	1.390029	0.000000		
4	C	2.207185	2.220473	1.344238	0.000000	
5	N	1.382467	2.216230	2.178855	1.337563	0.000000
6	C	2.548972	3.648806	3.608092	2.501822	1.476836
7	H	1.075190	2.217321	3.264396	3.222677	2.151231
8	H	2.215047	1.078249	2.178353	3.247296	3.274160
9	H	3.293498	4.241133	3.962370	2.734985	2.090632
10	H	2.618521	3.916497	4.218040	3.317896	2.065075
11	Br	4.049241	3.255556	3.992583	4.972992	5.016975
12	H	3.249446	3.259917	2.153748	1.076175	2.153780
13	C	3.601892	2.534040	1.428053	2.439756	3.548052
14	C	4.320229	3.038956	2.427493	3.634720	4.584933
15	H	4.277394	3.406463	2.101567	2.615555	3.901524
16	H	5.383195	4.111099	3.393176	4.497668	5.558211
17	H	4.155330	2.833552	2.728570	4.021605	4.715521
18	C	4.714587	4.985332	5.721796	5.895299	5.337530
19	C	5.650014	6.110884	6.972103	7.060987	6.313559
20	O	4.325514	4.960425	5.830543	5.805725	4.950821
21	H	4.936390	5.189400	5.676569	5.726108	5.301443
22	H	4.463086	4.473997	5.292170	5.706013	5.271934
23	H	6.031123	6.422539	7.426810	7.646884	6.873815
24	C	6.771376	7.342810	8.074796	7.991347	7.226960
25	H	7.167454	7.878731	8.681896	8.522647	7.626949
26	H	7.639409	8.085752	8.800638	8.807615	8.132512
27	H	6.630010	7.240995	7.808556	7.591907	6.883138
28	C	3.499035	4.496761	4.354808	3.239172	2.506487
29	H	4.411368	5.501282	5.377301	4.199120	3.423916
30	H	3.955395	4.692608	4.245508	3.085250	2.816174
31	C	3.549007	4.521047	4.690496	3.908776	3.081773
32	O	4.464036	5.231931	5.302264	4.613734	4.031729
33	O	3.057203	4.182102	4.732210	4.162903	3.061930
34	H	3.538178	4.504484	5.193844	4.826930	3.811760

		6	7	8	9	10
6	C	0.000000				
7	H	2.830437	0.000000			
8	H	4.672456	2.754729	0.000000		
9	H	1.090954	3.678696	5.291042	0.000000	
10	H	1.089649	2.480775	4.828593	1.762732	0.000000
11	Br	6.246855	4.301175	2.612984	7.089694	6.429903
12	H	2.845395	4.221805	4.245369	2.762842	3.830195
13	C	4.907924	4.633813	2.873640	5.130260	5.603417

14	C	6.008610	5.240218	2.903085	6.345578	6.613778
15	H	5.091538	5.346427	3.885364	5.106594	5.905226
16	H	6.946595	6.317896	3.941622	7.202170	7.608121
17	H	6.167130	4.927193	2.372106	6.660332	6.640927
18	C	5.791726	4.448244	5.022415	6.864388	5.765515
19	C	6.550312	5.142138	6.125854	7.639768	6.321467
20	O	5.144287	3.783927	5.131641	6.234363	4.883819
21	H	5.681986	4.847219	5.370382	6.715709	5.826889
22	H	5.981757	4.277833	4.312793	7.026670	5.982982
23	H	7.200823	5.429128	6.279183	8.288872	6.873534
24	C	7.224865	6.275527	7.474163	8.286021	7.015668
25	H	7.475411	6.542282	8.037276	8.517272	7.127541
26	H	8.215042	7.189196	8.128710	9.278394	8.053019
27	H	6.776026	6.246628	7.507034	7.800003	6.682160
28	C	1.528940	3.720774	5.483983	2.177847	2.161285
29	H	2.134925	4.491746	6.490423	2.464181	2.482440
30	H	2.193169	4.408257	5.696683	2.556271	3.085483
31	C	2.568595	3.525333	5.329900	3.510735	2.797993
32	O	3.663572	4.505670	5.960121	4.530633	3.998676
33	O	2.710987	2.659609	4.859518	3.767896	2.461887
34	H	3.672777	3.037021	5.002467	4.745200	3.403113

		11	12	13	14	15
11	Br	0.000000				
12	H	5.840693	0.000000			
13	C	4.266926	2.768469	0.000000		
14	C	3.706329	4.055308	1.326395	0.000000	
15	H	5.315742	2.514142	1.084270	2.127696	0.000000
16	H	4.507404	4.737166	2.073250	1.083638	2.441691
17	H	2.720339	4.646471	2.129095	1.090678	3.107747
18	C	3.687460	6.647345	6.565430	6.600839	7.402195
19	C	4.879776	7.833096	7.917104	7.977343	8.759557
20	O	4.463937	6.601419	6.915576	7.152299	7.717833
21	H	4.069490	6.335755	6.440292	6.547620	7.174083
22	H	2.681305	6.532808	6.022721	5.889999	6.944899
23	H	4.948048	8.499298	8.355391	8.307820	9.268134
24	C	6.236936	8.645564	9.026255	9.166312	9.784119
25	H	7.014418	9.193565	9.732548	9.940274	10.484522
26	H	6.588819	9.452000	9.646878	9.669500	10.426487
27	H	6.398970	8.136787	8.746880	8.988478	9.414108
28	C	6.502900	3.357793	5.527420	6.564187	5.681655
29	H	7.539596	4.203497	6.550094	7.626901	6.631921
30	H	6.609302	2.910033	5.208691	6.273928	5.219344
31	C	5.793201	4.285607	5.873928	6.677499	6.255139
32	O	5.953862	4.879009	6.313815	7.008039	6.682177

33	O	5.400178	4.800810	6.042078	6.745113	6.584831
34	H	5.086947	5.526624	6.435798	6.970662	7.082366

		16	17	18	19	20
16	H	0.000000				
17	H	1.867087	0.000000			
18	C	7.501658	5.928291	0.000000		
19	C	8.903604	7.265440	1.466602	0.000000	
20	O	8.146147	6.540376	1.461089	1.445234	0.000000
21	H	7.390873	6.001256	1.086263	2.198166	2.138696
22	H	6.773087	5.111024	1.084892	2.237447	2.158486
23	H	9.233842	7.498114	2.187733	1.087999	2.109073
24	C	10.065736	8.527992	2.603611	1.504226	2.510121
25	H	10.882508	9.305168	3.444976	2.151318	2.923872
26	H	10.510863	8.982581	3.141074	2.138993	3.414179
27	H	9.867116	8.459330	2.734782	2.150686	2.698740
28	C	7.460352	6.697355	5.351868	6.076993	4.793426
29	H	8.510237	7.780916	6.090568	6.631361	5.382021
30	H	7.069952	6.532306	5.688217	6.573592	5.386055
31	C	7.624291	6.582481	3.971824	4.604410	3.396770
32	O	7.884265	6.891014	3.726661	4.377167	3.464057
33	O	7.771718	6.491939	3.558629	3.991045	2.613804
34	H	7.995820	6.578281	2.719986	3.001033	1.647772

		21	22	23	24	25
21	H	0.000000				
22	H	1.839633	0.000000			
23	H	3.112006	2.534132	0.000000		
24	C	2.802514	3.556592	2.206965	0.000000	
25	H	3.754004	4.365033	2.561227	1.093752	0.000000
26	H	3.283404	3.954498	2.557785	1.094235	1.769151
27	H	2.522824	3.797437	3.098455	1.091838	1.775665
28	C	5.008548	5.767632	6.900772	6.483373	6.775221
29	H	5.744142	6.617728	7.468223	6.857858	7.013158
30	H	5.175167	6.061704	7.456322	6.943563	7.359196
31	C	3.633926	4.543319	5.481916	4.958017	5.289372
32	O	3.104598	4.442518	5.382536	4.480060	4.946300
33	O	3.600883	4.060600	4.696002	4.574185	4.770422
34	H	2.894404	3.341250	3.722832	3.623114	3.851901

		26	27	28	29	30
26	H	0.000000				
27	H	1.776209	0.000000			
28	C	7.446283	5.851094	0.000000		
29	H	7.852112	6.180552	1.095121	0.000000	
30	H	7.824858	6.218812	1.091584	1.753424	0.000000
31	C	5.919189	4.339939	1.527757	2.127469	2.133304

32	O	5.332210	3.676167	2.405282	2.875274	2.564529
33	O	5.605450	4.230139	2.365989	2.885831	3.221706
34	H	4.652021	3.390290	3.260608	3.772347	3.998599

		31	32	33	34
31	C	0.000000			
32	O	1.208002	0.000000		
33	O	1.328831	2.257702	0.000000	
34	H	1.939769	2.410929	0.999565	0.000000

Stoichiometry C11H17BrN2O3
Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.095906	1.025535	1.363878
2	6	0	-2.035137	0.122309	0.967160
3	7	0	-2.776179	0.735850	-0.036137
4	6	0	-2.285202	1.970960	-0.237188
5	7	0	-1.267914	2.170260	0.608080
6	6	0	-0.439193	3.390722	0.676946
7	1	0	-0.301648	0.938250	2.083301
8	1	0	-2.209421	-0.888229	1.300416
9	1	0	-1.107599	4.252474	0.705197
10	1	0	0.088775	3.345633	1.629075
11	35	0	-0.936257	-2.806094	0.064075
12	1	0	-2.660079	2.680773	-0.953977
13	6	0	-3.852520	0.187172	-0.797569
14	6	0	-4.089616	-1.113834	-0.900009
15	1	0	-4.448960	0.946581	-1.290720
16	1	0	-4.940234	-1.436988	-1.488474
17	1	0	-3.435087	-1.875440	-0.474420
18	6	0	2.480455	-1.495948	-0.390857
19	6	0	3.786995	-1.597105	0.267659
20	8	0	2.869572	-0.548196	0.650841
21	1	0	2.439943	-1.053944	-1.382299
22	1	0	1.656897	-2.153042	-0.132071
23	1	0	3.891913	-2.350116	1.045932
24	6	0	5.063006	-1.165650	-0.401920
25	1	0	5.767982	-0.760432	0.329586

26	1	0	5.536826	-2.025220	-0.885639
27	1	0	4.866983	-0.402886	-1.158146
28	6	0	0.560952	3.499151	-0.474406
29	1	0	1.110537	4.438429	-0.351912
30	1	0	0.073186	3.547824	-1.449737
31	6	0	1.592468	2.373158	-0.520799
32	8	0	2.139679	2.031957	-1.542274
33	8	0	1.773692	1.824648	0.675899
34	1	0	2.366290	1.020751	0.634579

Rotational constants (GHZ): 0.3256183 0.2670036 0.1604463

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 538 symmetry adapted cartesian basis functions of A symmetry.

There are 519 symmetry adapted basis functions of A symmetry.

519 basis functions, 823 primitive gaussians, 538 cartesian basis functions

78 alpha electrons 78 beta electrons

nuclear repulsion energy 1576.4570121335 Hartrees.

NAtoms= 34 NActive= 34 NUniq= 34 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 519 RedAO= T EigKep= 4.07D-06 NBF= 519

NBsUse= 519 1.00D-06 EigRej= -1.00D+00 NBFU= 519

Initial guess from the checkpoint file: "./coohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999180 -0.000543 -0.007448 -0.039787 Ang= -4.64 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3338.90033865 A.U. after 12 cycles
NFock= 12 Conv=0.86D-08 -V/T= 2.0019
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000989200	-0.000692124	0.001191745
2	6	-0.002639262	0.002963197	-0.000125719
3	7	0.001922985	0.000950205	-0.000176969
4	6	0.000035999	0.000389580	0.001165384
5	7	-0.000177718	0.000799802	-0.002484764
6	6	0.000381715	-0.000393029	0.002704693
7	1	-0.000356369	-0.000481125	-0.000124942
8	1	0.001224455	-0.002032045	-0.002548600
9	1	-0.000623878	-0.000501327	-0.001197593
10	1	-0.000917110	-0.000093318	-0.001015681
11	35	-0.001762301	-0.000990794	0.000809795
12	1	0.000344494	-0.000204645	-0.000159074
13	6	-0.001582299	-0.000890070	0.001235674
14	6	0.001064797	-0.001580753	-0.000197372
15	1	0.000394926	0.000368531	0.001110605
16	1	0.000793258	0.000143013	-0.000110680
17	1	-0.000312991	0.001276619	0.000130806
18	6	0.002065001	-0.000390416	-0.000928384
19	6	0.001550713	0.000072120	-0.002020412
20	8	-0.002109870	-0.000535450	0.002050521
21	1	0.000000306	0.000673930	-0.000290989
22	1	-0.001313937	0.000894712	0.001302571
23	1	-0.000263655	0.000166225	0.000193566
24	6	0.000206641	0.000291955	0.000520284
25	1	0.000276209	0.000069303	-0.000009723
26	1	0.000084034	-0.000012801	-0.000108864
27	1	-0.000061540	-0.000074931	-0.000097170
28	6	0.002055531	0.001665809	0.000891265
29	1	-0.000118871	0.000420965	-0.000431558
30	1	-0.000050962	-0.000242081	0.000491033
31	6	-0.002730995	-0.005613478	-0.004997408
32	8	-0.000135866	0.002874135	0.001717823
33	8	0.004043057	0.002541026	0.003683002
34	1	-0.000297297	-0.001832745	-0.002172865

Cartesian Forces: Max 0.005613478 RMS 0.001493010

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.010371561 RMS 0.002004086
Search for a local minimum.
Step number 14 out of a maximum of 175
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 12 13 14
DE= -1.77D-03 DEPred=-2.48D-03 R= 7.16D-01
TightC=F SS= 1.41D+00 RLast= 3.07D-01 DXNew= 1.0091D+00 9.2170D-01
Trust test= 7.16D-01 RLast= 3.07D-01 DXMaxT set to 9.22D-01
ITU= 1 0 0 -1 1 1 1 0 1 0 -1 0 1 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00167	0.00297	0.00360	0.00627	0.00698
Eigenvalues ---	0.00945	0.01077	0.01431	0.01647	0.01795
Eigenvalues ---	0.01853	0.02010	0.02216	0.02323	0.02347
Eigenvalues ---	0.02458	0.02508	0.02857	0.02953	0.03057
Eigenvalues ---	0.03096	0.03519	0.03621	0.04001	0.04242
Eigenvalues ---	0.04516	0.04987	0.05181	0.05644	0.05795
Eigenvalues ---	0.05905	0.06444	0.07709	0.09542	0.09668
Eigenvalues ---	0.11907	0.12623	0.12777	0.13304	0.14351
Eigenvalues ---	0.15075	0.15411	0.15886	0.15983	0.15989
Eigenvalues ---	0.16000	0.16001	0.16004	0.16021	0.16418
Eigenvalues ---	0.16984	0.17979	0.19065	0.20477	0.21825
Eigenvalues ---	0.22799	0.23147	0.23832	0.24863	0.25664
Eigenvalues ---	0.25918	0.28453	0.29190	0.29907	0.31838
Eigenvalues ---	0.32353	0.34497	0.34580	0.34611	0.34764
Eigenvalues ---	0.34863	0.34894	0.34976	0.35007	0.35180
Eigenvalues ---	0.35242	0.35704	0.35750	0.36543	0.36673
Eigenvalues ---	0.36841	0.37036	0.37241	0.37674	0.40348
Eigenvalues ---	0.41089	0.43212	0.46020	0.49029	0.51661
Eigenvalues ---	0.53385	0.55575	0.56174	0.60516	0.89715
Eigenvalues ---	1.10356				

RFO step: Lambda=-1.47319107D-03 EMin= 1.67052011D-03
Quartic linear search produced a step of -0.20448.
Iteration 1 RMS(Cart)= 0.12555232 RMS(Int)= 0.00480991
Iteration 2 RMS(Cart)= 0.00835560 RMS(Int)= 0.00005818
Iteration 3 RMS(Cart)= 0.00003853 RMS(Int)= 0.00005632
Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00005632

Variable	Old X	-DE/DX	Delta X	Delta X	Delta X	New X

			(Linear)	(Quad)	(Total)	
R1	2.57402	0.00015	-0.00077	0.00145	0.00068	2.57471
R2	2.61248	0.00208	0.00000	0.00200	0.00199	2.61448
R3	2.03181	-0.00050	-0.00012	-0.00045	-0.00057	2.03125
R4	2.62677	-0.00434	-0.00034	-0.00381	-0.00415	2.62263
R5	2.03760	0.00098	-0.00007	0.00391	0.00385	2.04144
R6	2.54024	-0.00063	0.00072	-0.00156	-0.00084	2.53940
R7	2.69863	-0.00032	-0.00192	0.00545	0.00353	2.70216
R8	2.52763	0.00013	-0.00024	0.00095	0.00072	2.52835
R9	2.03368	-0.00008	0.00020	-0.00018	0.00001	2.03369
R10	2.79082	0.00070	-0.00176	0.00534	0.00358	2.79440
R11	2.06160	0.00047	0.00029	0.00003	0.00033	2.06193
R12	2.05914	-0.00127	0.00019	-0.00250	-0.00232	2.05682
R13	2.88928	0.00201	-0.00223	0.00865	0.00641	2.89569
R14	4.93783	-0.00043	-0.00911	-0.00993	-0.01905	4.91878
R15	2.50652	0.00008	0.00045	0.00000	0.00044	2.50696
R16	2.04897	-0.00087	-0.00037	0.00024	-0.00013	2.04884
R17	2.04778	-0.00063	-0.00076	0.00135	0.00059	2.04837
R18	2.06108	-0.00060	-0.00317	0.00937	0.00619	2.06728
R19	2.77148	0.00030	-0.00022	0.00216	0.00173	2.77320
R20	2.76106	-0.00147	0.00153	-0.00599	-0.00439	2.75667
R21	2.05274	0.00026	0.00054	-0.00077	-0.00023	2.05251
R22	2.05015	0.00104	0.00077	-0.00029	0.00048	2.05063
R23	2.73110	0.00093	-0.00049	0.00216	0.00179	2.73289
R24	2.05602	0.00007	0.00000	0.00016	0.00016	2.05618
R25	2.84257	0.00027	0.00054	-0.00088	-0.00034	2.84224
R26	3.11384	-0.00047	-0.00697	-0.00532	-0.01230	3.10154
R27	2.06689	0.00020	0.00006	-0.00007	-0.00001	2.06688
R28	2.06780	0.00007	-0.00004	0.00015	0.00011	2.06791
R29	2.06328	0.00009	0.00003	-0.00009	-0.00006	2.06322
R30	2.06948	0.00047	-0.00020	0.00014	-0.00006	2.06941
R31	2.06279	-0.00026	0.00064	-0.00327	-0.00263	2.06016
R32	2.88704	0.00128	-0.00005	0.00431	0.00425	2.89129
R33	2.28279	-0.00280	0.00001	0.00117	0.00118	2.28397
R34	2.51113	0.00305	0.00014	-0.00080	-0.00066	2.51047
R35	1.88890	0.00014	0.00086	-0.00218	-0.00133	1.88758
A1	1.87974	-0.00059	-0.00005	0.00099	0.00095	1.88069
A2	2.27893	-0.00002	0.00093	-0.00363	-0.00269	2.27624
A3	2.12344	0.00065	-0.00076	0.00263	0.00187	2.12531
A4	1.85994	0.00070	0.00018	-0.00101	-0.00082	1.85913
A5	2.26908	0.00397	0.00279	0.00568	0.00847	2.27755
A6	2.15386	-0.00466	-0.00292	-0.00464	-0.00756	2.14629
A7	1.89525	0.00108	0.00009	0.00182	0.00193	1.89718
A8	2.23582	-0.00504	-0.00054	-0.00954	-0.01007	2.22575

A9	2.15144	0.00395	0.00030	0.00780	0.00810	2.15954
A10	1.89671	0.00013	-0.00062	0.00092	0.00034	1.89705
A11	2.18758	-0.00003	0.00009	0.00010	0.00021	2.18779
A12	2.19884	-0.00010	0.00052	-0.00108	-0.00055	2.19829
A13	1.89308	-0.00132	0.00036	-0.00283	-0.00247	1.89062
A14	2.20059	0.00369	-0.00098	0.00485	0.00387	2.20445
A15	2.18877	-0.00233	0.00062	-0.00186	-0.00125	2.18752
A16	1.88618	-0.00371	0.00278	-0.01450	-0.01163	1.87455
A17	1.85297	-0.00055	0.00108	0.00336	0.00437	1.85734
A18	1.97204	0.00682	-0.00477	0.01639	0.01160	1.98364
A19	1.88275	0.00112	-0.00009	0.00223	0.00216	1.88491
A20	1.94364	-0.00278	-0.00247	-0.00467	-0.00711	1.93653
A21	1.92195	-0.00101	0.00377	-0.00308	0.00060	1.92255
A22	2.05205	0.00809	-0.00111	0.06055	0.05943	2.11148
A23	2.15648	-0.00310	0.00292	-0.01658	-0.01362	2.14286
A24	1.96927	0.00103	-0.00148	0.00407	0.00264	1.97192
A25	2.15739	0.00207	-0.00177	0.01274	0.01101	2.16840
A26	2.06549	0.00086	0.00094	-0.00109	-0.00015	2.06534
A27	2.15019	-0.00143	0.00225	-0.01135	-0.00909	2.14109
A28	2.06545	0.00057	-0.00341	0.01303	0.00963	2.07508
A29	2.06134	-0.00097	-0.00121	0.00313	0.00196	2.06330
A30	2.12632	0.00088	0.00251	-0.00005	0.00237	2.12868
A31	1.97873	0.00000	-0.00091	-0.00122	-0.00218	1.97655
A32	2.00974	-0.00146	-0.00118	-0.00938	-0.01058	1.99915
A33	2.02178	0.00049	0.00003	0.00171	0.00169	2.02347
A34	2.04298	-0.00025	0.00040	-0.00138	-0.00102	2.04196
A35	2.13655	0.00063	-0.00029	0.00286	0.00258	2.13914
A36	1.95397	-0.00080	0.00054	-0.00493	-0.00437	1.94960
A37	2.03570	0.00128	-0.00059	0.00240	0.00175	2.03744
A38	2.02098	-0.00022	-0.00031	0.00107	0.00077	2.02175
A39	2.12851	-0.00033	-0.00181	-0.01411	-0.01638	2.11213
A40	2.65157	-0.00173	0.00351	-0.02145	-0.01815	2.63342
A41	1.93405	0.00027	-0.00014	0.00093	0.00078	1.93484
A42	1.91642	0.00010	0.00051	-0.00110	-0.00059	1.91582
A43	1.93520	-0.00013	-0.00024	-0.00002	-0.00026	1.93494
A44	1.88345	-0.00016	0.00001	-0.00039	-0.00038	1.88307
A45	1.89665	-0.00002	-0.00013	0.00066	0.00053	1.89719
A46	1.89689	-0.00007	0.00000	-0.00010	-0.00010	1.89679
A47	1.88060	-0.00195	0.00039	0.00573	0.00617	1.88677
A48	1.96460	-0.00379	-0.00226	-0.00655	-0.00878	1.95582
A49	1.99574	0.01037	0.00467	0.00914	0.01382	2.00956
A50	1.86079	0.00134	-0.00250	0.00319	0.00069	1.86148
A51	1.87203	-0.00399	0.00188	-0.00716	-0.00532	1.86671
A52	1.88329	-0.00253	-0.00252	-0.00467	-0.00719	1.87610

A53	2.14088	-0.00197	-0.00428	0.00584	0.00144	2.14232
A54	1.94869	0.00455	0.00696	-0.00233	0.00451	1.95320
A55	2.19339	-0.00249	-0.00266	-0.00296	-0.00573	2.18765
A56	1.95584	-0.00246	-0.01089	0.00599	-0.00490	1.95094
A57	2.81283	0.00515	-0.00785	0.03003	0.02218	2.83501
D1	-0.00062	0.00064	0.00205	-0.00353	-0.00148	-0.00210
D2	3.11446	0.00090	0.00519	-0.00259	0.00259	3.11706
D3	-3.09193	-0.00031	-0.00157	-0.00325	-0.00480	-3.09674
D4	0.02316	-0.00005	0.00158	-0.00231	-0.00073	0.02243
D5	-0.00508	-0.00065	0.00147	-0.00317	-0.00171	-0.00678
D6	-3.10690	-0.00159	0.00134	-0.00722	-0.00590	-3.11281
D7	3.09164	0.00018	0.00473	-0.00363	0.00112	3.09276
D8	-0.01018	-0.00076	0.00460	-0.00768	-0.00308	-0.01326
D9	0.00609	-0.00041	-0.00485	0.00900	0.00416	0.01025
D10	3.10883	-0.00040	-0.00827	0.01150	0.00323	3.11206
D11	-3.11118	-0.00080	-0.00778	0.00796	0.00017	-3.11101
D12	-0.00844	-0.00080	-0.01120	0.01045	-0.00076	-0.00919
D13	-1.55746	-0.00320	-0.01299	0.02277	0.00978	-1.54768
D14	1.55370	-0.00280	-0.00936	0.02393	0.01457	1.56828
D15	-0.00937	0.00000	0.00584	-0.01115	-0.00531	-0.01468
D16	-3.14048	0.00024	0.00082	-0.00608	-0.00527	3.13743
D17	-3.11440	0.00024	0.00910	-0.01304	-0.00394	-3.11834
D18	0.03767	0.00047	0.00408	-0.00797	-0.00390	0.03377
D19	-0.31740	-0.00078	-0.00838	-0.08608	-0.09448	-0.41188
D20	2.83416	-0.00033	0.00205	-0.11009	-0.10802	2.72614
D21	2.78015	-0.00087	-0.01228	-0.08345	-0.09574	2.68440
D22	-0.35148	-0.00042	-0.00185	-0.10746	-0.10929	-0.46077
D23	0.00895	0.00039	-0.00454	0.00887	0.00433	0.01328
D24	3.11111	0.00149	-0.00445	0.01308	0.00862	3.11973
D25	3.13998	0.00015	0.00052	0.00378	0.00430	-3.13891
D26	-0.04104	0.00125	0.00061	0.00798	0.00859	-0.03246
D27	-2.33829	0.00030	0.00896	0.02421	0.03318	-2.30511
D28	-0.32219	-0.00044	0.01077	0.02155	0.03229	-0.28991
D29	1.78616	0.00196	0.01330	0.02966	0.04298	1.82915
D30	0.84959	-0.00084	0.00882	0.01947	0.02830	0.87788
D31	2.86568	-0.00159	0.01062	0.01681	0.02740	2.89308
D32	-1.30915	0.00081	0.01316	0.02493	0.03810	-1.27105
D33	3.12036	-0.00324	-0.01072	0.02824	0.01746	3.13782
D34	1.07367	-0.00146	-0.00664	0.02446	0.01780	1.09147
D35	-1.08361	-0.00320	-0.00506	0.02887	0.02379	-1.05981
D36	0.99362	-0.00126	-0.00918	0.03876	0.02958	1.02320
D37	-1.05307	0.00051	-0.00510	0.03499	0.02992	-1.02315
D38	3.07284	-0.00123	-0.00352	0.03939	0.03592	3.10875
D39	-1.09417	-0.00021	-0.00994	0.04101	0.03105	-1.06311

D40	-3.14086	0.00157	-0.00586	0.03723	0.03139	-3.10947
D41	0.98505	-0.00018	-0.00428	0.04163	0.03739	1.02244
D42	3.12523	0.00071	0.00940	-0.01938	-0.01000	3.11523
D43	-0.08655	0.00081	0.00593	-0.00873	-0.00281	-0.08936
D44	-0.02740	0.00021	-0.00211	0.00711	0.00502	-0.02238
D45	3.04401	0.00030	-0.00558	0.01776	0.01220	3.05622
D46	-2.74251	-0.00047	0.00008	-0.00912	-0.00904	-2.75155
D47	-0.04484	-0.00016	-0.00049	-0.00241	-0.00291	-0.04775
D48	-0.02089	0.00074	0.00375	0.00428	0.00803	-0.01287
D49	2.67678	0.00106	0.00318	0.01099	0.01416	2.69093
D50	0.65470	-0.00095	0.00531	-0.02857	-0.02320	0.63151
D51	-1.73069	-0.00009	0.00760	-0.01930	-0.01165	-1.74234
D52	2.56373	0.00016	0.00461	0.02427	0.02884	2.59256
D53	0.17894	0.00000	0.00514	0.02560	0.03072	0.20965
D54	2.55797	-0.00016	-0.00016	0.00022	0.00008	2.55805
D55	-1.64621	-0.00013	0.00008	-0.00038	-0.00027	-1.64649
D56	0.45021	-0.00023	0.00026	-0.00122	-0.00094	0.44926
D57	1.33357	0.00009	-0.00075	0.00236	0.00159	1.33516
D58	-2.87061	0.00012	-0.00050	0.00176	0.00124	-2.86938
D59	-0.77419	0.00002	-0.00033	0.00092	0.00057	-0.77362
D60	-1.02238	0.00014	-0.00055	0.00627	0.00572	-1.01666
D61	1.05662	0.00017	-0.00031	0.00567	0.00536	1.06198
D62	-3.13014	0.00007	-0.00014	0.00483	0.00469	-3.12545
D63	1.16699	0.00128	0.00142	-0.05467	-0.05345	1.11354
D64	2.67819	0.00033	-0.00097	-0.08782	-0.08860	2.58960
D65	2.69136	0.00120	0.00771	-0.05162	-0.04386	2.64749
D66	-0.42820	-0.00283	0.00702	-0.07740	-0.07037	-0.49857
D67	-1.50779	0.00232	0.01253	-0.04380	-0.03129	-1.53908
D68	1.65584	-0.00171	0.01184	-0.06958	-0.05780	1.59804
D69	0.49100	0.00065	0.00933	-0.04594	-0.03657	0.45443
D70	-2.62856	-0.00338	0.00864	-0.07172	-0.06308	-2.69164
D71	3.02666	0.00477	0.01145	-0.00607	0.00533	3.03199
D72	-0.09210	0.00059	0.01075	-0.03293	-0.02212	-0.11422
D73	-1.86961	0.00090	-0.00190	-0.03014	-0.03203	-1.90165

Item	Value	Threshold	Converged?
Maximum Force	0.010372	0.000450	NO
RMS Force	0.002004	0.000300	NO
Maximum Displacement	0.593700	0.001800	NO
RMS Displacement	0.129152	0.001200	NO

Predicted change in Energy=-9.333169D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.112957	1.676551	1.659069
2	6	0	-1.870793	0.546895	1.735896
3	7	0	-2.642485	0.510215	0.582974
4	6	0	-2.344136	1.582866	-0.169479
5	7	0	-1.423109	2.312639	0.470233
6	6	0	-0.813464	3.559168	-0.040791
7	1	0	-0.359612	2.057005	2.324739
8	1	0	-1.906854	-0.223547	2.492289
9	1	0	-1.626624	4.214254	-0.357323
10	1	0	-0.314690	4.027246	0.805845
11	35	0	-0.330177	-2.291253	2.374817
12	1	0	-2.784509	1.816330	-1.123280
13	6	0	-3.573391	-0.501465	0.189788
14	6	0	-3.508560	-1.749371	0.635287
15	1	0	-4.327506	-0.138103	-0.499245
16	1	0	-4.266761	-2.452077	0.309269
17	1	0	-2.692185	-2.108715	1.268646
18	6	0	2.908205	-0.742094	0.950897
19	6	0	4.281739	-0.362328	1.301306
20	8	0	3.224879	0.623380	1.354884
21	1	0	2.652015	-0.829481	-0.100974
22	1	0	2.266681	-1.279280	1.641851
23	1	0	4.630505	-0.632809	2.295854
24	6	0	5.352293	-0.150997	0.266217
25	1	0	6.047570	0.633040	0.579524
26	1	0	5.924680	-1.073942	0.131983
27	1	0	4.914972	0.131918	-0.693342
28	6	0	0.183821	3.332910	-1.181965
29	1	0	0.574145	4.308234	-1.491167
30	1	0	-0.290975	2.893857	-2.059643
31	6	0	1.390404	2.461455	-0.827505
32	8	0	1.974081	1.789273	-1.644984
33	8	0	1.702132	2.546843	0.461061
34	1	0	2.423740	1.903096	0.711260

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.362475	0.000000			
3	N	2.204036	1.387834	0.000000		
4	C	2.206393	2.219852	1.343793	0.000000	

5	N	1.383521	2.218146	2.179064	1.337944	0.000000
6	C	2.554108	3.653539	3.609781	2.503056	1.478732
7	H	1.074890	2.216040	3.261566	3.222463	2.153036
8	H	2.221464	1.080284	2.173716	3.246437	3.279475
9	H	3.281711	4.229741	3.954244	2.733919	2.083845
10	H	2.625069	3.924192	4.223483	3.323387	2.069083
11	Br	4.107130	3.291930	4.050394	5.053541	5.100761
12	H	3.248860	3.259023	2.153465	1.076183	2.153838
13	C	3.599484	2.527519	1.429923	2.446339	3.552682
14	C	4.303951	3.027617	2.420445	3.620405	4.569056
15	H	4.276052	3.391242	2.104950	2.646552	3.921932
16	H	5.367868	4.095090	3.389448	4.495158	5.551106
17	H	4.120028	2.818736	2.707657	3.977073	4.668660
18	C	4.745640	5.011640	5.702088	5.852159	5.321908
19	C	5.778216	6.234517	7.015855	7.060398	6.355424
20	O	4.474206	5.110469	5.919004	5.853053	5.023942
21	H	4.853139	5.071912	5.504025	5.548480	5.177434
22	H	4.489899	4.523544	5.331362	5.721226	5.281015
23	H	6.223022	6.631149	7.558892	7.722222	6.975299
24	C	6.861445	7.404051	8.028325	7.901337	7.212294
25	H	7.316248	8.002817	8.690923	8.478437	7.657939
26	H	7.708797	8.122133	8.724063	8.690387	8.097737
27	H	6.652493	7.219418	7.673802	7.421208	6.802993
28	C	3.535057	4.527386	4.366992	3.237028	2.520503
29	H	4.438024	5.526239	5.392005	4.206050	3.437807
30	H	3.998288	4.733938	4.265534	3.083324	2.831928
31	C	3.614684	4.568585	4.696912	3.892520	3.101955
32	O	4.523193	5.268482	5.283225	4.568010	4.035957
33	O	3.180779	4.288447	4.799834	4.207032	3.134017
34	H	3.668500	4.618676	5.255779	4.859104	3.876089

		6	7	8	9	10
6	C	0.000000				
7	H	2.838698	0.000000			
8	H	4.681979	2.760969	0.000000		
9	H	1.091128	3.667765	5.281373	0.000000	
10	H	1.088423	2.488153	4.842347	1.763265	0.000000
11	Br	6.347925	4.348646	2.602906	7.174050	6.510403
12	H	2.845045	4.222189	4.243079	2.770817	3.835320
13	C	4.915191	4.629488	2.855888	5.131008	5.613188
14	C	5.991762	5.220979	2.888262	6.331808	6.602969
15	H	5.121376	5.342057	3.849174	5.124249	5.929257
16	H	6.941388	6.297599	3.911659	7.201017	7.605726
17	H	6.113028	4.889729	2.380736	6.615069	6.596717
18	C	5.773657	4.516749	5.082280	6.844085	5.758011

19	C	6.568139	5.333173	6.303681	7.655385	6.375030
20	O	5.184108	3.980512	5.324065	6.274003	4.941285
21	H	5.592263	4.825534	5.279721	6.619043	5.762938
22	H	5.977387	4.300529	4.388190	7.023777	5.960000
23	H	7.257368	5.668969	6.553102	8.347757	6.956378
24	C	7.202509	6.460545	7.593147	8.255271	7.061417
25	H	7.484705	6.791571	8.225890	8.520330	7.214583
26	H	8.179129	7.355497	8.223573	9.231827	8.087395
27	H	6.707223	6.374638	7.537368	7.718216	6.691077
28	C	1.532334	3.770971	5.524441	2.175893	2.163794
29	H	2.142464	4.527811	6.523827	2.477462	2.478962
30	H	2.188926	4.464060	5.748858	2.534817	3.081583
31	C	2.584749	3.628054	5.394644	3.520772	2.833175
32	O	3.671018	4.612646	6.019147	4.528099	4.031571
33	O	2.757695	2.822060	4.982543	3.811906	2.525478
34	H	3.713172	3.220877	5.142832	4.784221	3.466981

		11	12	13	14	15
11	Br	0.000000				
12	H	5.927282	0.000000			
13	C	4.300713	2.778247	0.000000		
14	C	3.663566	4.041168	1.326628	0.000000	
15	H	5.373540	2.567113	1.084199	2.134015	0.000000
16	H	4.448488	4.740102	2.073625	1.083952	2.451909
17	H	2.614578	4.597370	2.126901	1.093955	3.111756
18	C	3.861938	6.576833	6.530565	6.503007	7.404272
19	C	5.113018	7.781840	7.934602	7.940796	8.798373
20	O	4.708904	6.608871	6.988505	7.175442	7.813845
21	H	4.142438	6.131983	6.240819	6.272237	7.024979
22	H	2.881840	6.537834	6.067943	5.881120	7.026371
23	H	5.231161	8.524740	8.470932	8.381443	9.396983
24	C	6.427858	8.485789	8.932889	9.011422	9.710026
25	H	7.242253	9.072228	9.695457	9.848787	10.459475
26	H	6.755398	9.261713	9.515484	9.470773	10.314145
27	H	6.541938	7.893294	8.557652	8.732720	9.248459
28	C	6.674287	3.333832	5.540828	6.539546	5.732897
29	H	7.701744	4.198271	6.569694	7.608211	6.691787
30	H	6.822855	2.873248	5.230909	6.259000	5.284053
31	C	5.983603	4.234804	5.869672	6.623494	6.289671
32	O	6.174067	4.787179	6.276011	6.912380	6.688610
33	O	5.585689	4.813910	6.098927	6.755673	6.669907
34	H	5.286214	5.522583	6.482240	6.966956	7.156197

		16	17	18	19	20
16	H	0.000000				
17	H	1.875524	0.000000			

18	C	7.403774	5.773473	0.000000		
19	C	8.855961	7.189337	1.467517	0.000000	
20	O	8.165563	6.517931	1.458768	1.446183	0.000000
21	H	7.118327	5.663283	1.086142	2.200142	2.135064
22	H	6.770310	5.041587	1.085145	2.239918	2.149560
23	H	9.296107	7.540242	2.187960	1.088083	2.106946
24	C	9.890552	8.339733	2.606098	1.504046	2.512119
25	H	10.769234	9.185610	3.447393	2.151716	2.927261
26	H	10.285727	8.752893	3.143226	2.138449	3.415452
27	H	9.590958	8.169374	2.737614	2.150321	2.700588
28	C	7.449666	6.624816	5.345748	6.050979	4.798457
29	H	8.507511	7.711207	6.075963	6.584702	5.357662
30	H	7.070901	6.470629	5.702477	6.542815	5.401416
31	C	7.578824	6.476715	3.966000	4.567866	3.392144
32	O	7.794630	6.742224	3.744196	4.316861	3.452971
33	O	7.787164	6.452630	3.537182	3.977897	2.611013
34	H	7.993243	6.525182	2.699845	2.988722	1.641265

		21	22	23	24	25
21	H	0.000000				
22	H	1.840718	0.000000			
23	H	3.114144	2.536397	0.000000		
24	C	2.808322	3.561796	2.207385	0.000000	
25	H	3.759234	4.368138	2.560515	1.093748	0.000000
26	H	3.290041	3.962679	2.559654	1.094292	1.768949
27	H	2.529063	3.802374	3.098552	1.091808	1.775975
28	C	4.958429	5.795217	6.898924	6.399058	6.691464
29	H	5.713693	6.625767	7.430309	6.767853	6.910368
30	H	5.134279	6.136590	7.458465	6.821087	7.228668
31	C	3.598578	4.567130	5.461510	4.870081	5.197309
32	O	3.114712	4.506097	5.334161	4.339314	4.783160
33	O	3.552143	4.043785	4.695959	4.543124	4.749685
34	H	2.859862	3.319366	3.716392	3.604689	3.842205

		26	27	28	29	30
26	H	0.000000				
27	H	1.776168	0.000000			
28	C	7.355561	5.733140	0.000000		
29	H	7.760841	6.076258	1.095087	0.000000	
30	H	7.692920	6.049543	1.090191	1.752729	0.000000
31	C	5.829177	4.226975	1.530007	2.125399	2.128890
32	O	5.192576	3.507319	2.408783	2.885939	2.553924
33	O	5.572100	4.181728	2.371224	2.861127	3.232157
34	H	4.631944	3.363958	3.262807	3.749183	4.003647

		31	32	33	34
31	C	0.000000			

32 O 1.208627 0.000000

33 O 1.328482 2.254616 0.000000

34 H 1.935806 2.401465 0.998864 0.000000

Stoichiometry C11H17BrN2O3

Framework group C1[X(C11H17BrN2O3)]

Deg. of freedom 96

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.058920	1.132831	1.374089
2	6	0	-2.066660	0.342458	0.909212
3	7	0	-2.661030	1.034983	-0.136358
4	6	0	-2.017023	2.202887	-0.300781
5	7	0	-1.044645	2.288895	0.614192
6	6	0	-0.092702	3.412586	0.747505
7	1	0	-0.334345	0.955227	2.147934
8	1	0	-2.387124	-0.641182	1.220288
9	1	0	-0.676184	4.334459	0.763580
10	1	0	0.383263	3.298850	1.719712
11	35	0	-1.345965	-2.783633	0.170998
12	1	0	-2.255579	2.946643	-1.041110
13	6	0	-3.743371	0.601600	-0.964245
14	6	0	-4.038015	-0.678580	-1.149357
15	1	0	-4.288786	1.424191	-1.412971
16	1	0	-4.889954	-0.925550	-1.772379
17	1	0	-3.424201	-1.490008	-0.747418
18	6	0	2.330242	-1.714738	-0.336475
19	6	0	3.693981	-1.922327	0.164250
20	8	0	2.904393	-0.816433	0.659219
21	1	0	2.205922	-1.251382	-1.310923
22	1	0	1.491738	-2.304750	0.018963
23	1	0	3.830099	-2.690724	0.922513
24	6	0	4.914450	-1.574506	-0.642986
25	1	0	5.726918	-1.235309	0.005955
26	1	0	5.263928	-2.458504	-1.185100
27	1	0	4.691361	-0.786848	-1.365392
28	6	0	0.967733	3.454415	-0.357834
29	1	0	1.616882	4.317019	-0.174164
30	1	0	0.525943	3.600154	-1.343785

```
      31        6        0        1.873060        2.223542       -0.436929
      32        8        0        2.385767        1.854203       -1.467219
      33        8        0        2.018176        1.638023        0.746699
      34        1        0        2.525304        0.780361        0.676242
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.3177449           0.2592678           0.1570185
 Standard basis: 6-311++G(d,p) (5D, 7F)
 There are     538 symmetry adapted cartesian basis functions of A      symmetry.
 There are     519 symmetry adapted basis functions of A      symmetry.
    519 basis functions,      823 primitive gaussians,      538 cartesian basis functions
     78 alpha electrons              78 beta electrons
          nuclear repulsion energy           1564.1030091018 Hartrees.
 NAtoms=       34 NActive=       34 NUniq=       34 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      519 RedAO= T EigKep=    4.72D-06    NBF=      519
 NBsUse=      519 1.00D-06 EigRej= -1.00D+00 NBFU=      519
 Initial guess from the checkpoint file:    "./coohpo.chk"
 B after Tr=          0.000000        0.000000        0.000000
             Rot=        0.998646      -0.002570        0.003018        0.051863 Ang=    -5.96 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn=                5 AccDes=
0.00D+00
 Harris functional with IExCor=    402 and IRadAn=             5 diagonalized for initial guess.
 HarFok:    IExCor=    402 AccDes= 0.00D+00 IRadAn=                5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=    3500011 ScaDFX=    1.000000    1.000000    1.000000    1.000000
 FoFCou: FMM=F IPFlag=                  0 FMFlag=           100000 FMFlg1=                  0
             NFxFlg=                   0 DoJE=T BraDBF=F KetDBF=T FulRan=T
             wScrn=      0.000000  ICntrl=             500  IOpCl=      0  I1Cent=        200000004  NGrid=
0
             NMat0=        1 NMatS0=            1 NMatT0=        0 NMatD0=        1 NMtDS0=        0
NMtDT0=        0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                      energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3338.90110615          A.U. after      13 cycles
                  NFock= 13    Conv=0.39D-08         -V/T= 2.0019
 Calling FoFJK, ICntrl=             2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
```

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000137549	-0.000590876	0.000620966
2	6	-0.002598763	0.003071196	0.000549514
3	7	0.002437939	0.001553982	-0.001260235
4	6	-0.000951118	0.000581788	0.001249092
5	7	0.001798018	-0.000128549	-0.002700123
6	6	0.000462305	-0.000423240	0.001644882
7	1	0.000050587	-0.000081257	0.000076863
8	1	0.002347493	-0.001532418	-0.002439372
9	1	0.000175184	0.000419867	-0.001049090
10	1	-0.000561532	-0.000287105	0.000078455
11	35	-0.000022856	0.000181353	0.000185171
12	1	0.000228281	-0.000216166	-0.000130348
13	6	-0.001982311	-0.001368690	0.001277312
14	6	0.001095564	-0.000868553	-0.001269625
15	1	0.000380312	0.000088409	0.000766143
16	1	0.000989646	0.000040413	0.000107455
17	1	-0.001616215	0.000657112	0.000740648
18	6	0.000144200	0.000171884	-0.000069844
19	6	0.000665292	0.000108852	-0.001200518
20	8	-0.000981172	0.000349065	0.002387678
21	1	0.000066815	-0.000206343	-0.000193995
22	1	-0.000529436	-0.000511529	0.000380872
23	1	-0.000112507	-0.000060617	-0.000008029
24	6	-0.000005603	-0.000043074	0.000081960
25	1	0.000057603	0.000028634	0.000050314
26	1	0.000046467	0.000000131	-0.000065435
27	1	-0.000099934	0.000031652	-0.000026836
28	6	0.001584950	-0.001567776	0.001353769
29	1	-0.000770056	0.000689253	0.000214891
30	1	-0.000365871	-0.000334087	-0.000571666
31	6	-0.000778644	-0.002935690	-0.003837364
32	8	-0.001875068	0.002167606	0.001290165
33	8	0.000270177	0.002518387	0.003590369
34	1	0.000587801	-0.001503614	-0.001824042

Cartesian Forces: Max 0.003837364 RMS 0.001223906

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.005645213 RMS 0.001067126
Search for a local minimum.
Step number 15 out of a maximum of 175
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 13 14 15
DE= -7.67D-04 DEPred=-9.33D-04 R= 8.22D-01
TightC=F SS= 1.41D+00 RLast= 3.10D-01 DXNew= 1.5501D+00 9.2979D-01
Trust test= 8.22D-01 RLast= 3.10D-01 DXMaxT set to 9.30D-01
ITU= 1 1 0 0 -1 1 1 1 0 1 0 -1 0 1 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00170	0.00336	0.00364	0.00626	0.00698
Eigenvalues ---	0.00950	0.01070	0.01354	0.01641	0.01761
Eigenvalues ---	0.01953	0.02020	0.02225	0.02319	0.02363
Eigenvalues ---	0.02451	0.02666	0.02851	0.02924	0.03068
Eigenvalues ---	0.03150	0.03311	0.03626	0.03991	0.04090
Eigenvalues ---	0.04338	0.04884	0.05203	0.05541	0.05758
Eigenvalues ---	0.05906	0.06161	0.07582	0.09664	0.09754
Eigenvalues ---	0.11937	0.12678	0.12743	0.13535	0.14299
Eigenvalues ---	0.14813	0.15443	0.15888	0.15966	0.15992
Eigenvalues ---	0.15999	0.16001	0.16003	0.16007	0.16445
Eigenvalues ---	0.16969	0.17721	0.19890	0.20655	0.21797
Eigenvalues ---	0.22583	0.23312	0.23870	0.24786	0.25208
Eigenvalues ---	0.25996	0.28732	0.29385	0.30219	0.31844
Eigenvalues ---	0.32380	0.34497	0.34516	0.34608	0.34764
Eigenvalues ---	0.34880	0.34936	0.34951	0.35059	0.35073
Eigenvalues ---	0.35604	0.35709	0.35850	0.36538	0.36768
Eigenvalues ---	0.36847	0.37207	0.37534	0.38218	0.40725
Eigenvalues ---	0.41051	0.42678	0.46020	0.49051	0.51599
Eigenvalues ---	0.53744	0.55564	0.56164	0.60526	0.89708
Eigenvalues ---	1.25520				

RFO step: Lambda=-9.67403381D-04 EMin= 1.70314522D-03
Quartic linear search produced a step of -0.09207.
Iteration 1 RMS(Cart)= 0.05788926 RMS(Int)= 0.00064771
Iteration 2 RMS(Cart)= 0.00093507 RMS(Int)= 0.00006523
Iteration 3 RMS(Cart)= 0.00000241 RMS(Int)= 0.00006522
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00006522

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.57471	-0.00215	-0.00006	-0.00242	-0.00242	2.57228
R2	2.61448	-0.00045	-0.00018	0.00223	0.00204	2.61651
R3	2.03125	0.00006	0.00005	-0.00061	-0.00056	2.03069

R4	2.62263	-0.00144	0.00038	-0.00642	-0.00600	2.61663
R5	2.04144	-0.00069	-0.00035	0.00174	0.00138	2.04282
R6	2.53940	-0.00027	0.00008	-0.00067	-0.00062	2.53878
R7	2.70216	0.00131	-0.00033	0.00516	0.00483	2.70700
R8	2.52835	0.00000	-0.00007	0.00079	0.00066	2.52901
R9	2.03369	-0.00002	0.00000	-0.00025	-0.00025	2.03344
R10	2.79440	-0.00278	-0.00033	-0.00174	-0.00206	2.79233
R11	2.06193	0.00043	-0.00003	0.00129	0.00126	2.06319
R12	2.05682	-0.00032	0.00021	-0.00323	-0.00302	2.05381
R13	2.89569	-0.00234	-0.00059	0.00305	0.00246	2.89815
R14	4.91878	-0.00017	0.00175	0.00181	0.00357	4.92234
R15	2.50696	0.00004	-0.00004	0.00003	-0.00001	2.50695
R16	2.04884	-0.00072	0.00001	-0.00208	-0.00207	2.04677
R17	2.04837	-0.00075	-0.00005	-0.00133	-0.00139	2.04698
R18	2.06728	-0.00099	-0.00057	0.00165	0.00108	2.06835
R19	2.77320	0.00031	-0.00016	0.00149	0.00122	2.77443
R20	2.75667	0.00038	0.00040	-0.00198	-0.00153	2.75514
R21	2.05251	0.00019	0.00002	-0.00037	-0.00035	2.05216
R22	2.05063	0.00081	-0.00004	0.00191	0.00186	2.05249
R23	2.73289	0.00026	-0.00017	0.00229	0.00220	2.73508
R24	2.05618	-0.00003	-0.00001	0.00032	0.00031	2.05649
R25	2.84224	-0.00003	0.00003	-0.00086	-0.00083	2.84140
R26	3.10154	0.00027	0.00113	0.00568	0.00682	3.10836
R27	2.06688	0.00007	0.00000	0.00011	0.00012	2.06700
R28	2.06791	0.00003	-0.00001	0.00023	0.00022	2.06813
R29	2.06322	0.00007	0.00001	0.00010	0.00010	2.06332
R30	2.06941	0.00028	0.00001	0.00053	0.00053	2.06995
R31	2.06016	0.00076	0.00024	-0.00086	-0.00061	2.05955
R32	2.89129	-0.00194	-0.00039	-0.00453	-0.00492	2.88638
R33	2.28397	-0.00298	-0.00011	-0.00177	-0.00188	2.28209
R34	2.51047	0.00309	0.00006	0.00678	0.00684	2.51731
R35	1.88758	0.00082	0.00012	-0.00176	-0.00164	1.88594
A1	1.88069	-0.00045	-0.00009	-0.00031	-0.00036	1.88033
A2	2.27624	0.00010	0.00025	-0.00276	-0.00266	2.27359
A3	2.12531	0.00030	-0.00017	0.00208	0.00174	2.12705
A4	1.85913	0.00091	0.00008	0.00177	0.00171	1.86084
A5	2.27755	-0.00046	-0.00078	0.00358	0.00239	2.27994
A6	2.14629	-0.00047	0.00070	-0.00624	-0.00593	2.14037
A7	1.89718	0.00006	-0.00018	0.00090	0.00081	1.89799
A8	2.22575	-0.00229	0.00093	-0.01516	-0.01428	2.21146
A9	2.15954	0.00222	-0.00075	0.01416	0.01337	2.17292
A10	1.89705	-0.00089	-0.00003	-0.00003	-0.00011	1.89694
A11	2.18779	0.00041	-0.00002	0.00017	0.00011	2.18790
A12	2.19829	0.00049	0.00005	0.00003	0.00003	2.19833

A13	1.89062	0.00038	0.00023	-0.00222	-0.00198	1.88864
A14	2.20445	-0.00274	-0.00036	-0.00486	-0.00522	2.19923
A15	2.18752	0.00235	0.00012	0.00700	0.00710	2.19462
A16	1.87455	0.00312	0.00107	-0.00003	0.00100	1.87555
A17	1.85734	0.00077	-0.00040	0.00157	0.00118	1.85851
A18	1.98364	-0.00565	-0.00107	-0.00297	-0.00405	1.97959
A19	1.88491	-0.00058	-0.00020	0.00476	0.00457	1.88948
A20	1.93653	0.00078	0.00065	-0.00822	-0.00757	1.92895
A21	1.92255	0.00175	-0.00006	0.00557	0.00553	1.92808
A22	2.11148	0.00051	-0.00547	0.03954	0.03407	2.14555
A23	2.14286	-0.00060	0.00125	-0.01384	-0.01259	2.13028
A24	1.97192	0.00004	-0.00024	0.00228	0.00204	1.97396
A25	2.16840	0.00057	-0.00101	0.01156	0.01055	2.17895
A26	2.06534	0.00058	0.00001	0.00411	0.00399	2.06932
A27	2.14109	-0.00015	0.00084	-0.00776	-0.00706	2.13403
A28	2.07508	-0.00037	-0.00089	0.00535	0.00433	2.07941
A29	2.06330	-0.00076	-0.00018	0.00017	0.00001	2.06331
A30	2.12868	0.00078	-0.00022	0.00205	0.00180	2.13049
A31	1.97655	0.00004	0.00020	0.00088	0.00105	1.97760
A32	1.99915	0.00014	0.00097	-0.00512	-0.00414	1.99502
A33	2.02347	-0.00008	-0.00016	-0.00025	-0.00040	2.02307
A34	2.04196	-0.00018	0.00009	-0.00139	-0.00133	2.04063
A35	2.13914	0.00006	-0.00024	0.00245	0.00223	2.14137
A36	1.94960	-0.00021	0.00040	-0.00352	-0.00311	1.94649
A37	2.03744	0.00011	-0.00016	0.00079	0.00061	2.03805
A38	2.02175	0.00011	-0.00007	0.00088	0.00082	2.02256
A39	2.11213	-0.00003	0.00151	-0.00924	-0.00801	2.10413
A40	2.63342	-0.00127	0.00167	-0.02789	-0.02628	2.60714
A41	1.93484	-0.00002	-0.00007	0.00036	0.00029	1.93512
A42	1.91582	0.00013	0.00005	0.00028	0.00034	1.91616
A43	1.93494	-0.00013	0.00002	-0.00112	-0.00109	1.93385
A44	1.88307	-0.00004	0.00003	-0.00018	-0.00015	1.88293
A45	1.89719	0.00006	-0.00005	0.00083	0.00078	1.89796
A46	1.89679	0.00000	0.00001	-0.00015	-0.00014	1.89665
A47	1.88677	0.00013	-0.00057	0.00660	0.00601	1.89279
A48	1.95582	0.00089	0.00081	-0.00673	-0.00593	1.94989
A49	2.00956	-0.00325	-0.00127	0.00452	0.00322	2.01278
A50	1.86148	-0.00031	-0.00006	0.00043	0.00039	1.86186
A51	1.86671	0.00235	0.00049	0.00315	0.00361	1.87032
A52	1.87610	0.00045	0.00066	-0.00772	-0.00707	1.86903
A53	2.14232	-0.00084	-0.00013	0.00215	0.00194	2.14426
A54	1.95320	-0.00047	-0.00042	-0.00226	-0.00275	1.95045
A55	2.18765	0.00132	0.00053	-0.00001	0.00044	2.18810
A56	1.95094	-0.00056	0.00045	-0.00863	-0.00818	1.94276

A57	2.83501	-0.00175	-0.00204	0.01277	0.01073	2.84574
D1	-0.00210	-0.00057	0.00014	-0.00188	-0.00175	-0.00385
D2	3.11706	-0.00172	-0.00024	-0.04770	-0.04806	3.06900
D3	-3.09674	0.00059	0.00044	0.02272	0.02315	-3.07358
D4	0.02243	-0.00055	0.00007	-0.02310	-0.02316	-0.00073
D5	-0.00678	0.00082	0.00016	0.00554	0.00569	-0.00109
D6	-3.11281	0.00124	0.00054	0.00774	0.00828	-3.10453
D7	3.09276	-0.00023	-0.00010	-0.01664	-0.01681	3.07594
D8	-0.01326	0.00019	0.00028	-0.01444	-0.01423	-0.02749
D9	0.01025	0.00013	-0.00038	-0.00241	-0.00279	0.00746
D10	3.11206	-0.00017	-0.00030	-0.00479	-0.00503	3.10703
D11	-3.11101	0.00117	-0.00002	0.03898	0.03882	-3.07219
D12	-0.00919	0.00087	0.00007	0.03660	0.03657	0.02738
D13	-1.54768	0.00102	-0.00090	0.01262	0.01168	-1.53600
D14	1.56828	-0.00027	-0.00134	-0.03963	-0.04092	1.52736
D15	-0.01468	0.00039	0.00049	0.00593	0.00641	-0.00827
D16	3.13743	-0.00055	0.00049	-0.01102	-0.01054	3.12690
D17	-3.11834	0.00080	0.00036	0.00899	0.00935	-3.10899
D18	0.03377	-0.00014	0.00036	-0.00795	-0.00759	0.02618
D19	-0.41188	0.00029	0.00870	-0.01971	-0.01103	-0.42291
D20	2.72614	0.00064	0.00995	-0.01935	-0.00942	2.71672
D21	2.68440	-0.00011	0.00882	-0.02284	-0.01400	2.67040
D22	-0.46077	0.00023	0.01006	-0.02247	-0.01240	-0.47317
D23	0.01328	-0.00075	-0.00040	-0.00710	-0.00748	0.00580
D24	3.11973	-0.00129	-0.00079	-0.00957	-0.01037	3.10936
D25	-3.13891	0.00020	-0.00040	0.00997	0.00959	-3.12932
D26	-0.03246	-0.00034	-0.00079	0.00751	0.00670	-0.02576
D27	-2.30511	-0.00114	-0.00306	-0.03611	-0.03918	-2.34429
D28	-0.28991	0.00005	-0.00297	-0.02989	-0.03287	-0.32277
D29	1.82915	-0.00068	-0.00396	-0.02365	-0.02762	1.80152
D30	0.87788	-0.00059	-0.00261	-0.03332	-0.03592	0.84196
D31	2.89308	0.00060	-0.00252	-0.02710	-0.02960	2.86348
D32	-1.27105	-0.00013	-0.00351	-0.02086	-0.02436	-1.29541
D33	3.13782	0.00092	-0.00161	0.03248	0.03087	-3.11449
D34	1.09147	0.00071	-0.00164	0.03171	0.03009	1.12156
D35	-1.05981	0.00193	-0.00219	0.04418	0.04201	-1.01781
D36	1.02320	0.00030	-0.00272	0.04073	0.03799	1.06119
D37	-1.02315	0.00008	-0.00275	0.03997	0.03721	-0.98595
D38	3.10875	0.00130	-0.00331	0.05244	0.04912	-3.12531
D39	-1.06311	-0.00061	-0.00286	0.03644	0.03358	-1.02954
D40	-3.10947	-0.00083	-0.00289	0.03568	0.03280	-3.07668
D41	1.02244	0.00040	-0.00344	0.04815	0.04471	1.06715
D42	3.11523	0.00060	0.00092	0.01047	0.01139	3.12661
D43	-0.08936	0.00161	0.00026	0.04252	0.04278	-0.04658

D44	-0.02238	0.00022	-0.00046	0.01008	0.00961	-0.01277
D45	3.05622	0.00123	-0.00112	0.04214	0.04101	3.09722
D46	-2.75155	0.00026	0.00083	-0.00285	-0.00200	-2.75355
D47	-0.04775	0.00028	0.00027	0.00233	0.00260	-0.04515
D48	-0.01287	0.00006	-0.00074	0.00266	0.00193	-0.01094
D49	2.69093	0.00008	-0.00130	0.00784	0.00653	2.69746
D50	0.63151	-0.00056	0.00214	-0.03157	-0.02943	0.60208
D51	-1.74234	-0.00064	0.00107	-0.02656	-0.02546	-1.76779
D52	2.59256	-0.00008	-0.00266	0.01297	0.01028	2.60284
D53	0.20965	-0.00013	-0.00283	0.01475	0.01190	0.22156
D54	2.55805	0.00006	-0.00001	0.00104	0.00105	2.55910
D55	-1.64649	0.00008	0.00003	0.00122	0.00126	-1.64523
D56	0.44926	0.00008	0.00009	0.00051	0.00061	0.44987
D57	1.33516	-0.00007	-0.00015	0.00189	0.00173	1.33689
D58	-2.86938	-0.00004	-0.00011	0.00207	0.00194	-2.86744
D59	-0.77362	-0.00004	-0.00005	0.00135	0.00129	-0.77234
D60	-1.01666	0.00001	-0.00053	0.00563	0.00510	-1.01156
D61	1.06198	0.00003	-0.00049	0.00581	0.00531	1.06730
D62	-3.12545	0.00003	-0.00043	0.00509	0.00466	-3.12079
D63	1.11354	0.00007	0.00492	0.09838	0.10321	1.21675
D64	2.58960	-0.00054	0.00816	0.07137	0.07963	2.66922
D65	2.64749	-0.00056	0.00404	-0.04537	-0.04134	2.60616
D66	-0.49857	-0.00001	0.00648	-0.07163	-0.06515	-0.56373
D67	-1.53908	-0.00074	0.00288	-0.03190	-0.02901	-1.56808
D68	1.59804	-0.00019	0.00532	-0.05816	-0.05282	1.54522
D69	0.45443	0.00025	0.00337	-0.03356	-0.03020	0.42423
D70	-2.69164	0.00080	0.00581	-0.05982	-0.05401	-2.74566
D71	3.03199	-0.00207	-0.00049	-0.02219	-0.02269	3.00930
D72	-0.11422	-0.00151	0.00204	-0.04926	-0.04722	-0.16144
D73	-1.90165	-0.00073	0.00295	-0.01801	-0.01506	-1.91670

Item	Value	Threshold	Converged?
Maximum Force	0.005645	0.000450	NO
RMS Force	0.001067	0.000300	NO
Maximum Displacement	0.242840	0.001800	NO
RMS Displacement	0.057787	0.001200	NO

Predicted change in Energy=-5.287887D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.089300	1.699365	1.642562

2	6	0	-1.831063	0.560853	1.722708
3	7	0	-2.615630	0.518296	0.582564
4	6	0	-2.345112	1.599000	-0.168295
5	7	0	-1.421123	2.336500	0.458896
6	6	0	-0.822345	3.587065	-0.051953
7	1	0	-0.319974	2.074292	2.292422
8	1	0	-1.823205	-0.234340	2.454964
9	1	0	-1.639337	4.226126	-0.392746
10	1	0	-0.344171	4.069161	0.796650
11	35	0	-0.251372	-2.304118	2.280893
12	1	0	-2.795490	1.825282	-1.118998
13	6	0	-3.530799	-0.519268	0.211178
14	6	0	-3.405661	-1.761882	0.658589
15	1	0	-4.312868	-0.177447	-0.455633
16	1	0	-4.138256	-2.498778	0.352569
17	1	0	-2.574308	-2.071186	1.299814
18	6	0	2.840878	-0.751509	0.935409
19	6	0	4.214565	-0.393550	1.310049
20	8	0	3.165163	0.601316	1.371694
21	1	0	2.596804	-0.815449	-0.120831
22	1	0	2.181966	-1.292412	1.608418
23	1	0	4.546233	-0.686217	2.304344
24	6	0	5.301081	-0.169888	0.295019
25	1	0	6.000463	0.599002	0.635739
26	1	0	5.865586	-1.095624	0.146457
27	1	0	4.878843	0.139614	-0.663147
28	6	0	0.190440	3.361145	-1.181230
29	1	0	0.601597	4.332226	-1.477513
30	1	0	-0.281612	2.937771	-2.067644
31	6	0	1.372194	2.460080	-0.828377
32	8	0	1.928880	1.761357	-1.640941
33	8	0	1.715588	2.575596	0.453511
34	1	0	2.404415	1.899336	0.706852

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.361193	0.000000			
3	N	2.201863	1.384660	0.000000		
4	C	2.205978	2.217631	1.343462	0.000000	
5	N	1.384598	2.217700	2.178991	1.338294	0.000000
6	C	2.550698	3.650328	3.610516	2.506942	1.477639
7	H	1.074593	2.213247	3.258032	3.222144	2.154785
8	H	2.222123	1.081015	2.168013	3.242686	3.279508

9	H	3.290827	4.236287	3.956309	2.729522	2.084130
10	H	2.624255	3.921308	4.220663	3.322135	2.067854
11	Br	4.139743	3.318894	4.054634	5.061284	5.120872
12	H	3.248561	3.256408	2.153108	1.076048	2.154061
13	C	3.596124	2.518032	1.432481	2.457013	3.559144
14	C	4.279482	3.001134	2.414362	3.619949	4.557960
15	H	4.279747	3.383727	2.107731	2.666532	3.939350
16	H	5.346458	4.069614	3.387333	4.503160	5.547434
17	H	4.066912	2.767468	2.687298	3.959563	4.632998
18	C	4.685419	4.916215	5.613411	5.799788	5.284649
19	C	5.711553	6.134394	6.929088	7.013210	6.319700
20	O	4.402219	5.008705	5.834996	5.807759	4.987793
21	H	4.798042	4.989875	5.426151	5.500396	5.139514
22	H	4.433179	4.421771	5.229528	5.657862	5.241436
23	H	6.155338	6.524062	7.463756	7.669862	6.939152
24	C	6.793155	7.310251	7.951767	7.861800	7.176132
25	H	7.244946	7.906691	8.616635	8.443642	7.624311
26	H	7.643346	8.029128	8.644417	8.647290	8.060597
27	H	6.585427	7.133905	7.606729	7.386488	6.765712
28	C	3.517535	4.512313	4.366553	3.249649	2.517350
29	H	4.418819	5.512033	5.398197	4.227017	3.438604
30	H	3.993950	4.734692	4.280783	3.107711	2.836092
31	C	3.569759	4.513973	4.654462	3.872406	3.078143
32	O	4.460341	5.185799	5.209774	4.523500	3.995325
33	O	3.170019	4.271860	4.796727	4.222519	3.145815
34	H	3.622373	4.556619	5.208029	4.838811	3.858411

		6	7	8	9	10
6	C	0.000000				
7	H	2.834952	0.000000			
8	H	4.678621	2.759693	0.000000		
9	H	1.091794	3.685272	5.295188	0.000000	
10	H	1.086828	2.493475	4.843312	1.765434	0.000000
11	Br	6.361936	4.378963	2.604793	7.191584	6.544484
12	H	2.852327	4.222318	4.237993	2.761917	3.835840
13	C	4.926148	4.622502	2.834014	5.144037	5.617032
14	C	5.982444	5.187206	2.839809	6.330991	6.587325
15	H	5.149589	5.344655	3.830566	5.152007	5.945792
16	H	6.942362	6.265403	3.860985	7.212796	7.598033
17	H	6.075562	4.822061	2.296199	6.587493	6.552140
18	C	5.763446	4.451699	4.932564	6.827384	5.779502
19	C	6.562835	5.255221	6.147426	7.649123	6.400112
20	O	5.180896	3.894044	5.172583	6.271818	4.967096
21	H	5.574716	4.762562	5.148679	6.590623	5.774991
22	H	5.965904	4.249973	4.228186	7.004375	5.982207

23	H	7.254977	5.594687	6.387223	8.346656	6.985900
24	C	7.192456	6.373557	7.444795	8.244232	7.077431
25	H	7.480117	6.698434	8.075508	8.519410	7.233413
26	H	8.166723	7.274249	8.073941	9.216053	8.103014
27	H	6.690442	6.285386	7.401346	7.698010	6.697180
28	C	1.533636	3.739355	5.495834	2.172092	2.167742
29	H	2.148277	4.489985	6.495966	2.491939	2.476994
30	H	2.185631	4.444912	5.735223	2.511684	3.080282
31	C	2.586297	3.570946	5.315149	3.518240	2.859329
32	O	3.664332	4.541653	5.902321	4.512787	4.053957
33	O	2.778429	2.788622	4.942127	3.833526	2.567311
34	H	3.719704	3.157046	5.047895	4.793224	3.502988

		11	12	13	14	15
11	Br	0.000000				
12	H	5.923153	0.000000			
13	C	4.268964	2.794094	0.000000		
14	C	3.588235	4.049675	1.326622	0.000000	
15	H	5.339200	2.598733	1.083102	2.138913	0.000000
16	H	4.343293	4.760885	2.075441	1.083217	2.464195
17	H	2.532351	4.591518	2.123312	1.094526	3.112946
18	C	3.712537	6.529095	6.416908	6.333777	7.310309
19	C	4.953524	7.743665	7.823936	7.769464	8.710995
20	O	4.576123	6.575030	6.887554	7.019184	7.737347
21	H	4.012047	6.086595	6.143734	6.126403	6.947136
22	H	2.719725	6.475637	5.931754	5.687192	6.905528
23	H	5.063118	8.481025	8.345517	8.191348	9.293007
24	C	6.271233	8.457814	8.839185	8.858554	9.643213
25	H	7.086613	9.052715	9.606026	9.697911	10.399940
26	H	6.590405	9.227530	9.414267	9.309253	10.237503
27	H	6.399868	7.870493	8.480604	8.602074	9.199518
28	C	6.654074	3.358352	5.553740	6.523978	5.773033
29	H	7.674258	4.237157	6.592827	7.599948	6.747841
30	H	6.810880	2.908117	5.263209	6.267278	5.343612
31	C	5.916173	4.225756	5.830654	6.547055	6.278169
32	O	6.054945	4.753544	6.199975	6.793995	6.642539
33	O	5.569548	4.835864	6.096022	6.714385	6.689400
34	H	5.215346	5.511644	6.428227	6.867593	7.126450

		16	17	18	19	20
16	H	0.000000				
17	H	1.877776	0.000000			
18	C	7.218099	5.585568	0.000000		
19	C	8.667085	6.993093	1.468164	0.000000	
20	O	7.999320	6.331584	1.457959	1.447344	0.000000
21	H	6.958357	5.507768	1.085957	2.200583	2.134921

22	H	6.555736	4.829479	1.086132	2.242417	2.146840
23	H	9.083785	7.323204	2.187803	1.088247	2.105928
24	C	9.722558	8.163719	2.607870	1.503605	2.513192
25	H	10.605190	9.005421	3.449154	2.151578	2.929260
26	H	10.103869	8.574017	3.144792	2.138393	3.416592
27	H	9.449914	8.018124	2.739121	2.149194	2.700083
28	C	7.445055	6.581005	5.330938	6.041340	4.794064
29	H	8.513403	7.668351	6.056479	6.569399	5.348788
30	H	7.091347	6.456460	5.690260	6.536216	5.400770
31	C	7.506661	6.374672	3.947439	4.560169	3.392646
32	O	7.676781	6.604175	3.712656	4.310025	3.456885
33	O	7.747706	6.380597	3.545156	3.974213	2.615742
34	H	7.891481	6.395649	2.696241	2.982920	1.644872

		21	22	23	24	25
21	H	0.000000				
22	H	1.841164	0.000000			
23	H	3.114233	2.538020	0.000000		
24	C	2.811191	3.565664	2.207664	0.000000	
25	H	3.762707	4.370867	2.559457	1.093809	0.000000
26	H	3.291637	3.968011	2.562184	1.094406	1.768997
27	H	2.532579	3.805766	3.098166	1.091861	1.776562
28	C	4.935481	5.779611	6.892263	6.384838	6.684846
29	H	5.685068	6.607351	7.419391	6.745076	6.895690
30	H	5.114883	6.121854	7.453566	6.812208	7.227903
31	C	3.567826	4.546966	5.457806	4.859517	5.198858
32	O	3.065418	4.466306	5.329768	4.341588	4.807507
33	O	3.550437	4.063596	4.698676	4.518690	4.722318
34	H	2.844667	3.324088	3.718124	3.583569	3.824590

		26	27	28	29	30
26	H	0.000000				
27	H	1.776213	0.000000			
28	C	7.337085	5.712074	0.000000		
29	H	7.733590	6.044503	1.095369	0.000000	
30	H	7.678448	6.035941	1.089866	1.752945	0.000000
31	C	5.812392	4.208141	1.527405	2.126060	2.121095
32	O	5.182160	3.505483	2.406829	2.897888	2.540138
33	O	5.549290	4.145735	2.369713	2.838235	3.236696
34	H	4.611240	3.331113	3.256290	3.733706	3.998865

		31	32	33	34
31	C	0.000000			
32	O	1.207631	0.000000		
33	O	1.332104	2.257256	0.000000	
34	H	1.933092	2.399438	0.997994	0.000000

Stoichiometry C11H17BrN2O3

Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.061880	1.150680	1.374460
2	6	0	-2.041736	0.318620	0.926793
3	7	0	-2.670722	0.973821	-0.118372
4	6	0	-2.077540	2.165416	-0.300378
5	7	0	-1.096834	2.298240	0.600512
6	6	0	-0.177778	3.449855	0.712480
7	1	0	-0.313970	0.999121	2.131039
8	1	0	-2.300028	-0.688334	1.223307
9	1	0	-0.784744	4.357037	0.687431
10	1	0	0.287929	3.378676	1.691891
11	35	0	-1.217126	-2.801585	0.152589
12	1	0	-2.346785	2.886662	-1.052170
13	6	0	-3.740722	0.468421	-0.925635
14	6	0	-3.949938	-0.832045	-1.083566
15	1	0	-4.339944	1.250694	-1.375181
16	1	0	-4.784635	-1.151791	-1.695449
17	1	0	-3.292697	-1.587581	-0.641764
18	6	0	2.283177	-1.658362	-0.320539
19	6	0	3.645645	-1.858416	0.188544
20	8	0	2.843527	-0.758753	0.680637
21	1	0	2.162061	-1.194752	-1.295064
22	1	0	1.443486	-2.250925	0.030844
23	1	0	3.779996	-2.625927	0.948252
24	6	0	4.870482	-1.500510	-0.606758
25	1	0	5.675899	-1.159696	0.050178
26	1	0	5.229468	-2.380034	-1.150165
27	1	0	4.647827	-0.711150	-1.327518
28	6	0	0.890006	3.486874	-0.387749
29	1	0	1.539338	4.351279	-0.211663
30	1	0	0.447867	3.623677	-1.374464
31	6	0	1.790268	2.255474	-0.466154
32	8	0	2.273240	1.861746	-1.500604
33	8	0	1.991307	1.713689	0.734076
34	1	0	2.476731	0.844605	0.663031

```
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.3166937           0.2688070           0.1599249
 Standard basis: 6-311++G(d,p) (5D, 7F)
 There are      538 symmetry adapted cartesian basis functions of A      symmetry.
 There are      519 symmetry adapted basis functions of A      symmetry.
    519 basis functions,      823 primitive gaussians,      538 cartesian basis functions
     78 alpha electrons              78 beta electrons
          nuclear repulsion energy           1572.5535389851 Hartrees.
 NAtoms=       34 NActive=       34 NUniq=       34 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      519 RedAO= T EigKep=    4.59D-06    NBF=      519
 NBsUse=      519 1.00D-06 EigRej= -1.00D+00 NBFU=      519
 Initial guess from the checkpoint file:    "./coohpo.chk"
 B after Tr=          0.000000        0.000000        0.000000
             Rot=        0.999916        0.003569      -0.001161      -0.012421 Ang=      1.49 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn=                5 AccDes=
0.00D+00
 Harris functional with IExCor=    402 and IRadAn=             5 diagonalized for initial guess.
 HarFok:    IExCor=    402 AccDes= 0.00D+00 IRadAn=                5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=    3500011 ScaDFX=    1.000000    1.000000    1.000000    1.000000
 FoFCou: FMM=F IPFlag=                  0 FMFlag=           100000 FMFlg1=                  0
             NFxFlg=                    0 DoJE=T BraDBF=F KetDBF=T FulRan=T
             wScrn=      0.000000  ICntrl=             500  IOpCl=      0  I1Cent=        200000004  NGrid=
0
             NMat0=         1 NMatS0=            1 NMatT0=         0 NMatD0=         1 NMtDS0=         0
NMtDT0=        0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                       energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3338.90143362          A.U. after      13 cycles
                   NFock= 13    Conv=0.14D-08         -V/T= 2.0019
 Calling FoFJK, ICntrl=             2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 ---------------------------------------------------------------------
 Center         Atomic                             Forces (Hartrees/Bohr)
 Number          Number                       X                       Y                       Z
 ---------------------------------------------------------------------
```

1	6	0.001110634	-0.000585911	-0.000001168
2	6	-0.000671515	0.001782930	0.001206618
3	7	0.000323533	0.001287703	-0.001249330
4	6	-0.001012400	-0.000289070	0.000238439
5	7	0.001294086	-0.000435239	-0.000376292
6	6	0.000051122	-0.000629588	-0.000790809
7	1	-0.000086853	0.000599344	0.000277577
8	1	0.001855322	-0.000343108	-0.001446711
9	1	0.000492198	0.000444801	-0.000229636
10	1	-0.000037306	0.000213699	0.000791293
11	35	-0.000294877	-0.000204039	0.001269081
12	1	-0.000108915	0.000075363	-0.000072028
13	6	-0.000388051	-0.000791619	0.000510628
14	6	-0.000942052	0.000954155	0.000247291
15	1	0.000397465	-0.000098349	-0.000401508
16	1	0.000601345	-0.000196384	0.000150219
17	1	-0.001144557	-0.001181779	-0.001197552
18	6	0.000593865	-0.000505993	0.000523563
19	6	-0.000313056	0.000137168	-0.000581243
20	8	-0.000617515	0.001735830	0.001796586
21	1	0.000100404	-0.000096471	-0.000487470
22	1	0.000195542	-0.000638316	-0.000302445
23	1	-0.000018039	-0.000155350	-0.000212175
24	6	-0.000024095	-0.000035202	-0.000058156
25	1	0.000053375	0.000051516	-0.000001059
26	1	-0.000007632	0.000046642	-0.000065179
27	1	0.000005722	0.000009151	-0.000085643
28	6	0.000176150	-0.002440863	0.000298228
29	1	-0.000873931	0.000542790	0.000726874
30	1	-0.000775876	-0.000082584	-0.000915505
31	6	0.001804429	0.001062828	-0.001035606
32	8	-0.002144269	0.000493728	0.001166993
33	8	-0.001731812	0.000749492	0.001061676
34	1	0.002137555	-0.001477276	-0.000755553

Cartesian Forces: Max 0.002440863 RMS 0.000843818

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.006248428 RMS 0.001169941

Search for a local minimum.

Step number 16 out of a maximum of 175
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 14 15 16
DE= -3.27D-04 DEPred=-5.29D-04 R= 6.19D-01
TightC=F SS= 1.41D+00 RLast= 2.68D-01 DXNew= 1.5637D+00 8.0269D-01
Trust test= 6.19D-01 RLast= 2.68D-01 DXMaxT set to 9.30D-01
ITU= 1 1 1 0 0 -1 1 1 1 0 1 0 -1 0 1 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00192	0.00247	0.00365	0.00656	0.00698
Eigenvalues ---	0.00925	0.01034	0.01384	0.01683	0.01782
Eigenvalues ---	0.01962	0.02102	0.02238	0.02333	0.02349
Eigenvalues ---	0.02428	0.02596	0.02849	0.02891	0.03045
Eigenvalues ---	0.03137	0.03584	0.03666	0.03950	0.04178
Eigenvalues ---	0.04600	0.04948	0.05164	0.05501	0.05759
Eigenvalues ---	0.05906	0.06159	0.07573	0.09667	0.09725
Eigenvalues ---	0.11948	0.12571	0.12689	0.13506	0.14003
Eigenvalues ---	0.14862	0.15444	0.15897	0.15962	0.15982
Eigenvalues ---	0.15997	0.16001	0.16003	0.16011	0.16635
Eigenvalues ---	0.17204	0.17342	0.19588	0.20898	0.22283
Eigenvalues ---	0.23240	0.23385	0.23920	0.24915	0.25731
Eigenvalues ---	0.28475	0.29197	0.30117	0.31841	0.32359
Eigenvalues ---	0.33037	0.34497	0.34607	0.34746	0.34775
Eigenvalues ---	0.34878	0.34906	0.34961	0.35036	0.35090
Eigenvalues ---	0.35603	0.35720	0.35835	0.36560	0.36773
Eigenvalues ---	0.36926	0.37148	0.37435	0.38244	0.39684
Eigenvalues ---	0.41091	0.44818	0.48820	0.49028	0.52241
Eigenvalues ---	0.53622	0.55807	0.56601	0.60549	0.88895
Eigenvalues ---	1.26619				

RFO step: Lambda=-6.95797006D-04 EMin= 1.92109031D-03
Quartic linear search produced a step of -0.25769.
Iteration 1 RMS(Cart)= 0.06891026 RMS(Int)= 0.00229926
Iteration 2 RMS(Cart)= 0.00306313 RMS(Int)= 0.00010407
Iteration 3 RMS(Cart)= 0.00000957 RMS(Int)= 0.00010397
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00010397

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.57228	0.00040	0.00062	-0.00201	-0.00140	2.57088
R2	2.61651	-0.00032	-0.00052	-0.00017	-0.00069	2.61582
R3	2.03069	0.00032	0.00014	0.00040	0.00054	2.03123
R4	2.61663	0.00243	0.00155	-0.00300	-0.00146	2.61517
R5	2.04282	0.00029	-0.00036	0.00156	0.00121	2.04403
R6	2.53878	-0.00121	0.00016	-0.00148	-0.00131	2.53747
R7	2.70700	0.00206	-0.00125	0.00856	0.00731	2.71431

R8	2.52901	-0.00015	-0.00017	0.00038	0.00022	2.52923
R9	2.03344	0.00013	0.00007	-0.00036	-0.00029	2.03315
R10	2.79233	-0.00118	0.00053	-0.00474	-0.00421	2.78813
R11	2.06319	-0.00004	-0.00032	0.00148	0.00116	2.06435
R12	2.05381	0.00069	0.00078	-0.00180	-0.00102	2.05279
R13	2.89815	-0.00164	-0.00063	-0.00569	-0.00632	2.89183
R14	4.92234	-0.00010	-0.00092	-0.06706	-0.06797	4.85437
R15	2.50695	-0.00002	0.00000	0.00043	0.00043	2.50738
R16	2.04677	-0.00007	0.00053	-0.00206	-0.00152	2.04524
R17	2.04698	-0.00032	0.00036	-0.00162	-0.00127	2.04572
R18	2.06835	-0.00124	-0.00028	0.00069	0.00041	2.06876
R19	2.77443	-0.00061	-0.00032	-0.00123	-0.00196	2.77247
R20	2.75514	0.00124	0.00039	0.00067	0.00124	2.75638
R21	2.05216	0.00046	0.00009	0.00081	0.00090	2.05307
R22	2.05249	0.00001	-0.00048	0.00221	0.00173	2.05422
R23	2.73508	0.00021	-0.00057	0.00295	0.00263	2.73771
R24	2.05649	-0.00016	-0.00008	-0.00026	-0.00034	2.05615
R25	2.84140	0.00017	0.00021	-0.00008	0.00013	2.84153
R26	3.10836	-0.00021	-0.00176	-0.00810	-0.00986	3.09850
R27	2.06700	0.00007	-0.00003	0.00042	0.00040	2.06739
R28	2.06813	-0.00003	-0.00006	0.00021	0.00015	2.06828
R29	2.06332	0.00007	-0.00003	0.00038	0.00035	2.06367
R30	2.06995	-0.00004	-0.00014	0.00205	0.00191	2.07186
R31	2.05955	0.00112	0.00016	0.00268	0.00284	2.06239
R32	2.88638	-0.00055	0.00127	-0.00595	-0.00469	2.88169
R33	2.28209	-0.00206	0.00049	-0.00441	-0.00392	2.27817
R34	2.51731	0.00088	-0.00176	0.00441	0.00264	2.51996
R35	1.88594	0.00204	0.00042	0.00451	0.00494	1.89087
A1	1.88033	-0.00056	0.00009	-0.00219	-0.00210	1.87823
A2	2.27359	0.00062	0.00068	-0.00006	0.00066	2.27424
A3	2.12705	0.00001	-0.00045	0.00206	0.00165	2.12870
A4	1.86084	0.00003	-0.00044	0.00226	0.00184	1.86268
A5	2.27994	-0.00124	-0.00062	-0.00143	-0.00198	2.27796
A6	2.14037	0.00125	0.00153	-0.00238	-0.00080	2.13957
A7	1.89799	-0.00067	-0.00021	0.00015	-0.00009	1.89790
A8	2.21146	0.00364	0.00368	-0.00629	-0.00263	2.20884
A9	2.17292	-0.00294	-0.00345	0.00655	0.00309	2.17601
A10	1.89694	0.00053	0.00003	-0.00126	-0.00121	1.89572
A11	2.18790	-0.00025	-0.00003	0.00086	0.00084	2.18874
A12	2.19833	-0.00027	-0.00001	0.00037	0.00037	2.19869
A13	1.88864	0.00068	0.00051	0.00108	0.00158	1.89022
A14	2.19923	0.00116	0.00135	-0.00608	-0.00474	2.19449
A15	2.19462	-0.00181	-0.00183	0.00516	0.00333	2.19795
A16	1.87555	-0.00079	-0.00026	0.00472	0.00445	1.88000

A17	1.85851	-0.00038	-0.00030	-0.00014	-0.00043	1.85808
A18	1.97959	0.00213	0.00104	-0.01037	-0.00933	1.97026
A19	1.88948	0.00017	-0.00118	0.00427	0.00309	1.89256
A20	1.92895	-0.00111	0.00195	-0.00437	-0.00242	1.92654
A21	1.92808	-0.00008	-0.00143	0.00659	0.00516	1.93324
A22	2.14555	0.00625	-0.00878	0.07669	0.06791	2.21346
A23	2.13028	0.00431	0.00324	0.00068	0.00391	2.13418
A24	1.97396	-0.00221	-0.00053	-0.00459	-0.00512	1.96884
A25	2.17895	-0.00210	-0.00272	0.00393	0.00120	2.18014
A26	2.06932	-0.00034	-0.00103	0.00089	-0.00011	2.06921
A27	2.13403	0.00169	0.00182	-0.00084	0.00101	2.13504
A28	2.07941	-0.00137	-0.00112	0.00037	-0.00071	2.07869
A29	2.06331	-0.00099	0.00000	-0.00242	-0.00227	2.06103
A30	2.13049	0.00085	-0.00047	0.00139	0.00074	2.13123
A31	1.97760	-0.00027	-0.00027	-0.00015	-0.00052	1.97709
A32	1.99502	0.00065	0.00107	-0.00319	-0.00212	1.99290
A33	2.02307	-0.00004	0.00010	0.00176	0.00188	2.02494
A34	2.04063	0.00009	0.00034	-0.00267	-0.00243	2.03820
A35	2.14137	-0.00039	-0.00058	0.00179	0.00128	2.14265
A36	1.94649	0.00008	0.00080	-0.00209	-0.00124	1.94526
A37	2.03805	-0.00047	-0.00016	0.00040	0.00011	2.03816
A38	2.02256	0.00021	-0.00021	0.00138	0.00119	2.02376
A39	2.10413	0.00020	0.00206	-0.02377	-0.02261	2.08152
A40	2.60714	-0.00135	0.00677	-0.03923	-0.03286	2.57428
A41	1.93512	0.00002	-0.00007	0.00063	0.00055	1.93567
A42	1.91616	0.00007	-0.00009	0.00053	0.00044	1.91660
A43	1.93385	0.00003	0.00028	-0.00081	-0.00053	1.93332
A44	1.88293	-0.00003	0.00004	-0.00042	-0.00039	1.88254
A45	1.89796	-0.00003	-0.00020	0.00059	0.00039	1.89835
A46	1.89665	-0.00007	0.00004	-0.00052	-0.00048	1.89617
A47	1.89279	-0.00182	-0.00155	-0.00499	-0.00655	1.88624
A48	1.94989	-0.00073	0.00153	-0.00508	-0.00356	1.94633
A49	2.01278	0.00264	-0.00083	0.00455	0.00373	2.01651
A50	1.86186	0.00051	-0.00010	0.00089	0.00076	1.86262
A51	1.87032	-0.00077	-0.00093	0.00646	0.00555	1.87587
A52	1.86903	0.00006	0.00182	-0.00152	0.00031	1.86934
A53	2.14426	-0.00162	-0.00050	-0.00799	-0.00846	2.13580
A54	1.95045	0.00160	0.00071	0.00236	0.00309	1.95354
A55	2.18810	0.00001	-0.00011	0.00544	0.00535	2.19345
A56	1.94276	-0.00082	0.00211	-0.00675	-0.00464	1.93812
A57	2.84574	0.00374	-0.00276	0.02172	0.01896	2.86470
D1	-0.00385	0.00039	0.00045	0.00218	0.00263	-0.00122
D2	3.06900	0.00120	0.01238	-0.02397	-0.01156	3.05744
D3	-3.07358	-0.00067	-0.00597	0.00518	-0.00078	-3.07436

D4	-0.00073	0.00013	0.00597	-0.02097	-0.01497	-0.01570
D5	-0.00109	-0.00050	-0.00147	0.00026	-0.00120	-0.00230
D6	-3.10453	-0.00122	-0.00213	-0.00432	-0.00644	-3.11097
D7	3.07594	0.00049	0.00433	-0.00252	0.00183	3.07778
D8	-0.02749	-0.00023	0.00367	-0.00710	-0.00341	-0.03090
D9	0.00746	-0.00015	0.00072	-0.00386	-0.00315	0.00431
D10	3.10703	0.00049	0.00130	0.00695	0.00820	3.11523
D11	-3.07219	-0.00075	-0.01000	0.01967	0.00972	-3.06247
D12	0.02738	-0.00012	-0.00942	0.03048	0.02107	0.04845
D13	-1.53600	0.00031	-0.00301	0.06976	0.06676	-1.46924
D14	1.52736	0.00117	0.01054	0.04016	0.05070	1.57805
D15	-0.00827	-0.00017	-0.00165	0.00411	0.00246	-0.00581
D16	3.12690	0.00056	0.00271	-0.00155	0.00117	3.12807
D17	-3.10899	-0.00097	-0.00241	-0.00603	-0.00846	-3.11745
D18	0.02618	-0.00025	0.00196	-0.01169	-0.00975	0.01643
D19	-0.42291	-0.00044	0.00284	-0.10382	-0.10097	-0.52387
D20	2.71672	-0.00020	0.00243	-0.09481	-0.09239	2.62433
D21	2.67040	0.00037	0.00361	-0.09161	-0.08799	2.58241
D22	-0.47317	0.00061	0.00319	-0.08260	-0.07941	-0.55258
D23	0.00580	0.00042	0.00193	-0.00270	-0.00078	0.00501
D24	3.10936	0.00122	0.00267	0.00155	0.00425	3.11361
D25	-3.12932	-0.00032	-0.00247	0.00299	0.00051	-3.12881
D26	-0.02576	0.00049	-0.00173	0.00725	0.00554	-0.02022
D27	-2.34429	0.00036	0.01010	-0.00827	0.00183	-2.34246
D28	-0.32277	-0.00001	0.00847	-0.00114	0.00732	-0.31545
D29	1.80152	0.00094	0.00712	0.00063	0.00776	1.80928
D30	0.84196	-0.00056	0.00926	-0.01348	-0.00424	0.83773
D31	2.86348	-0.00092	0.00763	-0.00636	0.00126	2.86474
D32	-1.29541	0.00003	0.00628	-0.00459	0.00170	-1.29371
D33	-3.11449	-0.00109	-0.00796	0.00453	-0.00340	-3.11790
D34	1.12156	-0.00016	-0.00775	0.00949	0.00174	1.12329
D35	-1.01781	-0.00168	-0.01083	0.01216	0.00134	-1.01646
D36	1.06119	-0.00075	-0.00979	0.00880	-0.00098	1.06021
D37	-0.98595	0.00018	-0.00959	0.01376	0.00416	-0.98179
D38	-3.12531	-0.00134	-0.01266	0.01644	0.00377	-3.12154
D39	-1.02954	-0.00020	-0.00865	0.00204	-0.00660	-1.03614
D40	-3.07668	0.00073	-0.00845	0.00700	-0.00146	-3.07814
D41	1.06715	-0.00079	-0.01152	0.00968	-0.00186	1.06529
D42	3.12661	0.00035	-0.00293	0.01558	0.01265	3.13927
D43	-0.04658	-0.00040	-0.01103	0.03133	0.02031	-0.02626
D44	-0.01277	0.00008	-0.00248	0.00550	0.00302	-0.00975
D45	3.09722	-0.00067	-0.01057	0.02125	0.01068	3.10790
D46	-2.75355	0.00044	0.00052	0.00032	0.00086	-2.75269
D47	-0.04515	0.00025	-0.00067	0.00188	0.00122	-0.04393

D48	-0.01094	-0.00009	-0.00050	0.00277	0.00226	-0.00868
D49	2.69746	-0.00029	-0.00168	0.00434	0.00261	2.70008
D50	0.60208	-0.00068	0.00758	-0.04041	-0.03272	0.56935
D51	-1.76779	-0.00102	0.00656	-0.03950	-0.03276	-1.80055
D52	2.60284	0.00001	-0.00265	0.04208	0.03932	2.64216
D53	0.22156	0.00011	-0.00307	0.04186	0.03873	0.26029
D54	2.55910	0.00020	-0.00027	0.00351	0.00328	2.56238
D55	-1.64523	0.00022	-0.00032	0.00371	0.00343	-1.64180
D56	0.44987	0.00020	-0.00016	0.00289	0.00278	0.45265
D57	1.33689	-0.00019	-0.00044	0.00284	0.00235	1.33924
D58	-2.86744	-0.00017	-0.00050	0.00304	0.00250	-2.86494
D59	-0.77234	-0.00019	-0.00033	0.00222	0.00184	-0.77049
D60	-1.01156	-0.00002	-0.00131	0.00413	0.00281	-1.00875
D61	1.06730	0.00000	-0.00137	0.00433	0.00295	1.07025
D62	-3.12079	-0.00002	-0.00120	0.00351	0.00230	-3.11849
D63	1.21675	0.00165	-0.02660	0.07146	0.04445	1.26119
D64	2.66922	0.00031	-0.02052	0.01466	-0.00544	2.66378
D65	2.60616	0.00087	0.01065	-0.05347	-0.04282	2.56334
D66	-0.56373	0.00043	0.01679	-0.06019	-0.04340	-0.60713
D67	-1.56808	-0.00032	0.00747	-0.05218	-0.04470	-1.61279
D68	1.54522	-0.00076	0.01361	-0.05890	-0.04528	1.49993
D69	0.42423	-0.00007	0.00778	-0.04881	-0.04103	0.38320
D70	-2.74566	-0.00051	0.01392	-0.05553	-0.04161	-2.78726
D71	3.00930	0.00325	0.00585	-0.00432	0.00153	3.01083
D72	-0.16144	0.00276	0.01217	-0.01151	0.00066	-0.16078
D73	-1.91670	0.00158	0.00388	-0.04716	-0.04328	-1.95998

Item	Value	Threshold	Converged?
Maximum Force	0.006248	0.000450	NO
RMS Force	0.001170	0.000300	NO
Maximum Displacement	0.422515	0.001800	NO
RMS Displacement	0.069223	0.001200	NO

Predicted change in Energy=-4.133069D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.109984	1.702669	1.643807
2	6	0	-1.858489	0.569009	1.717194
3	7	0	-2.624271	0.522172	0.565445
4	6	0	-2.339952	1.598232	-0.185749
5	7	0	-1.422547	2.334616	0.452571

6	6	0	-0.813646	3.582395	-0.046558
7	1	0	-0.350107	2.078131	2.304854
8	1	0	-1.857660	-0.227477	2.449029
9	1	0	-1.620611	4.226621	-0.403116
10	1	0	-0.345338	4.060159	0.809274
11	35	0	-0.295148	-2.265695	2.504478
12	1	0	-2.774751	1.821915	-1.144114
13	6	0	-3.546433	-0.514083	0.192759
14	6	0	-3.381321	-1.776987	0.564706
15	1	0	-4.363709	-0.149386	-0.415862
16	1	0	-4.114891	-2.508860	0.251423
17	1	0	-2.520650	-2.105336	1.156224
18	6	0	2.849988	-0.729670	1.014430
19	6	0	4.245083	-0.377626	1.301205
20	8	0	3.206623	0.625698	1.418583
21	1	0	2.543836	-0.801082	-0.025529
22	1	0	2.228495	-1.259356	1.731958
23	1	0	4.632743	-0.665137	2.276371
24	6	0	5.270137	-0.168525	0.221121
25	1	0	5.995457	0.596305	0.514070
26	1	0	5.817315	-1.099659	0.043684
27	1	0	4.792676	0.138973	-0.711641
28	6	0	0.208068	3.342089	-1.160177
29	1	0	0.626168	4.312292	-1.453341
30	1	0	-0.261922	2.920773	-2.050508
31	6	0	1.375675	2.431421	-0.795798
32	8	0	1.897717	1.698784	-1.598344
33	8	0	1.746168	2.581538	0.476377
34	1	0	2.428353	1.896800	0.735163

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.360452	0.000000			
3	N	2.202159	1.383886	0.000000		
4	C	2.207035	2.216370	1.342770	0.000000	
5	N	1.384231	2.215103	2.177575	1.338411	0.000000
6	C	2.545293	3.644586	3.608029	2.507167	1.475413
7	H	1.074880	2.213145	3.258585	3.223800	2.155659
8	H	2.221006	1.081654	2.167385	3.241585	3.277116
9	H	3.289524	4.234433	3.958331	2.733703	2.085933
10	H	2.615126	3.911786	4.215488	3.321091	2.065216
11	Br	4.141573	3.331576	4.117872	5.133076	5.161803
12	H	3.249334	3.255210	2.152804	1.075894	2.154233

13	C	3.599419	2.519155	1.436351	2.461857	3.562791
14	C	4.293185	3.025053	2.420591	3.611057	4.555727
15	H	4.273064	3.367810	2.107035	2.683787	3.946501
16	H	5.357721	4.088167	3.392302	4.495523	5.545126
17	H	4.090064	2.811631	2.695099	3.943343	4.627540
18	C	4.689751	4.934592	5.633490	5.813349	5.287730
19	C	5.755150	6.190538	6.966994	7.034041	6.340226
20	O	4.454626	5.074224	5.893886	5.855272	5.028201
21	H	4.733482	4.928966	5.367456	5.443691	5.078718
22	H	4.463945	4.477341	5.299428	5.719626	5.280490
23	H	6.243841	6.631130	7.549915	7.733262	6.999378
24	C	6.799363	7.321168	7.932042	7.823070	7.149217
25	H	7.279261	7.945611	8.620200	8.424527	7.619206
26	H	7.642049	8.031380	8.611792	8.594898	8.023531
27	H	6.544821	7.093813	7.535841	7.299342	6.693672
28	C	3.505322	4.498876	4.353371	3.237739	2.504968
29	H	4.406436	5.498907	5.385708	4.215541	3.426505
30	H	3.981325	4.719682	4.263471	3.089442	2.820645
31	C	3.558265	4.499280	4.636570	3.856456	3.065590
32	O	4.422423	5.135978	5.149250	4.468040	3.954073
33	O	3.208255	4.310852	4.832148	4.254607	3.178410
34	H	3.658298	4.593956	5.239028	4.865589	3.885997

		6	7	8	9	10
6	C	0.000000				
7	H	2.829632	0.000000			
8	H	4.672585	2.758502	0.000000		
9	H	1.092407	3.682837	5.294329	0.000000	
10	H	1.086288	2.482985	4.833192	1.767462	0.000000
11	Br	6.401311	4.348758	2.568822	7.236099	6.549249
12	H	2.854794	4.223734	4.236950	2.768344	3.837644
13	C	4.930165	4.625691	2.832817	5.151518	5.617009
14	C	5.974075	5.203682	2.876317	6.330884	6.584017
15	H	5.163867	5.336022	3.807097	5.164706	5.947145
16	H	6.934724	6.279384	3.889636	7.212251	7.594257
17	H	6.058946	4.850980	2.374290	6.582955	6.547189
18	C	5.756892	4.448544	4.946940	6.823526	5.761480
19	C	6.564219	5.306018	6.211563	7.649194	6.403741
20	O	5.201083	3.942761	5.238004	6.291854	4.978274
21	H	5.521594	4.700581	5.081892	6.539342	5.716283
22	H	5.988346	4.256315	4.275000	7.033499	5.981070
23	H	7.287021	5.688156	6.507433	8.379342	7.018695
24	C	7.152165	6.401292	7.468101	8.196913	7.054165
25	H	7.456200	6.757876	8.129829	8.486749	7.231259
26	H	8.117845	7.297146	8.090218	9.159238	8.073918

27	H	6.612892	6.269593	7.372319	7.611459	6.639885
28	C	1.530291	3.730360	5.480456	2.167857	2.168092
29	H	2.141226	4.479801	6.481311	2.481597	2.475241
30	H	2.181274	4.437003	5.718715	2.503033	3.079531
31	C	2.584420	3.566115	5.296517	3.514921	2.861980
32	O	3.647947	4.520129	5.847612	4.494125	4.050187
33	O	2.797824	2.826855	4.976896	3.849026	2.582932
34	H	3.736693	3.196349	5.081318	4.808103	3.518377

		11	12	13	14	15
11	Br	0.000000				
12	H	6.014084	0.000000			
13	C	4.356953	2.799931	0.000000		
14	C	3.677773	4.029900	1.326851	0.000000	
15	H	5.436942	2.634609	1.082296	2.139085	0.000000
16	H	4.441376	4.743323	2.075022	1.082547	2.464609
17	H	2.606983	4.558445	2.124283	1.094742	3.113528
18	C	3.804142	6.542750	6.452582	6.334692	7.376983
19	C	5.062250	7.752138	7.871150	7.788625	8.781327
20	O	4.669232	6.616282	6.957408	7.064206	7.827891
21	H	4.075029	6.034792	6.100934	6.033925	6.949190
22	H	2.824585	6.542056	6.022820	5.753300	7.021561
23	H	5.186321	8.529719	8.441752	8.269899	9.404800
24	C	6.370576	8.399163	8.823385	8.806413	9.654900
25	H	7.191974	9.009342	9.611653	9.672593	10.427519
26	H	6.691589	9.152599	9.383225	9.238244	10.235597
27	H	6.481652	7.764360	8.413392	8.492008	9.165698
28	C	6.717898	3.347894	5.549484	6.485667	5.800478
29	H	7.731951	4.226565	6.588941	7.563848	6.773611
30	H	6.902786	2.888486	5.255331	6.216023	5.377974
31	C	5.978827	4.209377	5.820686	6.495435	6.304399
32	O	6.112193	4.696109	6.143583	6.680420	6.634715
33	O	5.637005	4.862276	6.137991	6.730207	6.751639
34	H	5.279611	5.532592	6.465650	6.875905	7.186365

		16	17	18	19	20
16	H	0.000000				
17	H	1.876992	0.000000			
18	C	7.228916	5.545838	0.000000		
19	C	8.690993	6.984350	1.467129	0.000000	
20	O	8.049366	6.350515	1.458613	1.448736	0.000000
21	H	6.879815	5.361590	1.086436	2.198586	2.135521
22	H	6.632631	4.858141	1.087045	2.242682	2.146710
23	H	9.166287	7.382407	2.185149	1.088067	2.106151
24	C	9.672478	8.082204	2.607939	1.503675	2.514516
25	H	10.579706	8.957417	3.450007	2.152193	2.931996

26	H	10.033829	8.471765	3.143927	2.138833	3.418028
27	H	9.342551	7.874680	2.740055	2.149019	2.700059
28	C	7.410410	6.518133	5.318634	6.015993	4.797929
29	H	8.480093	7.609090	6.037934	6.532947	5.338321
30	H	7.044514	6.375481	5.692412	6.513564	5.415974
31	C	7.459850	6.290779	3.929760	4.530085	3.393596
32	O	7.568181	6.448329	3.691991	4.269543	3.459278
33	O	7.766258	6.374536	3.531574	3.959996	2.616485
34	H	7.903030	6.378638	2.674717	2.965456	1.639655

		21	22	23	24	25
21	H	0.000000				
22	H	1.843425	0.000000			
23	H	3.111391	2.535722	0.000000		
24	C	2.809569	3.567089	2.208381	0.000000	
25	H	3.762651	4.372268	2.560064	1.094018	0.000000
26	H	3.287796	3.969308	2.564549	1.094485	1.768981
27	H	2.532140	3.808087	3.098449	1.092048	1.777133
28	C	4.889694	5.798264	6.888067	6.313235	6.620899
29	H	5.644705	6.614895	7.398526	6.666933	6.819716
30	H	5.081833	6.163011	7.452407	6.731102	7.150874
31	C	3.522356	4.553975	5.443839	4.791730	5.140602
32	O	3.023334	4.466645	5.299236	4.262689	4.740172
33	O	3.511453	4.069593	4.702466	4.477316	4.690312
34	H	2.805451	3.315850	3.714590	3.550429	3.803209

		26	27	28	29	30
26	H	0.000000				
27	H	1.776122	0.000000			
28	C	7.255485	5.610684	0.000000		
29	H	7.647111	5.943611	1.096379	0.000000	
30	H	7.583313	5.922832	1.091369	1.755459	0.000000
31	C	5.735976	4.115617	1.524924	2.128802	2.120256
32	O	5.088300	3.405884	2.397364	2.910032	2.522251
33	O	5.505695	4.081511	2.371181	2.823778	3.245405
34	H	4.576240	3.282259	3.257428	3.724516	4.005753

		31	32	33	34
31	C	0.000000			
32	O	1.205556	0.000000		
33	O	1.333503	2.259799	0.000000	
34	H	1.933337	2.401258	1.000606	0.000000

Stoichiometry C11H17BrN2O3

Framework group C1[X(C11H17BrN2O3)]

Deg. of freedom 96

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.045706	1.158741	1.359014
2	6	0	-2.049040	0.377214	0.875934
3	7	0	-2.634417	1.078207	-0.163818
4	6	0	-1.995831	2.250689	-0.307093
5	7	0	-1.026108	2.324230	0.612458
6	6	0	-0.069599	3.435752	0.775101
7	1	0	-0.317773	0.961182	2.124816
8	1	0	-2.343468	-0.630066	1.137993
9	1	0	-0.638532	4.368244	0.763810
10	1	0	0.375895	3.317026	1.758696
11	35	0	-1.344409	-2.813095	0.224147
12	1	0	-2.225010	2.999180	-1.045190
13	6	0	-3.718471	0.631373	-0.993436
14	6	0	-3.917700	-0.651124	-1.269194
15	1	0	-4.329688	1.445955	-1.359817
16	1	0	-4.755320	-0.920823	-1.899720
17	1	0	-3.253627	-1.439326	-0.900135
18	6	0	2.255635	-1.714116	-0.326692
19	6	0	3.640164	-1.937906	0.103964
20	8	0	2.869560	-0.854159	0.678853
21	1	0	2.089961	-1.213446	-1.276547
22	1	0	1.430291	-2.315642	0.045655
23	1	0	3.806283	-2.734793	0.825951
24	6	0	4.826115	-1.554128	-0.737032
25	1	0	5.666639	-1.245000	-0.108672
26	1	0	5.150914	-2.412149	-1.333859
27	1	0	4.572681	-0.734649	-1.412897
28	6	0	1.009056	3.456342	-0.310197
29	1	0	1.686357	4.292674	-0.100772
30	1	0	0.580440	3.638971	-1.297122
31	6	0	1.858658	2.194506	-0.416688
32	8	0	2.294860	1.796864	-1.467865
33	8	0	2.072656	1.636151	0.775233
34	1	0	2.525665	0.749026	0.680345

Rotational constants (GHZ): 0.3130766 0.2647142 0.1585716

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 538 symmetry adapted cartesian basis functions of A symmetry.

There are 519 symmetry adapted basis functions of A symmetry.
519 basis functions, 823 primitive gaussians, 538 cartesian basis functions
78 alpha electrons 78 beta electrons
nuclear repulsion energy 1566.5418797811 Hartrees.
NAtoms= 34 NActive= 34 NUniq= 34 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 519 RedAO= T EigKep= 5.13D-06 NBF= 519
NBsUse= 519 1.00D-06 EigRej= -1.00D+00 NBFU= 519
Initial guess from the checkpoint file: "./coohpo.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999880 -0.003531 0.000204 0.015058 Ang= -1.77 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3338.90175839 A.U. after 13 cycles
NFock= 13 Conv=0.50D-08 -V/T= 2.0019
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000830560	-0.000548384	-0.000325111
2	6	-0.000392740	0.000450170	0.001594925
3	7	-0.000468221	-0.000033317	-0.000077217
4	6	-0.000976825	0.000330042	-0.000006952

5	7	0.000165527	-0.000375170	0.000593678
6	6	-0.000644796	-0.000931504	-0.001278276
7	1	-0.000136857	0.000538535	0.000208841
8	1	0.001835240	-0.001085291	-0.000642247
9	1	0.000624617	0.000206133	0.000332421
10	1	0.000266308	0.000599759	0.000902278
11	35	-0.000679393	0.000286219	0.000112572
12	1	-0.000175478	0.000150273	-0.000193583
13	6	0.001164458	-0.000075595	-0.000505283
14	6	0.001101221	0.001719045	0.000069008
15	1	-0.000385113	-0.000391123	-0.000712582
16	1	-0.000108609	-0.000359932	0.000523165
17	1	-0.001263248	-0.000545407	-0.000211511
18	6	-0.000624554	-0.000656148	0.000546792
19	6	-0.000053837	0.000402156	-0.000054545
20	8	-0.000493998	0.001066317	0.001498647
21	1	-0.000132127	-0.000205272	-0.000009791
22	1	0.000478987	-0.000575125	-0.000838923
23	1	0.000172423	0.000024573	-0.000163394
24	6	-0.000094893	-0.000077190	-0.000248242
25	1	-0.000165646	-0.000038974	0.000018361
26	1	-0.000066661	0.000059577	0.000009254
27	1	0.000066687	-0.000011701	0.000002026
28	6	-0.000273645	-0.000008673	-0.001550362
29	1	-0.000431869	-0.000273411	0.000524492
30	1	-0.000121234	0.000282358	-0.000149988
31	6	0.000147551	0.003663627	0.001279725
32	8	0.000663028	-0.002436756	-0.000171981
33	8	-0.001336279	-0.001085134	-0.000401284
34	1	0.001509415	-0.000064679	-0.000674915

Cartesian Forces: Max 0.003663627 RMS 0.000781639

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.003259555 RMS 0.000577458

Search for a local minimum.

Step number 17 out of a maximum of 175

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 15 16 17

DE= -3.25D-04 DEPred=-4.13D-04 R= 7.86D-01
TightC=F SS= 1.41D+00 RLast= 2.73D-01 DXNew= 1.5637D+00 8.1808D-01
Trust test= 7.86D-01 RLast= 2.73D-01 DXMaxT set to 9.30D-01
ITU= 1 1 1 1 0 0 -1 1 1 1 0 1 0 -1 0 1 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00148	0.00351	0.00435	0.00656	0.00698
Eigenvalues ---	0.00817	0.01011	0.01415	0.01698	0.01735
Eigenvalues ---	0.01922	0.02102	0.02260	0.02338	0.02389
Eigenvalues ---	0.02420	0.02535	0.02780	0.02889	0.03098
Eigenvalues ---	0.03190	0.03493	0.03680	0.03952	0.04175
Eigenvalues ---	0.04625	0.05012	0.05280	0.05736	0.05901
Eigenvalues ---	0.06010	0.06334	0.07568	0.09598	0.09661
Eigenvalues ---	0.11921	0.12354	0.12692	0.13365	0.13537
Eigenvalues ---	0.15004	0.15448	0.15890	0.15963	0.15986
Eigenvalues ---	0.15998	0.16002	0.16005	0.16021	0.16263
Eigenvalues ---	0.16918	0.17271	0.20478	0.21546	0.22493
Eigenvalues ---	0.23187	0.23458	0.23894	0.24921	0.26181
Eigenvalues ---	0.28711	0.29135	0.30168	0.31832	0.32304
Eigenvalues ---	0.32961	0.34497	0.34607	0.34724	0.34764
Eigenvalues ---	0.34884	0.34945	0.35010	0.35048	0.35192
Eigenvalues ---	0.35520	0.35737	0.35834	0.36572	0.36859
Eigenvalues ---	0.36913	0.37173	0.37333	0.37850	0.40647
Eigenvalues ---	0.41487	0.44799	0.48406	0.49042	0.52216
Eigenvalues ---	0.53291	0.55605	0.56331	0.60644	0.90556
Eigenvalues ---	1.27381				

RFO step: Lambda=-4.78543167D-04 EMin= 1.47858173D-03
Quartic linear search produced a step of -0.14907.
Iteration 1 RMS(Cart)= 0.03463218 RMS(Int)= 0.00058215
Iteration 2 RMS(Cart)= 0.00088899 RMS(Int)= 0.00003350
Iteration 3 RMS(Cart)= 0.00000062 RMS(Int)= 0.00003350

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.57088	0.00017	0.00021	-0.00062	-0.00041	2.57048
R2	2.61582	0.00023	0.00010	0.00200	0.00210	2.61792
R3	2.03123	0.00022	-0.00008	0.00045	0.00037	2.03160
R4	2.61517	0.00123	0.00022	-0.00023	0.00000	2.61516
R5	2.04403	0.00023	-0.00018	0.00215	0.00197	2.04600
R6	2.53747	-0.00027	0.00019	-0.00241	-0.00222	2.53525
R7	2.71431	-0.00037	-0.00109	0.00588	0.00479	2.71910
R8	2.52923	-0.00006	-0.00003	0.00000	-0.00004	2.52919
R9	2.03315	0.00027	0.00004	0.00068	0.00072	2.03387
R10	2.78813	-0.00012	0.00063	-0.00237	-0.00175	2.78638
R11	2.06435	-0.00045	-0.00017	-0.00019	-0.00036	2.06399
R12	2.05279	0.00109	0.00015	0.00087	0.00102	2.05381

R13	2.89183	-0.00022	0.00094	-0.00094	0.00001	2.89184
R14	4.85437	-0.00064	0.01013	-0.05277	-0.04264	4.81173
R15	2.50738	-0.00070	-0.00006	-0.00089	-0.00095	2.50643
R16	2.04524	0.00056	0.00023	-0.00031	-0.00008	2.04516
R17	2.04572	0.00016	0.00019	-0.00100	-0.00081	2.04490
R18	2.06876	-0.00094	-0.00006	-0.00205	-0.00211	2.06665
R19	2.77247	0.00009	0.00029	-0.00102	-0.00063	2.77185
R20	2.75638	0.00136	-0.00018	0.00175	0.00152	2.75790
R21	2.05307	0.00006	-0.00013	0.00085	0.00072	2.05378
R22	2.05422	-0.00055	-0.00026	0.00107	0.00082	2.05503
R23	2.73771	-0.00028	-0.00039	0.00223	0.00178	2.73950
R24	2.05615	-0.00009	0.00005	-0.00028	-0.00023	2.05592
R25	2.84153	-0.00003	-0.00002	-0.00031	-0.00033	2.84120
R26	3.09850	-0.00011	0.00147	0.00350	0.00496	3.10346
R27	2.06739	-0.00013	-0.00006	-0.00006	-0.00012	2.06727
R28	2.06828	-0.00008	-0.00002	-0.00008	-0.00010	2.06818
R29	2.06367	-0.00003	-0.00005	0.00017	0.00012	2.06379
R30	2.07186	-0.00055	-0.00028	-0.00067	-0.00096	2.07090
R31	2.06239	0.00007	-0.00042	0.00015	-0.00027	2.06212
R32	2.88169	0.00021	0.00070	-0.00195	-0.00125	2.88044
R33	2.27817	0.00188	0.00058	-0.00054	0.00005	2.27822
R34	2.51996	-0.00064	-0.00039	0.00505	0.00466	2.52461
R35	1.89087	0.00048	-0.00074	0.00016	-0.00057	1.89030
A1	1.87823	-0.00016	0.00031	-0.00195	-0.00162	1.87661
A2	2.27424	0.00036	-0.00010	0.00124	0.00113	2.27538
A3	2.12870	-0.00020	-0.00025	0.00089	0.00063	2.12933
A4	1.86268	-0.00039	-0.00027	0.00058	0.00027	1.86295
A5	2.27796	0.00042	0.00029	0.00089	0.00110	2.27906
A6	2.13957	-0.00006	0.00012	-0.00325	-0.00321	2.13636
A7	1.89790	0.00032	0.00001	0.00131	0.00133	1.89924
A8	2.20884	0.00038	0.00039	-0.00409	-0.00371	2.20513
A9	2.17601	-0.00070	-0.00046	0.00303	0.00256	2.17856
A10	1.89572	-0.00034	0.00018	-0.00105	-0.00088	1.89484
A11	2.18874	0.00021	-0.00013	0.00102	0.00089	2.18963
A12	2.19869	0.00013	-0.00005	-0.00002	-0.00009	2.19861
A13	1.89022	0.00058	-0.00024	0.00116	0.00091	1.89114
A14	2.19449	-0.00031	0.00071	-0.00171	-0.00101	2.19348
A15	2.19795	-0.00027	-0.00050	0.00087	0.00035	2.19831
A16	1.88000	0.00075	-0.00066	0.00262	0.00196	1.88196
A17	1.85808	0.00009	0.00006	0.00101	0.00107	1.85915
A18	1.97026	-0.00105	0.00139	-0.00081	0.00057	1.97083
A19	1.89256	-0.00034	-0.00046	0.00051	0.00005	1.89262
A20	1.92654	0.00042	0.00036	-0.00644	-0.00608	1.92046
A21	1.93324	0.00014	-0.00077	0.00342	0.00265	1.93589

A22	2.21346	0.00151	-0.01012	0.04360	0.03348	2.24694
A23	2.13418	0.00004	-0.00058	-0.00130	-0.00188	2.13230
A24	1.96884	0.00053	0.00076	-0.00024	0.00053	1.96936
A25	2.18014	-0.00057	-0.00018	0.00155	0.00137	2.18152
A26	2.06921	-0.00003	0.00002	0.00175	0.00166	2.07087
A27	2.13504	0.00101	-0.00015	0.00328	0.00301	2.13805
A28	2.07869	-0.00096	0.00011	-0.00442	-0.00443	2.07426
A29	2.06103	-0.00055	0.00034	-0.00176	-0.00146	2.05958
A30	2.13123	0.00072	-0.00011	-0.00083	-0.00091	2.13033
A31	1.97709	-0.00010	0.00008	0.00081	0.00090	1.97798
A32	1.99290	0.00087	0.00032	0.00213	0.00245	1.99535
A33	2.02494	-0.00032	-0.00028	0.00056	0.00027	2.02522
A34	2.03820	0.00019	0.00036	-0.00103	-0.00068	2.03752
A35	2.14265	-0.00045	-0.00019	0.00019	0.00001	2.14266
A36	1.94526	0.00018	0.00018	-0.00082	-0.00065	1.94461
A37	2.03816	-0.00055	-0.00002	-0.00034	-0.00033	2.03783
A38	2.02376	0.00017	-0.00018	0.00097	0.00079	2.02455
A39	2.08152	0.00001	0.00337	-0.00168	0.00186	2.08338
A40	2.57428	-0.00113	0.00490	-0.04471	-0.03968	2.53460
A41	1.93567	-0.00014	-0.00008	0.00019	0.00011	1.93579
A42	1.91660	-0.00001	-0.00007	0.00024	0.00018	1.91678
A43	1.93332	0.00010	0.00008	-0.00003	0.00005	1.93337
A44	1.88254	0.00008	0.00006	-0.00001	0.00005	1.88259
A45	1.89835	0.00000	-0.00006	0.00043	0.00037	1.89873
A46	1.89617	-0.00003	0.00007	-0.00086	-0.00078	1.89539
A47	1.88624	0.00033	0.00098	-0.00583	-0.00485	1.88139
A48	1.94633	0.00101	0.00053	-0.00331	-0.00277	1.94355
A49	2.01651	-0.00326	-0.00056	-0.00430	-0.00486	2.01165
A50	1.86262	-0.00035	-0.00011	0.00409	0.00395	1.86658
A51	1.87587	0.00125	-0.00083	0.00614	0.00529	1.88116
A52	1.86934	0.00120	-0.00005	0.00427	0.00421	1.87355
A53	2.13580	0.00151	0.00126	0.00469	0.00593	2.14172
A54	1.95354	-0.00056	-0.00046	0.00091	0.00042	1.95396
A55	2.19345	-0.00092	-0.00080	-0.00524	-0.00606	2.18739
A56	1.93812	0.00043	0.00069	-0.00777	-0.00708	1.93104
A57	2.86470	-0.00032	-0.00283	0.01212	0.00930	2.87400
D1	-0.00122	-0.00002	-0.00039	0.00458	0.00418	0.00297
D2	3.05744	-0.00038	0.00172	-0.02023	-0.01855	3.03890
D3	-3.07436	-0.00001	0.00012	0.00158	0.00170	-3.07267
D4	-0.01570	-0.00037	0.00223	-0.02324	-0.02103	-0.03674
D5	-0.00230	0.00010	0.00018	0.00053	0.00071	-0.00158
D6	-3.11097	0.00028	0.00096	-0.00973	-0.00876	-3.11974
D7	3.07778	0.00011	-0.00027	0.00327	0.00298	3.08076
D8	-0.03090	0.00029	0.00051	-0.00699	-0.00650	-0.03739

D9	0.00431	-0.00006	0.00047	-0.00811	-0.00765	-0.00334
D10	3.11523	-0.00022	-0.00122	0.00064	-0.00059	3.11465
D11	-3.06247	0.00023	-0.00145	0.01405	0.01256	-3.04991
D12	0.04845	0.00007	-0.00314	0.02280	0.01962	0.06807
D13	-1.46924	-0.00024	-0.00995	0.02180	0.01184	-1.45740
D14	1.57805	-0.00065	-0.00756	-0.00622	-0.01378	1.56428
D15	-0.00581	0.00013	-0.00037	0.00857	0.00820	0.00239
D16	3.12807	-0.00004	-0.00017	0.00069	0.00052	3.12859
D17	-3.11745	0.00026	0.00126	0.00017	0.00141	-3.11604
D18	0.01643	0.00009	0.00145	-0.00771	-0.00627	0.01016
D19	-0.52387	0.00093	0.01505	0.02813	0.04318	-0.48069
D20	2.62433	0.00065	0.01377	0.02531	0.03908	2.66341
D21	2.58241	0.00077	0.01312	0.03816	0.05127	2.63368
D22	-0.55258	0.00049	0.01184	0.03533	0.04718	-0.50540
D23	0.00501	-0.00014	0.00012	-0.00565	-0.00553	-0.00051
D24	3.11361	-0.00032	-0.00063	0.00458	0.00395	3.11756
D25	-3.12881	0.00002	-0.00008	0.00229	0.00220	-3.12661
D26	-0.02022	-0.00016	-0.00083	0.01251	0.01168	-0.00854
D27	-2.34246	-0.00019	-0.00027	-0.02700	-0.02727	-2.36974
D28	-0.31545	-0.00018	-0.00109	-0.02462	-0.02572	-0.34117
D29	1.80928	-0.00058	-0.00116	-0.02018	-0.02134	1.78795
D30	0.83773	0.00000	0.00063	-0.03902	-0.03839	0.79934
D31	2.86474	0.00002	-0.00019	-0.03665	-0.03683	2.82791
D32	-1.29371	-0.00039	-0.00025	-0.03220	-0.03245	-1.32616
D33	-3.11790	0.00064	0.00051	0.02999	0.03049	-3.08740
D34	1.12329	0.00029	-0.00026	0.03045	0.03020	1.15349
D35	-1.01646	0.00036	-0.00020	0.03072	0.03052	-0.98594
D36	1.06021	0.00009	0.00015	0.03177	0.03191	1.09212
D37	-0.98179	-0.00026	-0.00062	0.03223	0.03161	-0.95018
D38	-3.12154	-0.00019	-0.00056	0.03250	0.03194	-3.08960
D39	-1.03614	0.00015	0.00098	0.03312	0.03410	-1.00204
D40	-3.07814	-0.00020	0.00022	0.03358	0.03380	-3.04434
D41	1.06529	-0.00013	0.00028	0.03385	0.03413	1.09942
D42	3.13927	-0.00056	-0.00189	-0.00026	-0.00214	3.13712
D43	-0.02626	0.00017	-0.00303	0.02960	0.02657	0.00031
D44	-0.00975	-0.00024	-0.00045	0.00291	0.00246	-0.00729
D45	3.10790	0.00049	-0.00159	0.03277	0.03118	3.13908
D46	-2.75269	0.00035	-0.00013	0.00190	0.00177	-2.75092
D47	-0.04393	0.00017	-0.00018	0.00245	0.00227	-0.04166
D48	-0.00868	-0.00018	-0.00034	-0.00382	-0.00415	-0.01283
D49	2.70008	-0.00036	-0.00039	-0.00327	-0.00365	2.69643
D50	0.56935	-0.00064	0.00488	-0.04961	-0.04475	0.52460
D51	-1.80055	-0.00099	0.00488	-0.05365	-0.04881	-1.84936
D52	2.64216	-0.00034	-0.00586	-0.00833	-0.01420	2.62797

D53	0.26029	-0.00021	-0.00577	-0.00855	-0.01434	0.24595
D54	2.56238	0.00015	-0.00049	0.00124	0.00074	2.56312
D55	-1.64180	0.00016	-0.00051	0.00151	0.00099	-1.64081
D56	0.45265	0.00018	-0.00041	0.00059	0.00016	0.45281
D57	1.33924	-0.00018	-0.00035	0.00075	0.00041	1.33965
D58	-2.86494	-0.00018	-0.00037	0.00102	0.00066	-2.86428
D59	-0.77049	-0.00016	-0.00027	0.00009	-0.00017	-0.77067
D60	-1.00875	-0.00002	-0.00042	0.00133	0.00091	-1.00784
D61	1.07025	-0.00002	-0.00044	0.00160	0.00116	1.07141
D62	-3.11849	0.00000	-0.00034	0.00067	0.00033	-3.11816
D63	1.26119	0.00040	-0.00663	0.07578	0.06930	1.33050
D64	2.66378	-0.00031	0.00081	0.05737	0.05803	2.72181
D65	2.56334	-0.00030	0.00638	-0.07969	-0.07332	2.49001
D66	-0.60713	0.00091	0.00647	-0.06643	-0.05994	-0.66707
D67	-1.61279	-0.00105	0.00666	-0.08543	-0.07879	-1.69158
D68	1.49993	0.00015	0.00675	-0.07216	-0.06541	1.43452
D69	0.38320	-0.00028	0.00612	-0.07570	-0.06958	0.31362
D70	-2.78726	0.00092	0.00620	-0.06243	-0.05620	-2.84346
D71	3.01083	-0.00043	-0.00023	-0.01090	-0.01109	2.99974
D72	-0.16078	0.00087	-0.00010	0.00309	0.00295	-0.15783
D73	-1.95998	0.00004	0.00645	0.00709	0.01354	-1.94644

Item	Value	Threshold	Converged?
Maximum Force	0.003260	0.000450	NO
RMS Force	0.000577	0.000300	NO
Maximum Displacement	0.160358	0.001800	NO
RMS Displacement	0.034624	0.001200	NO

Predicted change in Energy=-2.682147D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.088294	1.691893	1.625109
2	6	0	-1.841170	0.561530	1.700640
3	7	0	-2.613200	0.519409	0.552888
4	6	0	-2.336783	1.598748	-0.194439
5	7	0	-1.409949	2.328685	0.437589
6	6	0	-0.807947	3.580329	-0.057489
7	1	0	-0.322173	2.063432	2.281469
8	1	0	-1.828188	-0.246519	2.421143
9	1	0	-1.614637	4.213753	-0.432931
10	1	0	-0.359331	4.069141	0.803325

11	35	0	-0.313855	-2.292226	2.494011
12	1	0	-2.778112	1.826708	-1.149235
13	6	0	-3.541622	-0.517284	0.187256
14	6	0	-3.400302	-1.769733	0.600292
15	1	0	-4.341651	-0.159769	-0.447885
16	1	0	-4.134856	-2.503030	0.294218
17	1	0	-2.572944	-2.087355	1.241082
18	6	0	2.843532	-0.743335	1.005180
19	6	0	4.234331	-0.379852	1.296818
20	8	0	3.182380	0.606745	1.443779
21	1	0	2.536763	-0.793283	-0.036245
22	1	0	2.233357	-1.303364	1.709922
23	1	0	4.628371	-0.687410	2.263132
24	6	0	5.252628	-0.128325	0.219638
25	1	0	5.968862	0.637860	0.530613
26	1	0	5.811290	-1.046960	0.015220
27	1	0	4.767868	0.197187	-0.703268
28	6	0	0.230973	3.347911	-1.156775
29	1	0	0.661657	4.320197	-1.421549
30	1	0	-0.230104	2.947382	-2.061075
31	6	0	1.378262	2.417305	-0.781172
32	8	0	1.863897	1.634863	-1.559225
33	8	0	1.772633	2.595554	0.482753
34	1	0	2.431385	1.891526	0.749204

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.360238	0.000000			
3	N	2.202207	1.383885	0.000000		
4	C	2.208655	2.216479	1.341596	0.000000	
5	N	1.385341	2.214517	2.175911	1.338390	0.000000
6	C	2.544783	3.643036	3.605653	2.506542	1.474490
7	H	1.075077	2.213690	3.258957	3.225632	2.157199
8	H	2.222286	1.082699	2.166395	3.241134	3.277360
9	H	3.297324	4.235821	3.951854	2.723348	2.086429
10	H	2.618783	3.912078	4.212273	3.317934	2.065610
11	Br	4.150656	3.332575	4.118281	5.143898	5.175241
12	H	3.251252	3.255814	2.152545	1.076277	2.154498
13	C	3.600930	2.519068	1.438883	2.464736	3.564581
14	C	4.287014	3.012714	2.421146	3.620683	4.559059
15	H	4.279053	3.374736	2.109591	2.678828	3.946055
16	H	5.352587	4.078057	3.393742	4.505158	5.548978
17	H	4.078526	2.786266	2.696377	3.962809	4.636763

18	C	4.666252	4.912512	5.619165	5.810345	5.277459
19	C	5.721035	6.161249	6.946279	7.022695	6.319204
20	O	4.410111	5.030316	5.864304	5.842002	5.006694
21	H	4.698641	4.900875	5.347182	5.431232	5.054477
22	H	4.473491	4.481036	5.305690	5.738904	5.299461
23	H	6.224822	6.612957	7.538017	7.731723	6.992191
24	C	6.745060	7.279508	7.899485	7.794446	7.104529
25	H	7.218889	7.897556	8.582909	8.392422	7.570627
26	H	7.595875	7.999251	8.585723	8.569412	7.982460
27	H	6.476891	7.042081	7.494126	7.259431	6.634023
28	C	3.495960	4.496945	4.360355	3.252542	2.504684
29	H	4.387760	5.489971	5.391575	4.231161	3.422582
30	H	3.987568	4.736911	4.290339	3.121095	2.831632
31	C	3.521407	4.468560	4.616654	3.849136	3.044232
32	O	4.342657	5.050375	5.074413	4.416974	3.897015
33	O	3.210372	4.322046	4.852920	4.282466	3.194071
34	H	3.632521	4.574806	5.231547	4.869456	3.878667

		6	7	8	9	10
6	C	0.000000				
7	H	2.829784	0.000000			
8	H	4.672181	2.761062	0.000000		
9	H	1.092214	3.696256	5.299564	0.000000	
10	H	1.086827	2.491818	4.837334	1.767777	0.000000
11	Br	6.421930	4.360849	2.546259	7.251675	6.582361
12	H	2.854583	4.225802	4.236535	2.750409	3.832948
13	C	4.931867	4.627166	2.828324	5.145932	5.616209
14	C	5.981317	5.195613	2.847319	6.329160	6.586439
15	H	5.160214	5.343052	3.815278	5.154079	5.942060
16	H	6.942570	6.272025	3.864760	7.210786	7.596526
17	H	6.076524	4.835019	2.309953	6.589738	6.556993
18	C	5.758181	4.419112	4.906806	6.820276	5.784376
19	C	6.552996	5.263166	6.167335	7.635684	6.413954
20	O	5.197954	3.886587	5.175818	6.288396	4.994205
21	H	5.505998	4.658984	5.038899	6.516279	5.721485
22	H	6.018615	4.265292	4.256631	7.059565	6.033884
23	H	7.290571	5.663511	6.473523	8.382440	7.045068
24	C	7.110660	6.335089	7.416101	8.151001	7.032317
25	H	7.411419	6.683927	8.071569	8.439484	7.203755
26	H	8.076595	7.240842	8.049273	9.111550	8.054325
27	H	6.553808	6.188704	7.312098	7.546010	6.599243
28	C	1.530295	3.711789	5.473716	2.163310	2.170397
29	H	2.137242	4.446713	6.466878	2.483992	2.460795
30	H	2.179193	4.432554	5.731070	2.484247	3.078933
31	C	2.579894	3.520863	5.256625	3.507983	2.873747

32	O	3.630262	4.439990	5.745818	4.474307	4.055871
33	O	2.814434	2.811894	4.980026	3.864020	2.611416
34	H	3.741134	3.155863	5.050800	4.812534	3.540202

		11	12	13	14	15
11	Br	0.000000				
12	H	6.025896	0.000000			
13	C	4.346264	2.804186	0.000000		
14	C	3.658596	4.047513	1.326348	0.000000	
15	H	5.424506	2.623479	1.082252	2.139346	0.000000
16	H	4.414021	4.761402	2.075224	1.082116	2.466648
17	H	2.591387	4.590817	2.124619	1.093625	3.113924
18	C	3.819002	6.545954	6.441295	6.340575	7.353830
19	C	5.077051	7.747673	7.855918	7.791312	8.754422
20	O	4.661618	6.613584	6.932134	7.049172	7.795960
21	H	4.095735	6.029178	6.088751	6.050403	6.919781
22	H	2.842698	6.564065	6.023854	5.760807	7.013892
23	H	5.201378	8.533523	8.431309	8.270190	9.385591
24	C	6.390694	8.377872	8.802906	8.815459	9.617524
25	H	7.205059	8.985811	9.586530	9.673810	10.387510
26	H	6.724024	9.131908	9.369478	9.258410	10.202147
27	H	6.499514	7.732790	8.387558	8.502180	9.120087
28	C	6.740639	3.371751	5.565844	6.516420	5.806482
29	H	7.746443	4.257188	6.607347	7.594380	6.786105
30	H	6.943293	2.929113	5.293869	6.275684	5.400147
31	C	5.980783	4.214228	5.809898	6.501877	6.282500
32	O	6.049244	4.664027	6.074666	6.630731	6.554740
33	O	5.682340	4.895282	6.165905	6.769698	6.770700
34	H	5.299479	5.545009	6.464902	6.887349	7.177385

		16	17	18	19	20
16	H	0.000000				
17	H	1.873208	0.000000			
18	C	7.231867	5.585719	0.000000		
19	C	8.692318	7.018381	1.466797	0.000000	
20	O	8.033314	6.357910	1.459419	1.449680	0.000000
21	H	6.895139	5.423587	1.086815	2.197662	2.137140
22	H	6.633066	4.892339	1.087477	2.242192	2.149417
23	H	9.163364	7.406981	2.184312	1.087944	2.106434
24	C	9.683473	8.131465	2.607500	1.503499	2.514911
25	H	10.583298	8.994110	3.449725	2.152070	2.932460
26	H	10.056034	8.537010	3.143214	2.138767	3.418580
27	H	9.356530	7.930142	2.739790	2.148949	2.700245
28	C	7.443074	6.569154	5.313926	5.995265	4.794546
29	H	8.515094	7.655650	6.024031	6.499537	5.324836
30	H	7.106440	6.460783	5.698294	6.502085	5.422881

31	C	7.467304	6.324042	3.915063	4.505470	3.388714
32	O	7.519472	6.432899	3.632036	4.223152	3.437071
33	O	7.805738	6.433409	3.545129	3.946606	2.620366
34	H	7.914207	6.412235	2.679158	2.951213	1.642282

		21	22	23	24	25
21	H	0.000000				
22	H	1.844271	0.000000			
23	H	3.110171	2.534074	0.000000		
24	C	2.807769	3.566183	2.208651	0.000000	
25	H	3.761490	4.371855	2.560250	1.093954	0.000000
26	H	3.284742	3.967287	2.565478	1.094432	1.768920
27	H	2.530570	3.807740	3.098629	1.092111	1.777369
28	C	4.870497	5.819093	6.878712	6.260650	6.566203
29	H	5.619854	6.625767	7.374810	6.599989	6.748108
30	H	5.074255	6.193375	7.450856	6.687449	7.104782
31	C	3.493553	4.558521	5.428651	4.742633	5.095176
32	O	2.944165	4.411009	5.257916	4.213868	4.712979
33	O	3.512473	4.113365	4.701366	4.427088	4.630679
34	H	2.799327	3.342083	3.710746	3.509936	3.759415

		26	27	28	29	30
26	H	0.000000				
27	H	1.775629	0.000000			
28	C	7.199194	5.542215	0.000000		
29	H	7.575579	5.863114	1.095872	0.000000	
30	H	7.534203	5.864038	1.091226	1.757513	0.000000
31	C	5.682175	4.052706	1.524262	2.131807	2.122728
32	O	5.025233	3.351510	2.400612	2.945395	2.521785
33	O	5.458685	4.016247	2.372932	2.799112	3.256655
34	H	4.538413	3.231039	3.255092	3.707094	4.011985

		31	32	33	34
31	C	0.000000			
32	O	1.205580	0.000000		
33	O	1.335967	2.258524	0.000000	
34	H	1.930690	2.390975	1.000303	0.000000

Stoichiometry C11H17BrN2O3
Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.984971	1.186612	1.343669
2	6	0	-2.012847	0.432305	0.869602
3	7	0	-2.589743	1.149259	-0.163987
4	6	0	-1.929934	2.308537	-0.307538
5	7	0	-0.947065	2.354638	0.599728
6	6	0	0.031266	3.445881	0.761526
7	1	0	-0.253740	0.969720	2.101330
8	1	0	-2.321091	-0.574983	1.119790
9	1	0	-0.514117	4.391600	0.728286
10	1	0	0.460738	3.331406	1.753313
11	35	0	-1.430559	-2.783896	0.219185
12	1	0	-2.148765	3.064722	-1.041479
13	6	0	-3.694783	0.725958	-0.982576
14	6	0	-3.952888	-0.554384	-1.213456
15	1	0	-4.268429	1.555359	-1.375379
16	1	0	-4.801680	-0.808773	-1.834596
17	1	0	-3.343474	-1.361146	-0.796604
18	6	0	2.208560	-1.769686	-0.340245
19	6	0	3.586893	-2.018166	0.095590
20	8	0	2.823984	-0.937513	0.688660
21	1	0	2.057189	-1.248419	-1.281805
22	1	0	1.374527	-2.372714	0.010971
23	1	0	3.737881	-2.832003	0.801630
24	6	0	4.783266	-1.629681	-0.727989
25	1	0	5.622584	-1.344349	-0.086999
26	1	0	5.102630	-2.477743	-1.341648
27	1	0	4.544160	-0.792856	-1.387729
28	6	0	1.122425	3.431976	-0.311312
29	1	0	1.829451	4.236785	-0.080378
30	1	0	0.710892	3.643946	-1.299484
31	6	0	1.913646	2.133489	-0.417510
32	8	0	2.284404	1.680824	-1.471577
33	8	0	2.149525	1.592875	0.781200
34	1	0	2.551381	0.681981	0.684298

Rotational constants (GHZ): 0.3146571 0.2650328 0.1587550

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 538 symmetry adapted cartesian basis functions of A symmetry.

There are 519 symmetry adapted basis functions of A symmetry.

519 basis functions, 823 primitive gaussians, 538 cartesian basis functions

78 alpha electrons 78 beta electrons

nuclear repulsion energy 1567.9281827399 Hartrees.

NAtoms= 34 NActive= 34 NUniq= 34 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F

Big=F
 Integral buffers will be 131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis= 519 RedAO= T EigKep= 4.92D-06 NBF= 519
 NBsUse= 519 1.00D-06 EigRej= -1.00D+00 NBFU= 519
 Initial guess from the checkpoint file: "./coohpo.chk"
 B after Tr= 0.000000 0.000000 0.000000
 Rot= 0.999909 0.000481 -0.001300 0.013394 Ang= 1.54 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
 Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
 HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
 FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
 NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
 wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
 NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on energy=1.00D-06.
 No special actions if energy rises.
 SCF Done: E(RB3LYP) = -3338.90208287 A.U. after 13 cycles
 NFock= 13 Conv=0.19D-08 -V/T= 2.0019
 Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
 ***** Axes restored to original set *****

 Center Atomic Forces (Hartrees/Bohr)
 Number Number X Y Z

1	6	0.000211223	-0.000399639	-0.000910407
2	6	0.000566052	-0.000436198	0.001127474
3	7	-0.002920697	-0.001561863	0.000553693
4	6	-0.000257688	0.000132053	-0.000761145
5	7	-0.000130616	0.000426818	0.001395825
6	6	-0.000473207	-0.000675803	-0.001167151
7	1	-0.000174852	0.000536278	0.000092992
8	1	0.001875911	-0.000504637	-0.000279659
9	1	0.000328719	0.000243604	0.000732624

10	1	0.000263796	0.000364773	0.000632558
11	35	-0.000582313	0.000231708	0.000423575
12	1	-0.000120783	0.000172756	0.000087643
13	6	0.002444304	0.001504532	-0.000285183
14	6	-0.000760325	0.001822053	0.001896640
15	1	0.000118262	-0.000429880	-0.001226668
16	1	-0.000289288	-0.000433961	0.000053794
17	1	0.000149249	-0.001098734	-0.001572289
18	6	-0.000567563	-0.001004074	0.000166254
19	6	-0.000236700	0.000568193	0.000165005
20	8	-0.000654149	0.000438959	0.001221103
21	1	-0.000225999	0.000064288	0.000324479
22	1	0.000507495	0.000087649	-0.000840660
23	1	0.000290047	0.000081992	-0.000118389
24	6	-0.000062995	-0.000077101	-0.000351005
25	1	-0.000114899	-0.000017167	0.000027267
26	1	-0.000022958	0.000029056	0.000033943
27	1	0.000064857	-0.000032608	0.000039081
28	6	0.000170349	0.000212981	-0.001472412
29	1	-0.000130455	-0.000145615	0.000178165
30	1	0.000211040	0.000004627	-0.000127627
31	6	0.000498043	0.002427369	0.003159519
32	8	0.000471900	-0.001710185	-0.000934390
33	8	-0.002381512	-0.000452188	-0.002123109
34	1	0.001935752	-0.000370038	-0.000141540

Cartesian Forces: Max 0.003159519 RMS 0.000932127

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.003718711 RMS 0.000721451
Search for a local minimum.
Step number 18 out of a maximum of 175
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 16 17 18
DE= -3.24D-04 DEPred=-2.68D-04 R= 1.21D+00
TightC=F SS= 1.41D+00 RLast= 2.70D-01 DXNew= 1.5637D+00 8.1047D-01
Trust test= 1.21D+00 RLast= 2.70D-01 DXMaxT set to 9.30D-01
ITU= 1 1 1 1 1 0 0 -1 1 1 1 0 1 0 -1 0 1 0

Eigenvalues --- 0.00131 0.00350 0.00438 0.00642 0.00661
Eigenvalues --- 0.00699 0.01032 0.01420 0.01645 0.01748
Eigenvalues --- 0.01866 0.02086 0.02229 0.02340 0.02410
Eigenvalues --- 0.02456 0.02493 0.02725 0.03014 0.03137
Eigenvalues --- 0.03413 0.03480 0.03827 0.04145 0.04556
Eigenvalues --- 0.04829 0.04976 0.05289 0.05678 0.05772
Eigenvalues --- 0.05904 0.06204 0.07578 0.09524 0.09658
Eigenvalues --- 0.11440 0.12020 0.12718 0.12988 0.13550
Eigenvalues --- 0.14976 0.15365 0.15735 0.15922 0.15977
Eigenvalues --- 0.15999 0.16002 0.16004 0.16026 0.16038
Eigenvalues --- 0.16857 0.17240 0.20308 0.21558 0.22661
Eigenvalues --- 0.23013 0.23581 0.23858 0.24986 0.25700
Eigenvalues --- 0.28868 0.29156 0.29780 0.31667 0.31877
Eigenvalues --- 0.33107 0.34497 0.34536 0.34618 0.34764
Eigenvalues --- 0.34875 0.34938 0.34974 0.35113 0.35200
Eigenvalues --- 0.35363 0.35734 0.35792 0.36555 0.36831
Eigenvalues --- 0.36939 0.37242 0.37547 0.37789 0.40870
Eigenvalues --- 0.44460 0.46818 0.47841 0.49130 0.51950
Eigenvalues --- 0.53962 0.56216 0.56662 0.60576 0.91525
Eigenvalues --- 1.32078
En-DIIS/RFO-DIIS IScMMF= 0 using points: 18 17
RFO step: Lambda=-1.92994281D-04.
DidBck=F Rises=F RFO-DIIS coefs: 1.34977 -0.34977
Iteration 1 RMS(Cart)= 0.11905598 RMS(Int)= 0.00540574
Iteration 2 RMS(Cart)= 0.00969845 RMS(Int)= 0.00045879
Iteration 3 RMS(Cart)= 0.00006040 RMS(Int)= 0.00045725
Iteration 4 RMS(Cart)= 0.00000006 RMS(Int)= 0.00045725

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.57048	0.00045	-0.00014	-0.00153	-0.00164	2.56884
R2	2.61792	-0.00035	0.00073	0.00168	0.00240	2.62031
R3	2.03160	0.00012	0.00013	0.00103	0.00116	2.03276
R4	2.61516	0.00193	0.00000	0.00296	0.00299	2.61816
R5	2.04600	0.00032	0.00069	0.00679	0.00748	2.05349
R6	2.53525	0.00048	-0.00078	-0.00279	-0.00358	2.53167
R7	2.71910	-0.00177	0.00167	0.00760	0.00927	2.72836
R8	2.52919	-0.00004	-0.00001	0.00044	0.00038	2.52957
R9	2.03387	0.00001	0.00025	0.00073	0.00099	2.03485
R10	2.78638	0.00020	-0.00061	-0.00544	-0.00605	2.78034
R11	2.06399	-0.00035	-0.00013	-0.00070	-0.00083	2.06316
R12	2.05381	0.00077	0.00036	0.00312	0.00348	2.05728
R13	2.89184	0.00039	0.00000	-0.00084	-0.00084	2.89100
R14	4.81173	-0.00052	-0.01491	-0.18843	-0.20335	4.60839
R15	2.50643	-0.00024	-0.00033	-0.00156	-0.00189	2.50454

R16	2.04516	0.00049	-0.00003	0.00014	0.00011	2.04527
R17	2.04490	0.00047	-0.00028	-0.00054	-0.00083	2.04407
R18	2.06665	-0.00048	-0.00074	-0.00397	-0.00470	2.06195
R19	2.77185	0.00026	-0.00022	-0.00214	-0.00406	2.76778
R20	2.75790	0.00069	0.00053	0.00834	0.00954	2.76745
R21	2.05378	-0.00025	0.00025	0.00055	0.00080	2.05459
R22	2.05503	-0.00088	0.00029	-0.00073	-0.00044	2.05459
R23	2.73950	-0.00042	0.00062	0.00390	0.00556	2.74506
R24	2.05592	-0.00002	-0.00008	-0.00065	-0.00074	2.05518
R25	2.84120	0.00007	-0.00012	-0.00001	-0.00013	2.84107
R26	3.10346	-0.00031	0.00174	-0.02093	-0.01919	3.08427
R27	2.06727	-0.00008	-0.00004	-0.00015	-0.00020	2.06708
R28	2.06818	-0.00004	-0.00004	-0.00020	-0.00023	2.06794
R29	2.06379	-0.00007	0.00004	0.00013	0.00018	2.06397
R30	2.07090	-0.00023	-0.00034	-0.00061	-0.00094	2.06996
R31	2.06212	0.00002	-0.00009	0.00221	0.00212	2.06423
R32	2.88044	-0.00026	-0.00044	-0.00683	-0.00727	2.87317
R33	2.27822	0.00191	0.00002	0.00010	0.00011	2.27833
R34	2.52461	-0.00203	0.00163	0.00324	0.00487	2.52948
R35	1.89030	0.00089	-0.00020	0.00814	0.00794	1.89823
A1	1.87661	0.00056	-0.00057	-0.00034	-0.00087	1.87574
A2	2.27538	0.00006	0.00040	0.00261	0.00295	2.27833
A3	2.12933	-0.00061	0.00022	-0.00154	-0.00138	2.12795
A4	1.86295	-0.00068	0.00009	-0.00148	-0.00151	1.86144
A5	2.27906	-0.00041	0.00038	-0.00025	-0.00018	2.27888
A6	2.13636	0.00112	-0.00112	-0.00111	-0.00253	2.13383
A7	1.89924	-0.00023	0.00047	0.00237	0.00289	1.90213
A8	2.20513	0.00225	-0.00130	-0.00140	-0.00275	2.20238
A9	2.17856	-0.00202	0.00089	-0.00083	0.00002	2.17858
A10	1.89484	0.00015	-0.00031	-0.00191	-0.00232	1.89252
A11	2.18963	-0.00001	0.00031	0.00218	0.00241	2.19204
A12	2.19861	-0.00014	-0.00003	-0.00056	-0.00066	2.19794
A13	1.89114	0.00021	0.00032	0.00135	0.00165	1.89279
A14	2.19348	-0.00001	-0.00035	-0.00523	-0.00558	2.18789
A15	2.19831	-0.00020	0.00012	0.00377	0.00389	2.20220
A16	1.88196	0.00044	0.00068	0.01497	0.01566	1.89762
A17	1.85915	0.00025	0.00038	-0.00399	-0.00363	1.85553
A18	1.97083	-0.00115	0.00020	-0.01176	-0.01156	1.95927
A19	1.89262	-0.00041	0.00002	-0.00187	-0.00185	1.89077
A20	1.92046	0.00094	-0.00213	-0.00047	-0.00256	1.91790
A21	1.93589	-0.00007	0.00093	0.00361	0.00450	1.94039
A22	2.24694	0.00265	0.01171	0.15335	0.16506	2.41200
A23	2.13230	0.00160	-0.00066	0.00394	0.00328	2.13558
A24	1.96936	-0.00040	0.00018	-0.00302	-0.00283	1.96653

A25	2.18152	-0.00120	0.00048	-0.00092	-0.00044	2.18107
A26	2.07087	-0.00040	0.00058	-0.00083	-0.00030	2.07057
A27	2.13805	0.00122	0.00105	0.01309	0.01409	2.15214
A28	2.07426	-0.00081	-0.00155	-0.01225	-0.01385	2.06041
A29	2.05958	-0.00031	-0.00051	-0.00245	-0.00247	2.05711
A30	2.13033	0.00059	-0.00032	0.00195	0.00098	2.13131
A31	1.97798	-0.00007	0.00031	-0.00200	-0.00223	1.97575
A32	1.99535	0.00046	0.00086	0.00719	0.00822	2.00357
A33	2.02522	-0.00026	0.00010	-0.00190	-0.00178	2.02344
A34	2.03752	0.00028	-0.00024	0.00038	-0.00074	2.03678
A35	2.14266	-0.00036	0.00000	-0.00154	-0.00078	2.14188
A36	1.94461	0.00013	-0.00023	-0.00133	-0.00136	1.94325
A37	2.03783	-0.00027	-0.00011	-0.00137	-0.00204	2.03580
A38	2.02455	0.00002	0.00028	0.00105	0.00143	2.02598
A39	2.08338	-0.00019	0.00065	-0.02812	-0.03164	2.05174
A40	2.53460	-0.00099	-0.01388	-0.11515	-0.12980	2.40480
A41	1.93579	-0.00012	0.00004	-0.00083	-0.00079	1.93499
A42	1.91678	-0.00002	0.00006	0.00067	0.00073	1.91751
A43	1.93337	0.00008	0.00002	0.00006	0.00008	1.93345
A44	1.88259	0.00006	0.00002	0.00025	0.00027	1.88286
A45	1.89873	0.00001	0.00013	0.00104	0.00117	1.89990
A46	1.89539	-0.00001	-0.00027	-0.00119	-0.00146	1.89392
A47	1.88139	0.00074	-0.00170	-0.00864	-0.01021	1.87118
A48	1.94355	0.00136	-0.00097	0.00087	-0.00008	1.94347
A49	2.01165	-0.00372	-0.00170	-0.02490	-0.02664	1.98501
A50	1.86658	-0.00047	0.00138	0.00896	0.01016	1.87674
A51	1.88116	0.00118	0.00185	0.01917	0.02078	1.90194
A52	1.87355	0.00110	0.00147	0.00757	0.00886	1.88240
A53	2.14172	0.00099	0.00207	0.00280	0.00473	2.14646
A54	1.95396	-0.00159	0.00015	0.00078	0.00079	1.95475
A55	2.18739	0.00062	-0.00212	-0.00323	-0.00548	2.18190
A56	1.93104	0.00136	-0.00248	-0.01291	-0.01539	1.91565
A57	2.87400	-0.00101	0.00325	0.02387	0.02712	2.90112
D1	0.00297	-0.00017	0.00146	-0.00248	-0.00102	0.00194
D2	3.03890	0.00013	-0.00649	-0.03362	-0.04015	2.99875
D3	-3.07267	-0.00023	0.00059	-0.01524	-0.01466	-3.08732
D4	-0.03674	0.00007	-0.00736	-0.04638	-0.05378	-0.09052
D5	-0.00158	0.00011	0.00025	0.01001	0.01027	0.00869
D6	-3.11974	0.00036	-0.00307	0.01518	0.01212	-3.10762
D7	3.08076	0.00018	0.00104	0.02166	0.02267	3.10343
D8	-0.03739	0.00043	-0.00227	0.02683	0.02452	-0.01287
D9	-0.00334	0.00018	-0.00267	-0.00592	-0.00861	-0.01194
D10	3.11465	0.00004	-0.00021	0.00068	0.00046	3.11511
D11	-3.04991	0.00001	0.00439	0.02202	0.02635	-3.02357

D12	0.06807	-0.00014	0.00686	0.02862	0.03542	0.10348
D13	-1.45740	-0.00016	0.00414	0.05503	0.05916	-1.39824
D14	1.56428	0.00007	-0.00482	0.01968	0.01488	1.57915
D15	0.00239	-0.00012	0.00287	0.01229	0.01515	0.01754
D16	3.12859	-0.00005	0.00018	-0.00761	-0.00744	3.12115
D17	-3.11604	-0.00004	0.00049	0.00583	0.00628	-3.10975
D18	0.01016	0.00002	-0.00219	-0.01407	-0.01631	-0.00615
D19	-0.48069	0.00033	0.01510	-0.03739	-0.02228	-0.50298
D20	2.66341	0.00032	0.01367	-0.03814	-0.02446	2.63895
D21	2.63368	0.00020	0.01793	-0.02974	-0.01181	2.62187
D22	-0.50540	0.00019	0.01650	-0.03049	-0.01399	-0.51939
D23	-0.00051	0.00001	-0.00193	-0.01377	-0.01570	-0.01621
D24	3.11756	-0.00024	0.00138	-0.01911	-0.01773	3.09984
D25	-3.12661	-0.00006	0.00077	0.00622	0.00696	-3.11965
D26	-0.00854	-0.00031	0.00409	0.00088	0.00493	-0.00360
D27	-2.36974	-0.00008	-0.00954	-0.05529	-0.06485	-2.43458
D28	-0.34117	-0.00021	-0.00899	-0.05214	-0.06115	-0.40232
D29	1.78795	-0.00084	-0.00746	-0.05759	-0.06501	1.72293
D30	0.79934	0.00020	-0.01343	-0.04916	-0.06261	0.73673
D31	2.82791	0.00008	-0.01288	-0.04602	-0.05892	2.76899
D32	-1.32616	-0.00055	-0.01135	-0.05147	-0.06278	-1.38894
D33	-3.08740	0.00066	0.01067	0.04389	0.05448	-3.03293
D34	1.15349	0.00003	0.01056	0.03776	0.04838	1.20186
D35	-0.98594	0.00030	0.01068	0.04594	0.05667	-0.92927
D36	1.09212	0.00021	0.01116	0.03301	0.04408	1.13620
D37	-0.95018	-0.00043	0.01106	0.02689	0.03798	-0.91220
D38	-3.08960	-0.00016	0.01117	0.03507	0.04627	-3.04333
D39	-1.00204	0.00015	0.01193	0.03334	0.04518	-0.95686
D40	-3.04434	-0.00049	0.01182	0.02721	0.03908	-3.00526
D41	1.09942	-0.00022	0.01194	0.03539	0.04737	1.14679
D42	3.13712	-0.00011	-0.00075	0.00162	0.00087	3.13800
D43	0.00031	-0.00138	0.00929	-0.00060	0.00870	0.00901
D44	-0.00729	-0.00009	0.00086	0.00246	0.00332	-0.00397
D45	3.13908	-0.00137	0.01090	0.00024	0.01115	-3.13296
D46	-2.75092	0.00007	0.00062	-0.00165	-0.00083	-2.75175
D47	-0.04166	-0.00007	0.00079	-0.00167	-0.00073	-0.04238
D48	-0.01283	0.00004	-0.00145	-0.00894	-0.01041	-0.02324
D49	2.69643	-0.00009	-0.00128	-0.00897	-0.01030	2.68613
D50	0.52460	-0.00068	-0.01565	-0.12727	-0.14267	0.38194
D51	-1.84936	-0.00069	-0.01707	-0.12996	-0.14644	-1.99580
D52	2.62797	-0.00037	-0.00497	0.01653	0.01061	2.63858
D53	0.24595	-0.00026	-0.00501	0.01791	0.01216	0.25811
D54	2.56312	0.00006	0.00026	0.00146	0.00196	2.56509
D55	-1.64081	0.00004	0.00035	0.00167	0.00227	-1.63854

D56	0.45281	0.00007	0.00006	0.00066	0.00097	0.45378
D57	1.33965	-0.00009	0.00014	-0.00125	-0.00134	1.33831
D58	-2.86428	-0.00011	0.00023	-0.00104	-0.00104	-2.86532
D59	-0.77067	-0.00008	-0.00006	-0.00205	-0.00234	-0.77300
D60	-1.00784	-0.00002	0.00032	0.00128	0.00158	-1.00627
D61	1.07141	-0.00003	0.00040	0.00150	0.00188	1.07329
D62	-3.11816	0.00000	0.00011	0.00049	0.00058	-3.11758
D63	1.33050	0.00005	0.02424	0.10795	0.13038	1.46088
D64	2.72181	-0.00044	0.02030	0.02764	0.04975	2.77156
D65	2.49001	-0.00009	-0.02565	-0.13135	-0.15696	2.33306
D66	-0.66707	0.00064	-0.02097	-0.10780	-0.12867	-0.79574
D67	-1.69158	-0.00070	-0.02756	-0.14449	-0.17227	-1.86386
D68	1.43452	0.00004	-0.02288	-0.12094	-0.14398	1.29053
D69	0.31362	-0.00012	-0.02434	-0.12087	-0.14512	0.16851
D70	-2.84346	0.00062	-0.01966	-0.09732	-0.11683	-2.96029
D71	2.99974	-0.00052	-0.00388	-0.00067	-0.00446	2.99528
D72	-0.15783	0.00024	0.00103	0.02368	0.02462	-0.13321
D73	-1.94644	-0.00044	0.00474	-0.04063	-0.03590	-1.98234

Item	Value	Threshold	Converged?
Maximum Force	0.003719	0.000450	NO
RMS Force	0.000721	0.000300	NO
Maximum Displacement	0.535848	0.001800	NO
RMS Displacement	0.121727	0.001200	NO

Predicted change in Energy=-5.210405D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.008581	1.681085	1.579031
2	6	0	-1.749338	0.543811	1.655045
3	7	0	-2.548453	0.514120	0.523647
4	6	0	-2.308672	1.610372	-0.208154
5	7	0	-1.364245	2.332056	0.407525
6	6	0	-0.771622	3.586090	-0.083281
7	1	0	-0.237535	2.057908	2.227572
8	1	0	-1.690778	-0.292917	2.345904
9	1	0	-1.566431	4.212656	-0.492755
10	1	0	-0.353980	4.088367	0.787633
11	35	0	-0.349163	-2.306007	2.653411
12	1	0	-2.771497	1.848222	-1.150871
13	6	0	-3.479671	-0.529262	0.164880

14	6	0	-3.308010	-1.790750	0.533290
15	1	0	-4.309863	-0.162826	-0.424952
16	1	0	-4.045457	-2.523189	0.233741
17	1	0	-2.463563	-2.129473	1.135580
18	6	0	2.756676	-0.722310	1.141631
19	6	0	4.167887	-0.361090	1.293925
20	8	0	3.137567	0.622356	1.579200
21	1	0	2.343502	-0.744611	0.136205
22	1	0	2.227171	-1.311312	1.886481
23	1	0	4.661605	-0.692549	2.204502
24	6	0	5.065093	-0.076837	0.121522
25	1	0	5.810043	0.682604	0.376097
26	1	0	5.598808	-0.987353	-0.167647
27	1	0	4.484309	0.271659	-0.735304
28	6	0	0.299948	3.342948	-1.147733
29	1	0	0.760699	4.311318	-1.370915
30	1	0	-0.138379	2.965765	-2.074460
31	6	0	1.383277	2.368301	-0.713995
32	8	0	1.773897	1.467339	-1.413460
33	8	0	1.823984	2.626580	0.523245
34	1	0	2.433846	1.888641	0.827447

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.359372	0.000000			
3	N	2.201556	1.385470	0.000000		
4	C	2.211168	2.218539	1.339700	0.000000	
5	N	1.386609	2.214142	2.172723	1.338592	0.000000
6	C	2.539385	3.637742	3.600347	2.506308	1.471290
7	H	1.075692	2.214910	3.259906	3.228414	2.158056
8	H	2.224898	1.086660	2.169685	3.244613	3.279393
9	H	3.318485	4.255223	3.959370	2.720992	2.094765
10	H	2.617216	3.906828	4.202457	3.309511	2.061491
11	Br	4.181630	3.328467	4.162438	5.231277	5.252240
12	H	3.253947	3.258751	2.152577	1.076799	2.154774
13	C	3.604406	2.523119	1.443788	2.467474	3.566657
14	C	4.293551	3.022906	2.426817	3.621608	4.559777
15	H	4.279535	3.373723	2.112028	2.682537	3.948939
16	H	5.358017	4.086411	3.398575	4.505333	5.549100
17	H	4.102923	2.815388	2.714821	3.976941	4.652291
18	C	4.488295	4.708590	5.482250	5.737689	5.181704
19	C	5.572036	5.996900	6.816784	6.934602	6.216367
20	O	4.279188	4.888125	5.784180	5.816556	4.956027

21	H	4.382033	4.551730	5.066137	5.225634	4.825649
22	H	4.418038	4.394050	5.291135	5.787711	5.325384
23	H	6.178703	6.552152	7.501085	7.727167	6.977696
24	C	6.488770	7.012372	7.647027	7.571510	6.871750
25	H	6.995545	7.668064	8.361496	8.192412	7.361527
26	H	7.336827	7.724113	8.313253	8.323343	7.735205
27	H	6.124906	6.681781	7.148671	6.943676	6.305306
28	C	3.450982	4.459855	4.348467	3.269483	2.492041
29	H	4.330203	5.445258	5.381317	4.250665	3.405248
30	H	3.969339	4.729721	4.309198	3.167074	2.839821
31	C	3.383965	4.330634	4.519762	3.802738	2.967827
32	O	4.091806	4.762543	4.831534	4.259177	3.729833
33	O	3.167344	4.288068	4.855996	4.318155	3.203895
34	H	3.529626	4.471299	5.177345	4.862239	3.846874

		6	7	8	9	10
6	C	0.000000				
7	H	2.821459	0.000000			
8	H	4.668242	2.766279	0.000000		
9	H	1.091776	3.716057	5.326691	0.000000	
10	H	1.088667	2.491936	4.838480	1.767732	0.000000
11	Br	6.510359	4.386064	2.438652	7.339828	6.661019
12	H	2.856472	4.228334	4.240267	2.734200	3.823667
13	C	4.932671	4.632450	2.830700	5.155459	5.610727
14	C	5.976942	5.206782	2.853859	6.334567	6.584451
15	H	5.166263	5.343351	3.814993	5.164868	5.932286
16	H	6.938429	6.281886	3.870383	7.214221	7.592527
17	H	6.084074	4.866396	2.331313	6.609003	6.575176
18	C	5.701895	4.227786	4.627581	6.761240	5.739696
19	C	6.471141	5.111848	5.952753	7.549422	6.364061
20	O	5.179702	3.724581	4.973779	6.269836	4.983042
21	H	5.339209	4.346226	4.621928	6.344893	5.573010
22	H	6.071019	4.188408	4.074129	7.111006	6.084927
23	H	7.284275	5.618462	6.366513	8.374047	7.072537
24	C	6.893926	6.091834	7.115923	7.921754	6.867239
25	H	7.208298	6.472450	7.816271	8.223657	7.054343
26	H	7.842567	7.005253	7.741979	8.859257	7.881064
27	H	6.247832	5.853643	6.924182	7.225078	6.347885
28	C	1.529849	3.651424	5.421070	2.160731	2.174606
29	H	2.128841	4.361586	6.404956	2.489264	2.439579
30	H	2.179586	4.397899	5.706888	2.468980	3.081930
31	C	2.554290	3.372861	5.088702	3.485881	2.869072
32	O	3.569054	4.201398	5.406967	4.420662	4.030193
33	O	2.832967	2.734589	4.919258	3.878506	2.636332
34	H	3.739757	3.020807	4.906876	4.811049	3.551387

		11	12	13	14	15
11	Br	0.000000				
12	H	6.131712	0.000000			
13	C	4.376036	2.808049	0.000000		
14	C	3.676299	4.045536	1.325347	0.000000	
15	H	5.454969	2.633979	1.082310	2.138241	0.000000
16	H	4.423185	4.759135	2.073790	1.081678	2.464772
17	H	2.608766	4.598342	2.129651	1.091136	3.116374
18	C	3.799975	6.513363	6.315326	6.188057	7.259696
19	C	5.102416	7.682001	7.732281	7.649282	8.652519
20	O	4.678304	6.623675	6.863990	6.961499	7.752248
21	H	4.003090	5.877292	5.827224	5.761221	6.702286
22	H	2.866200	6.647921	6.011952	5.718322	7.028126
23	H	5.283235	8.541959	8.394469	8.216676	9.363860
24	C	6.379172	8.169270	8.556843	8.556629	9.391263
25	H	7.214830	8.793925	9.370806	9.448866	10.186703
26	H	6.713835	8.892087	9.096109	8.970404	9.946246
27	H	6.441289	7.436731	8.054613	8.159847	8.810367
28	C	6.839644	3.415843	5.567987	6.496002	5.836370
29	H	7.824065	4.311805	6.615936	7.577309	6.828134
30	H	7.084404	3.005865	5.328610	6.282623	5.469025
31	C	6.015807	4.209927	5.728574	6.392308	6.237146
32	O	5.940115	4.568876	5.837598	6.342772	6.375478
33	O	5.795739	4.952469	6.181951	6.771282	6.804700
34	H	5.354844	5.568749	6.423000	6.825932	7.159233

		16	17	18	19	20
16	H	0.000000				
17	H	1.862986	0.000000			
18	C	7.094818	5.406574	0.000000		
19	C	8.559070	6.865011	1.464647	0.000000	
20	O	7.956164	6.256358	1.464470	1.452621	0.000000
21	H	6.632620	5.101418	1.087241	2.194489	2.140414
22	H	6.598944	4.820397	1.087244	2.240630	2.159239
23	H	9.113072	7.346793	2.181590	1.087555	2.107765
24	C	9.433947	7.869071	2.605004	1.503431	2.515761
25	H	10.364760	8.771382	3.447154	2.151367	2.931418
26	H	9.774034	8.246494	3.140409	2.139142	3.420576
27	H	9.028131	7.585418	2.737805	2.149014	2.700672
28	C	7.429843	6.542010	5.272857	5.885791	4.784335
29	H	8.507911	7.626413	5.969441	6.367236	5.287828
30	H	7.121915	6.455408	5.685639	6.399836	5.438071
31	C	7.368584	6.200732	3.857649	4.385815	3.374107
32	O	7.245859	6.114796	3.505554	4.050218	3.395527
33	O	7.813724	6.432578	3.530918	3.874790	2.618674

34	H	7.861176	6.342302	2.649527	2.878505	1.632125
		21	22	23	24	25
21	H	0.000000				
22	H	1.843407	0.000000			
23	H	3.107116	2.531892	0.000000		
24	C	2.802355	3.562697	2.209233	0.000000	
25	H	3.756514	4.369660	2.559886	1.093851	0.000000
26	H	3.278454	3.961354	2.567557	1.094307	1.768907
27	H	2.524953	3.804501	3.098966	1.092204	1.778105
28	C	4.746868	5.880713	6.822520	6.001045	6.305603
29	H	5.508094	6.661467	7.282813	6.325431	6.458753
30	H	4.981332	6.291127	7.398151	6.415285	6.826549
31	C	3.366764	4.584124	5.351062	4.498061	4.860672
32	O	2.760187	4.337738	5.108192	3.946216	4.484283
33	O	3.432875	4.186641	4.679245	4.239650	4.437269
34	H	2.723967	3.376976	3.677192	3.359300	3.613440
		26	27	28	29	30
26	H	0.000000				
27	H	1.774669	0.000000			
28	C	6.913030	5.206899	0.000000		
29	H	7.275374	5.530653	1.095374	0.000000	
30	H	7.223461	5.515505	1.092346	1.764605	0.000000
31	C	5.415682	3.743363	1.520417	2.143470	2.126797
32	O	4.712483	3.039059	2.400218	3.019371	2.517738
33	O	5.271350	3.769208	2.372349	2.748956	3.273223
34	H	4.390733	3.043226	3.251133	3.674450	4.024624
		31	32	33	34	
31	C	0.000000				
32	O	1.205640	0.000000			
33	O	1.338542	2.257693	0.000000		
34	H	1.926087	2.373750	1.004502	0.000000	

Stoichiometry C11H17BrN2O3
Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.721935	1.278839	1.296151
2	6	0	-1.834024	0.666856	0.809709

3	7	0	-2.338254	1.490717	-0.183534
4	6	0	-1.561540	2.577631	-0.284185
5	7	0	-0.561573	2.466517	0.598736
6	6	0	0.544544	3.419099	0.782548
7	1	0	-0.014836	0.955904	2.039683
8	1	0	-2.235224	-0.324990	0.999736
9	1	0	0.143872	4.433825	0.740468
10	1	0	0.933930	3.245967	1.784346
11	35	0	-1.839486	-2.617084	0.267122
12	1	0	-1.699538	3.383905	-0.984453
13	6	0	-3.499120	1.228359	-1.000897
14	6	0	-3.891929	-0.001263	-1.301359
15	1	0	-3.992776	2.134437	-1.327579
16	1	0	-4.772901	-0.128368	-1.915979
17	1	0	-3.377512	-0.897215	-0.950330
18	6	0	1.870653	-2.020298	-0.297265
19	6	0	3.251632	-2.406415	0.001062
20	8	0	2.630813	-1.321692	0.741376
21	1	0	1.692689	-1.411611	-1.180396
22	1	0	1.019558	-2.590793	0.066429
23	1	0	3.388976	-3.285056	0.627083
24	6	0	4.407752	-2.040912	-0.887814
25	1	0	5.314771	-1.875654	-0.299158
26	1	0	4.607568	-2.854772	-1.591529
27	1	0	4.187143	-1.135807	-1.457923
28	6	0	1.638587	3.247394	-0.272927
29	1	0	2.463930	3.911908	0.004692
30	1	0	1.288754	3.552651	-1.261691
31	6	0	2.164694	1.825168	-0.383170
32	8	0	2.321960	1.263483	-1.438322
33	8	0	2.409036	1.286461	0.817574
34	1	0	2.622016	0.310193	0.714791

Rotational constants (GHZ): 0.3177172 0.2685145 0.1613493

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 538 symmetry adapted cartesian basis functions of A symmetry.

There are 519 symmetry adapted basis functions of A symmetry.

519 basis functions, 823 primitive gaussians, 538 cartesian basis functions

78 alpha electrons 78 beta electrons

nuclear repulsion energy 1575.5752878021 Hartrees.

NAtoms= 34 NActive= 34 NUniq= 34 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 519 RedAO= T EigKep= 4.90D-06 NBF= 519
NBsUse= 519 1.00D-06 EigRej= -1.00D+00 NBFU= 519
Initial guess from the checkpoint file: "./coohpo.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.997650 -0.002425 -0.003632 0.068375 Ang= -7.86 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3338.90250512 A.U. after 13 cycles
NFock= 13 Conv=0.55D-08 -V/T= 2.0019
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000042261	-0.000107539	-0.001507890
2	6	0.000322340	-0.001262069	-0.000419289
3	7	-0.005009460	-0.004352870	0.001543812
4	6	0.001662707	-0.000110456	-0.001857447
5	7	-0.003212179	0.001904194	0.002814248
6	6	0.000038703	0.000275313	-0.000324022
7	1	-0.000262629	0.000115133	-0.000287764
8	1	0.001307398	-0.000564130	0.001082333
9	1	-0.000777230	-0.000555409	0.001209835
10	1	0.000419070	0.000249538	-0.000692852
11	35	-0.000279813	-0.000477225	0.000308322
12	1	-0.000097768	0.000234905	0.000447322

13	6	0.003732169	0.004039803	-0.000061063
14	6	-0.001170277	0.000408138	0.000868676
15	1	0.000050528	-0.000513445	-0.001168610
16	1	-0.001061933	-0.000302820	-0.000250902
17	1	0.001455834	0.000052721	0.000057121
18	6	-0.000615043	-0.000868253	-0.000685419
19	6	0.000280303	0.001006954	0.000181525
20	8	-0.001121263	-0.001522861	0.000624179
21	1	-0.000173482	0.000142423	0.001021226
22	1	0.000099720	0.001237527	-0.000652216
23	1	0.000489862	0.000256403	0.000026328
24	6	-0.000044710	0.000029586	-0.000477553
25	1	0.000031324	0.000001056	0.000025059
26	1	0.000063669	-0.000057508	0.000141433
27	1	0.000088186	-0.000155533	0.000110848
28	6	-0.000140360	0.002311323	-0.001523285
29	1	0.000943397	-0.000665173	-0.000482239
30	1	0.000726219	-0.000042031	0.000886709
31	6	0.001174780	0.002530907	0.005111017
32	8	0.001243281	-0.002218744	-0.002139472
33	8	-0.001911420	-0.001609549	-0.004910572
34	1	0.001790338	0.000589691	0.000980602

Cartesian Forces: Max 0.005111017 RMS 0.001482972

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.004459664 RMS 0.000966866
Search for a local minimum.
Step number 19 out of a maximum of 175
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 18 19
DE= -4.22D-04 DEPred=-5.21D-04 R= 8.10D-01
TightC=F SS= 1.41D+00 RLast= 5.82D-01 DXNew= 1.5637D+00 1.7464D+00
Trust test= 8.10D-01 RLast= 5.82D-01 DXMaxT set to 1.56D+00
ITU= 1 1 1 1 1 1 0 0 -1 1 1 1 0 1 0 -1 0 1 0
Eigenvalues --- 0.00141 0.00364 0.00526 0.00580 0.00685
Eigenvalues --- 0.00700 0.01032 0.01376 0.01578 0.01773
Eigenvalues --- 0.01917 0.02097 0.02251 0.02344 0.02411

Eigenvalues --- 0.02472 0.02707 0.02815 0.03085 0.03120
Eigenvalues --- 0.03481 0.03495 0.03847 0.04193 0.04621
Eigenvalues --- 0.04838 0.05020 0.05291 0.05644 0.05779
Eigenvalues --- 0.05902 0.06296 0.07527 0.09366 0.09570
Eigenvalues --- 0.11237 0.12023 0.12591 0.12791 0.13531
Eigenvalues --- 0.15119 0.15387 0.15826 0.15977 0.15996
Eigenvalues --- 0.15999 0.16003 0.16006 0.16016 0.16234
Eigenvalues --- 0.17050 0.17190 0.20476 0.21537 0.22640
Eigenvalues --- 0.23000 0.23624 0.23982 0.24980 0.25815
Eigenvalues --- 0.28657 0.29368 0.30354 0.31424 0.31863
Eigenvalues --- 0.32893 0.34497 0.34566 0.34626 0.34765
Eigenvalues --- 0.34877 0.34943 0.34969 0.35110 0.35156
Eigenvalues --- 0.35464 0.35746 0.35814 0.36556 0.36831
Eigenvalues --- 0.36950 0.37230 0.37647 0.38176 0.41071
Eigenvalues --- 0.43954 0.46377 0.47377 0.49096 0.51764
Eigenvalues --- 0.54057 0.56177 0.57171 0.60563 0.91346
Eigenvalues --- 1.33647

En-DIIS/RFO-DIIS IScMMF= 0 using points: 19 18 17

RFO step: Lambda=-2.49369388D-04.

DidBck=F Rises=F RFO-DIIS coefs: 0.81758 0.23297 -0.05055

Iteration 1 RMS(Cart)= 0.03393892 RMS(Int)= 0.00063550

Iteration 2 RMS(Cart)= 0.00101837 RMS(Int)= 0.00010887

Iteration 3 RMS(Cart)= 0.00000068 RMS(Int)= 0.00010887

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56884	0.00159	0.00028	0.00108	0.00136	2.57020
R2	2.62031	-0.00011	-0.00033	-0.00017	-0.00050	2.61981
R3	2.03276	-0.00032	-0.00019	-0.00003	-0.00022	2.03254
R4	2.61816	0.00095	-0.00055	0.00380	0.00325	2.62141
R5	2.05349	0.00174	-0.00127	0.00481	0.00355	2.05703
R6	2.53167	0.00169	0.00054	0.00069	0.00122	2.53289
R7	2.72836	-0.00446	-0.00145	-0.00541	-0.00686	2.72151
R8	2.52957	0.00000	-0.00007	-0.00017	-0.00024	2.52933
R9	2.03485	-0.00030	-0.00014	-0.00008	-0.00022	2.03463
R10	2.78034	0.00236	0.00101	0.00065	0.00167	2.78200
R11	2.06316	-0.00021	0.00013	-0.00078	-0.00065	2.06251
R12	2.05728	-0.00028	-0.00058	0.00118	0.00059	2.05788
R13	2.89100	0.00310	0.00015	0.00469	0.00484	2.89584
R14	4.60839	0.00028	0.03494	-0.05005	-0.01511	4.59328
R15	2.50454	-0.00007	0.00030	-0.00044	-0.00015	2.50440
R16	2.04527	0.00043	-0.00002	0.00063	0.00061	2.04588
R17	2.04407	0.00100	0.00011	0.00126	0.00137	2.04544
R18	2.06195	0.00114	0.00075	-0.00114	-0.00039	2.06156
R19	2.76778	0.00089	0.00071	0.00106	0.00218	2.76996

R20	2.76745	-0.00080	-0.00166	0.00167	-0.00016	2.76729
R21	2.05459	-0.00088	-0.00011	-0.00134	-0.00145	2.05314
R22	2.05459	-0.00116	0.00012	-0.00247	-0.00235	2.05224
R23	2.74506	-0.00038	-0.00092	0.00061	-0.00056	2.74449
R24	2.05518	0.00017	0.00012	0.00003	0.00015	2.05533
R25	2.84107	0.00019	0.00001	0.00058	0.00059	2.84166
R26	3.08427	-0.00028	0.00375	-0.00187	0.00189	3.08616
R27	2.06708	0.00003	0.00003	0.00006	0.00009	2.06717
R28	2.06794	0.00004	0.00004	-0.00003	0.00001	2.06795
R29	2.06397	-0.00019	-0.00003	-0.00034	-0.00037	2.06360
R30	2.06996	-0.00009	0.00012	-0.00093	-0.00080	2.06915
R31	2.06423	-0.00103	-0.00040	-0.00106	-0.00146	2.06277
R32	2.87317	0.00123	0.00126	0.00100	0.00226	2.87543
R33	2.27833	0.00330	-0.00002	0.00200	0.00198	2.28031
R34	2.52948	-0.00384	-0.00065	-0.00284	-0.00349	2.52598
R35	1.89823	0.00046	-0.00148	0.00273	0.00125	1.89949
A1	1.87574	0.00132	0.00008	0.00270	0.00275	1.87849
A2	2.27833	-0.00042	-0.00048	0.00136	0.00084	2.27917
A3	2.12795	-0.00088	0.00028	-0.00322	-0.00297	2.12498
A4	1.86144	-0.00102	0.00029	-0.00260	-0.00231	1.85913
A5	2.27888	0.00015	0.00009	-0.00144	-0.00134	2.27754
A6	2.13383	0.00091	0.00030	0.00442	0.00474	2.13857
A7	1.90213	-0.00031	-0.00046	-0.00003	-0.00051	1.90161
A8	2.20238	0.00173	0.00031	0.00599	0.00631	2.20869
A9	2.17858	-0.00142	0.00013	-0.00603	-0.00590	2.17269
A10	1.89252	0.00082	0.00038	0.00133	0.00169	1.89421
A11	2.19204	-0.00028	-0.00039	0.00059	0.00020	2.19223
A12	2.19794	-0.00052	0.00012	-0.00169	-0.00158	2.19637
A13	1.89279	-0.00080	-0.00025	-0.00122	-0.00151	1.89127
A14	2.18789	0.00158	0.00097	0.00163	0.00255	2.19045
A15	2.20220	-0.00080	-0.00069	-0.00079	-0.00152	2.20067
A16	1.89762	-0.00216	-0.00276	-0.00314	-0.00591	1.89171
A17	1.85553	0.00031	0.00072	0.00205	0.00277	1.85829
A18	1.95927	0.00225	0.00214	0.00311	0.00524	1.96451
A19	1.89077	0.00012	0.00034	-0.00286	-0.00251	1.88825
A20	1.91790	0.00082	0.00016	0.00388	0.00404	1.92194
A21	1.94039	-0.00146	-0.00069	-0.00336	-0.00404	1.93635
A22	2.41200	0.00235	-0.02842	0.04031	0.01189	2.42389
A23	2.13558	0.00002	-0.00069	0.00537	0.00467	2.14025
A24	1.96653	0.00051	0.00054	-0.00027	0.00027	1.96680
A25	2.18107	-0.00052	0.00015	-0.00510	-0.00495	2.17612
A26	2.07057	-0.00023	0.00014	-0.00053	-0.00042	2.07015
A27	2.15214	-0.00046	-0.00242	0.00470	0.00225	2.15440
A28	2.06041	0.00070	0.00230	-0.00404	-0.00177	2.05864

A29	2.05711	0.00019	0.00038	0.00098	0.00125	2.05836
A30	2.13131	0.00039	-0.00023	0.00478	0.00467	2.13598
A31	1.97575	0.00039	0.00045	-0.00059	-0.00003	1.97572
A32	2.00357	-0.00061	-0.00138	-0.00127	-0.00267	2.00090
A33	2.02344	-0.00028	0.00034	-0.00350	-0.00319	2.02025
A34	2.03678	0.00033	0.00010	0.00313	0.00340	2.04018
A35	2.14188	0.00003	0.00014	-0.00203	-0.00202	2.13986
A36	1.94325	-0.00026	0.00022	-0.00081	-0.00063	1.94262
A37	2.03580	0.00075	0.00035	0.00149	0.00197	2.03777
A38	2.02598	-0.00035	-0.00022	-0.00123	-0.00147	2.02450
A39	2.05174	-0.00048	0.00586	0.00539	0.01220	2.06394
A40	2.40480	-0.00058	0.02167	-0.04532	-0.02344	2.38136
A41	1.93499	0.00000	0.00015	0.00003	0.00018	1.93517
A42	1.91751	-0.00018	-0.00012	-0.00081	-0.00094	1.91657
A43	1.93345	0.00005	-0.00001	0.00053	0.00052	1.93397
A44	1.88286	0.00002	-0.00005	-0.00029	-0.00033	1.88252
A45	1.89990	0.00004	-0.00019	0.00082	0.00063	1.90052
A46	1.89392	0.00006	0.00023	-0.00029	-0.00007	1.89386
A47	1.87118	0.00109	0.00162	-0.00162	-0.00002	1.87116
A48	1.94347	-0.00009	-0.00012	0.00105	0.00092	1.94439
A49	1.98501	0.00027	0.00461	-0.00963	-0.00501	1.98000
A50	1.87674	-0.00007	-0.00165	0.00566	0.00403	1.88076
A51	1.90194	-0.00115	-0.00352	0.00430	0.00081	1.90275
A52	1.88240	-0.00010	-0.00140	0.00117	-0.00021	1.88219
A53	2.14646	0.00077	-0.00056	0.00215	0.00159	2.14805
A54	1.95475	-0.00182	-0.00012	-0.00153	-0.00164	1.95311
A55	2.18190	0.00105	0.00069	-0.00076	-0.00006	2.18185
A56	1.91565	0.00379	0.00245	0.00609	0.00853	1.92419
A57	2.90112	-0.00192	-0.00448	-0.00067	-0.00515	2.89597
D1	0.00194	0.00008	0.00040	0.00604	0.00643	0.00838
D2	2.99875	0.00048	0.00639	0.00944	0.01581	3.01456
D3	-3.08732	-0.00024	0.00276	-0.01272	-0.00996	-3.09729
D4	-0.09052	0.00016	0.00875	-0.00931	-0.00059	-0.09111
D5	0.00869	-0.00047	-0.00184	-0.01091	-0.01275	-0.00406
D6	-3.10762	-0.00002	-0.00265	0.00521	0.00258	-3.10503
D7	3.10343	-0.00017	-0.00399	0.00602	0.00201	3.10545
D8	-0.01287	0.00027	-0.00480	0.02215	0.01734	0.00447
D9	-0.01194	0.00034	0.00118	0.00090	0.00208	-0.00986
D10	3.11511	0.00004	-0.00011	-0.00408	-0.00421	3.11090
D11	-3.02357	0.00004	-0.00417	-0.00163	-0.00582	-3.02938
D12	0.10348	-0.00026	-0.00547	-0.00661	-0.01211	0.09137
D13	-1.39824	-0.00054	-0.01019	-0.00447	-0.01467	-1.41291
D14	1.57915	-0.00024	-0.00341	-0.00119	-0.00459	1.57456
D15	0.01754	-0.00062	-0.00235	-0.00773	-0.01008	0.00746

D16	3.12115	0.00002	0.00138	-0.00141	-0.00001	3.12114
D17	-3.10975	-0.00036	-0.00108	-0.00296	-0.00407	-3.11382
D18	-0.00615	0.00029	0.00266	0.00336	0.00600	-0.00015
D19	-0.50298	0.00093	0.00625	0.07636	0.08260	-0.42037
D20	2.63895	0.00080	0.00644	0.08106	0.08750	2.72645
D21	2.62187	0.00059	0.00475	0.07070	0.07545	2.69731
D22	-0.51939	0.00046	0.00494	0.07540	0.08034	-0.43905
D23	-0.01621	0.00068	0.00258	0.01149	0.01407	-0.00214
D24	3.09984	0.00027	0.00343	-0.00476	-0.00130	3.09853
D25	-3.11965	0.00002	-0.00116	0.00509	0.00391	-3.11574
D26	-0.00360	-0.00039	-0.00031	-0.01116	-0.01145	-0.01506
D27	-2.43458	0.00034	0.01045	-0.02038	-0.00994	-2.44452
D28	-0.40232	-0.00042	0.00986	-0.02420	-0.01435	-0.41667
D29	1.72293	-0.00067	0.01078	-0.02513	-0.01435	1.70858
D30	0.73673	0.00086	0.00948	-0.00143	0.00805	0.74478
D31	2.76899	0.00009	0.00889	-0.00525	0.00364	2.77263
D32	-1.38894	-0.00016	0.00981	-0.00618	0.00364	-1.38531
D33	-3.03293	-0.00040	-0.00840	0.00766	-0.00072	-3.03365
D34	1.20186	-0.00091	-0.00730	0.00122	-0.00608	1.19579
D35	-0.92927	-0.00092	-0.00879	0.00598	-0.00281	-0.93208
D36	1.13620	0.00027	-0.00643	0.00687	0.00045	1.13665
D37	-0.91220	-0.00025	-0.00533	0.00044	-0.00491	-0.91710
D38	-3.04333	-0.00025	-0.00683	0.00520	-0.00164	-3.04497
D39	-0.95686	0.00051	-0.00652	0.01005	0.00354	-0.95332
D40	-3.00526	-0.00001	-0.00542	0.00361	-0.00182	-3.00707
D41	1.14679	-0.00001	-0.00692	0.00837	0.00145	1.14824
D42	3.13800	-0.00033	-0.00027	0.00304	0.00277	3.14077
D43	0.00901	-0.00068	-0.00024	-0.01015	-0.01040	-0.00140
D44	-0.00397	-0.00018	-0.00048	-0.00225	-0.00272	-0.00669
D45	-3.13296	-0.00054	-0.00046	-0.01544	-0.01589	3.13433
D46	-2.75175	-0.00034	0.00024	-0.00372	-0.00353	-2.75528
D47	-0.04238	-0.00039	0.00025	-0.00427	-0.00405	-0.04644
D48	-0.02324	0.00039	0.00169	0.00165	0.00334	-0.01989
D49	2.68613	0.00034	0.00170	0.00110	0.00282	2.68895
D50	0.38194	-0.00041	0.02376	-0.05589	-0.03216	0.34978
D51	-1.99580	0.00027	0.02425	-0.04838	-0.02426	-2.02006
D52	2.63858	-0.00055	-0.00265	-0.03034	-0.03280	2.60578
D53	0.25811	-0.00053	-0.00294	-0.02912	-0.03193	0.22619
D54	2.56509	-0.00007	-0.00032	-0.00360	-0.00398	2.56111
D55	-1.63854	-0.00016	-0.00036	-0.00446	-0.00488	-1.64342
D56	0.45378	-0.00016	-0.00017	-0.00501	-0.00524	0.44854
D57	1.33831	0.00009	0.00026	-0.00416	-0.00384	1.33447
D58	-2.86532	0.00000	0.00022	-0.00502	-0.00474	-2.87006
D59	-0.77300	0.00000	0.00042	-0.00557	-0.00510	-0.77810

D60	-1.00627	0.00003	-0.00024	-0.00315	-0.00338	-1.00965
D61	1.07329	-0.00005	-0.00028	-0.00400	-0.00428	1.06900
D62	-3.11758	-0.00005	-0.00009	-0.00456	-0.00464	-3.12222
D63	1.46088	-0.00049	-0.02028	0.02089	0.00113	1.46201
D64	2.77156	-0.00017	-0.00614	0.01506	0.00839	2.77995
D65	2.33306	-0.00023	0.02493	-0.04788	-0.02297	2.31009
D66	-0.79574	-0.00048	0.02044	-0.03630	-0.01587	-0.81161
D67	-1.86386	0.00051	0.02744	-0.05312	-0.02565	-1.88951
D68	1.29053	0.00027	0.02296	-0.04154	-0.01856	1.27198
D69	0.16851	-0.00023	0.02296	-0.04351	-0.02057	0.14793
D70	-2.96029	-0.00048	0.01847	-0.03193	-0.01348	-2.97376
D71	2.99528	-0.00036	0.00025	-0.01411	-0.01386	2.98142
D72	-0.13321	-0.00061	-0.00434	-0.00227	-0.00661	-0.13982
D73	-1.98234	-0.00069	0.00723	0.01910	0.02633	-1.95600

Item	Value	Threshold	Converged?
Maximum Force	0.004460	0.000450	NO
RMS Force	0.000967	0.000300	NO
Maximum Displacement	0.179852	0.001800	NO
RMS Displacement	0.034180	0.001200	NO

Predicted change in Energy=-3.162755D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.984646	1.651468	1.566227
2	6	0	-1.729341	0.515777	1.640308
3	7	0	-2.541380	0.502488	0.515715
4	6	0	-2.301222	1.604964	-0.207748
5	7	0	-1.354720	2.321571	0.410389
6	6	0	-0.762484	3.578555	-0.075960
7	1	0	-0.210206	2.023879	2.213074
8	1	0	-1.669778	-0.324862	2.329285
9	1	0	-1.563274	4.206272	-0.470844
10	1	0	-0.337750	4.076781	0.794242
11	35	0	-0.367076	-2.354279	2.633462
12	1	0	-2.771744	1.855736	-1.143142
13	6	0	-3.477976	-0.527259	0.146301
14	6	0	-3.364131	-1.779903	0.563751
15	1	0	-4.264409	-0.163225	-0.502614
16	1	0	-4.106069	-2.501388	0.246608
17	1	0	-2.558736	-2.126353	1.212938

18	6	0	2.763304	-0.720548	1.162463
19	6	0	4.172548	-0.341426	1.299851
20	8	0	3.132998	0.630549	1.589411
21	1	0	2.340011	-0.752595	0.162353
22	1	0	2.242663	-1.306427	1.914177
23	1	0	4.681053	-0.658410	2.207535
24	6	0	5.054312	-0.057022	0.115431
25	1	0	5.790386	0.716169	0.354148
26	1	0	5.598961	-0.963008	-0.167524
27	1	0	4.460665	0.272012	-0.740023
28	6	0	0.305283	3.348138	-1.150701
29	1	0	0.762136	4.319438	-1.366968
30	1	0	-0.135600	2.974015	-2.076543
31	6	0	1.392529	2.372618	-0.724594
32	8	0	1.768884	1.461145	-1.420061
33	8	0	1.847227	2.638215	0.504006
34	1	0	2.450655	1.898629	0.819038

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.360093	0.000000			
3	N	2.201625	1.387189	0.000000		
4	C	2.209644	2.220065	1.340347	0.000000	
5	N	1.386346	2.216739	2.174469	1.338463	0.000000
6	C	2.541614	3.641565	3.602324	2.506022	1.472171
7	H	1.075574	2.215898	3.260373	3.226177	2.155970
8	H	2.226554	1.088536	2.175600	3.249537	3.284057
9	H	3.318357	4.254914	3.955756	2.716724	2.090972
10	H	2.626134	3.915751	4.208223	3.311962	2.064543
11	Br	4.191228	3.328565	4.168162	5.242996	5.270775
12	H	3.252096	3.260321	2.153173	1.076680	2.153699
13	C	3.602740	2.525412	1.440159	2.460991	3.562834
14	C	4.294323	3.016896	2.426630	3.630745	4.569829
15	H	4.281362	3.388175	2.109264	2.658485	3.933710
16	H	5.360120	4.085892	3.397637	4.508441	5.554968
17	H	4.107858	2.802033	2.719784	4.000923	4.677367
18	C	4.453832	4.684089	5.482133	5.738895	5.174769
19	C	5.535271	5.973524	6.812040	6.926109	6.199467
20	O	4.242382	4.863960	5.776487	5.806033	4.938549
21	H	4.336326	4.511401	5.052532	5.218822	4.812801
22	H	4.391553	4.378612	5.302353	5.798764	5.325873
23	H	6.151988	6.541682	7.508228	7.727135	6.967107
24	C	6.441488	6.976481	7.626783	7.547882	6.842544

25	H	6.945860	7.631556	8.336072	8.159645	7.323457
26	H	7.292823	7.691493	8.299377	8.307165	7.712077
27	H	6.072322	6.636382	7.117488	6.912539	6.272387
28	C	3.453159	4.466732	4.356393	3.274398	2.499290
29	H	4.332777	5.451515	5.387656	4.253978	3.410507
30	H	3.967340	4.732645	4.314630	3.171217	2.845482
31	C	3.379184	4.334362	4.528951	3.807916	2.972907
32	O	4.066457	4.743117	4.821269	4.249253	3.721261
33	O	3.181429	4.311353	4.880711	4.334032	3.218928
34	H	3.524298	4.478742	5.192459	4.870407	3.850553

		6	7	8	9	10
6	C	0.000000				
7	H	2.821650	0.000000			
8	H	4.673869	2.767750	0.000000		
9	H	1.091434	3.714438	5.327592	0.000000	
10	H	1.088982	2.498752	4.848208	1.766103	0.000000
11	Br	6.534205	4.401091	2.430657	7.355844	6.688956
12	H	2.853789	4.225392	4.245832	2.727161	3.822412
13	C	4.927576	4.632297	2.841824	5.143274	5.610529
14	C	5.990899	5.209248	2.846944	6.336226	6.596428
15	H	5.142609	5.347425	3.844202	5.137085	5.922680
16	H	6.946172	6.286714	3.874316	7.209247	7.600818
17	H	6.118313	4.872401	2.298227	6.627835	6.602042
18	C	5.696241	4.180601	4.601116	6.757258	5.724202
19	C	6.450864	5.063317	5.932351	7.531041	6.333955
20	O	5.161296	3.675233	4.952463	6.251833	4.955290
21	H	5.333022	4.291605	4.577877	6.342470	5.558107
22	H	6.070799	4.146908	4.054995	7.110790	6.073856
23	H	7.266244	5.578451	6.360750	8.356462	7.043281
24	C	6.862154	6.037003	7.084228	7.893785	6.828136
25	H	7.163682	6.416605	7.787102	8.181549	7.002960
26	H	7.816787	6.952350	7.712060	8.838047	7.846592
27	H	6.217354	5.797142	6.881805	7.199910	6.313083
28	C	1.532411	3.651626	5.431583	2.165665	2.174216
29	H	2.130746	4.362539	6.414517	2.494670	2.437102
30	H	2.181922	4.394217	5.713809	2.476889	3.081942
31	C	2.553251	3.364562	5.097088	3.487614	2.864420
32	O	3.563405	4.175301	5.391829	4.420409	4.022760
33	O	2.833936	2.744332	4.947807	3.878228	2.632078
34	H	3.734626	3.006528	4.919627	4.806313	3.538385

		11	12	13	14	15
11	Br	0.000000				
12	H	6.145681	0.000000			
13	C	4.381972	2.800016	0.000000		

14	C	3.687269	4.059837	1.325271	0.000000	
15	H	5.461218	2.591240	1.082631	2.135716	0.000000
16	H	4.438331	4.764069	2.074065	1.082401	2.460368
17	H	2.621682	4.631794	2.130685	1.090932	3.115495
18	C	3.825205	6.526087	6.326415	6.247092	7.243745
19	C	5.141816	7.682378	7.739233	7.707956	8.629188
20	O	4.716965	6.620719	6.864989	7.005351	7.728408
21	H	4.000011	5.885384	5.822371	5.809795	6.663925
22	H	2.902775	6.670139	6.038063	5.786534	7.034898
23	H	5.342377	8.549395	8.416391	8.287627	9.360097
24	C	6.403852	8.154128	8.545292	8.604621	9.339798
25	H	7.248259	8.766445	9.353708	9.491021	10.129475
26	H	6.736079	8.886274	9.092808	9.029900	9.901415
27	H	6.448634	7.414744	8.027853	8.193754	8.739148
28	C	6.876737	3.419856	5.569018	6.534581	5.799290
29	H	7.862383	4.313727	6.615060	7.612866	6.790253
30	H	7.115367	3.011817	5.326485	6.324105	5.419095
31	C	6.059399	4.217052	5.734943	6.444306	6.203284
32	O	5.962452	4.566147	5.825529	6.386529	6.315134
33	O	5.861972	4.965911	6.205318	6.832393	6.798047
34	H	5.414699	5.579018	6.440976	6.885383	7.147733

		16	17	18	19	20
16	H	0.000000				
17	H	1.862440	0.000000			
18	C	7.155310	5.504812	0.000000		
19	C	8.620339	6.964460	1.465802	0.000000	
20	O	8.001015	6.335462	1.464384	1.452323	0.000000
21	H	6.679619	5.195061	1.086474	2.195713	2.139722
22	H	6.671965	4.921123	1.086000	2.243452	2.156397
23	H	9.189957	7.453766	2.184902	1.087633	2.107122
24	C	9.481809	7.965247	2.604853	1.503744	2.517304
25	H	10.406923	8.861450	3.446847	2.151804	2.931708
26	H	9.834924	8.355063	3.141433	2.138740	3.421581
27	H	9.058372	7.670606	2.735993	2.149512	2.705089
28	C	7.458515	6.615092	5.286474	5.879951	4.784295
29	H	8.533857	7.696255	5.983658	6.361328	5.288579
30	H	7.151342	6.534985	5.704788	6.399400	5.441947
31	C	7.411730	6.293431	3.873976	4.380972	3.379151
32	O	7.279734	6.207345	3.523931	4.052750	3.406996
33	O	7.869149	6.528109	3.543170	3.862479	2.619549
34	H	7.916972	6.438139	2.660033	2.865997	1.633124

		21	22	23	24	25
21	H	0.000000				
22	H	1.839863	0.000000			

23	H	3.110003	2.540026	0.000000		
24	C	2.802402	3.563969	2.208595	0.000000	
25	H	3.754882	4.371604	2.560299	1.093899	0.000000
26	H	3.282355	3.964360	2.564419	1.094311	1.768734
27	H	2.522156	3.802075	3.098766	1.092008	1.778382
28	C	4.762377	5.900161	6.817443	5.979254	6.267231
29	H	5.527570	6.678940	7.274198	6.306638	6.420988
30	H	5.002892	6.316975	7.399188	6.397431	6.791423
31	C	3.383985	4.606650	5.347794	4.474086	4.821685
32	O	2.780443	4.359022	5.112014	3.931489	4.458170
33	O	3.443422	4.207750	4.669081	4.207218	4.389216
34	H	2.733580	3.393372	3.666203	3.331465	3.573253

		26	27	28	29	30
26	H	0.000000				
27	H	1.774471	0.000000			
28	C	6.897510	5.186368	0.000000		
29	H	7.262078	5.518499	1.094948	0.000000	
30	H	7.213161	5.496613	1.091572	1.766236	0.000000
31	C	5.397296	3.718365	1.521614	2.144796	2.127116
32	O	4.702643	3.020293	2.403212	3.030875	2.519287
33	O	5.243593	3.738527	2.370577	2.739430	3.271635
34	H	4.367390	3.019386	3.253240	3.672879	4.028593

		31	32	33	34
31	C	0.000000			
32	O	1.206690	0.000000		
33	O	1.336693	2.256915	0.000000	
34	H	1.930569	2.381127	1.005166	0.000000

Stoichiometry C11H17BrN2O3
Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.650276	1.283218	1.282124
2	6	0	-1.789233	0.716372	0.801172
3	7	0	-2.273759	1.572957	-0.176474
4	6	0	-1.456611	2.631095	-0.272089
5	7	0	-0.457772	2.477875	0.605594
6	6	0	0.683815	3.389359	0.787984

7	1	0	0.049654	0.930795	2.018842
8	1	0	-2.226368	-0.262313	0.990905
9	1	0	0.312965	4.415475	0.759984
10	1	0	1.076353	3.196878	1.785354
11	35	0	-1.960316	-2.561585	0.248841
12	1	0	-1.571223	3.451482	-0.959888
13	6	0	-3.444633	1.370737	-0.990242
14	6	0	-3.942695	0.168146	-1.239345
15	1	0	-3.855312	2.298140	-1.368864
16	1	0	-4.826627	0.091466	-1.859326
17	1	0	-3.508088	-0.754520	-0.852128
18	6	0	1.799913	-2.094364	-0.275158
19	6	0	3.175807	-2.509985	0.012507
20	8	0	2.585720	-1.408609	0.752786
21	1	0	1.626157	-1.485642	-1.158160
22	1	0	0.937704	-2.637091	0.100925
23	1	0	3.303181	-3.386798	0.643316
24	6	0	4.329150	-2.176209	-0.892833
25	1	0	5.245769	-2.022504	-0.315946
26	1	0	4.505220	-3.001960	-1.589002
27	1	0	4.119842	-1.273858	-1.471134
28	6	0	1.769382	3.192022	-0.275447
29	1	0	2.616500	3.826703	0.004700
30	1	0	1.424937	3.512153	-1.260538
31	6	0	2.246439	1.751968	-0.393644
32	8	0	2.359578	1.180365	-1.450323
33	8	0	2.493899	1.208859	0.802411
34	1	0	2.661195	0.222169	0.708532

Rotational constants (GHZ): 0.3188553 0.2658546 0.1603439

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 538 symmetry adapted cartesian basis functions of A symmetry.

There are 519 symmetry adapted basis functions of A symmetry.

519 basis functions, 823 primitive gaussians, 538 cartesian basis functions

78 alpha electrons 78 beta electrons

nuclear repulsion energy 1573.5464936766 Hartrees.

NAtoms= 34 NActive= 34 NUniq= 34 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 519 RedAO= T EigKep= 4.67D-06 NBF= 519

NBsUse= 519 1.00D-06 EigRej= -1.00D+00 NBFU= 519

Initial guess from the checkpoint file: "./coohpo.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999819 -0.001234 -0.001132 0.018969 Ang= -2.18 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3338.90295670 A.U. after 11 cycles
NFock= 11 Conv=0.99D-08 -V/T= 2.0019
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000782458	0.000341892	-0.000389492
2	6	-0.000001373	-0.000641456	-0.000630709
3	7	-0.003384977	-0.003453212	0.001161381
4	6	0.000728828	0.000554450	-0.001120098
5	7	-0.001403585	0.000635874	0.001505550
6	6	0.000246974	0.000421085	-0.000360384
7	1	-0.000195671	-0.000113604	-0.000068529
8	1	0.001503047	-0.000191896	0.000014329
9	1	-0.000548782	-0.000268904	0.000623671
10	1	0.000205168	-0.000173354	-0.000593374
11	35	-0.000333374	-0.000273497	0.000346487
12	1	-0.000204238	0.000134152	0.000384613
13	6	0.002941513	0.003184383	0.000076371
14	6	-0.001359810	-0.000438224	0.000898094
15	1	0.000222910	-0.000334632	-0.000789424
16	1	-0.000638230	0.000085376	-0.000212483

17	1	0.001512276	0.000092617	-0.000101183
18	6	-0.000277692	0.000016066	-0.000480093
19	6	-0.000117316	0.000493615	0.000266940
20	8	-0.000800506	-0.000781689	0.000163903
21	1	-0.000106341	0.000055609	0.000466996
22	1	0.000134771	0.000462984	-0.000096712
23	1	0.000254404	0.000019472	-0.000033163
24	6	-0.000081219	0.000043599	-0.000296888
25	1	-0.000016237	0.000004560	0.000024384
26	1	0.000039247	-0.000043425	0.000132143
27	1	0.000045958	-0.000058700	0.000029232
28	6	-0.000462425	0.001433118	-0.000260875
29	1	0.000802732	-0.000456084	-0.000555619
30	1	0.000530090	-0.000017906	0.000477660
31	6	0.000891978	0.000813377	0.003828746
32	8	0.000776264	-0.000925052	-0.001547888
33	8	-0.001443152	-0.000987153	-0.003148805
34	1	0.001321226	0.000366557	0.000285217

Cartesian Forces: Max 0.003828746 RMS 0.001011039

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.003557052 RMS 0.000626760
Search for a local minimum.
Step number 20 out of a maximum of 175
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 19 20
DE= -4.52D-04 DEPred=-3.16D-04 R= 1.43D+00
TightC=F SS= 1.41D+00 RLast= 1.96D-01 DXNew= 2.6298D+00 5.8911D-01
Trust test= 1.43D+00 RLast= 1.96D-01 DXMaxT set to 1.56D+00
ITU= 1 1 1 1 1 1 1 0 0 -1 1 1 1 0 1 0 -1 0 1 0

Eigenvalues ---	0.00137	0.00366	0.00436	0.00573	0.00698
Eigenvalues ---	0.00709	0.00949	0.01223	0.01548	0.01770
Eigenvalues ---	0.01968	0.02046	0.02250	0.02335	0.02417
Eigenvalues ---	0.02443	0.02785	0.02929	0.03070	0.03120
Eigenvalues ---	0.03473	0.03553	0.04010	0.04191	0.04641
Eigenvalues ---	0.04872	0.05009	0.05322	0.05604	0.05779
Eigenvalues ---	0.05908	0.06345	0.07232	0.09226	0.09544

Eigenvalues --- 0.11076 0.12009 0.12553 0.12694 0.13379
Eigenvalues --- 0.15062 0.15409 0.15729 0.15979 0.15998
Eigenvalues --- 0.16000 0.16005 0.16016 0.16035 0.16281
Eigenvalues --- 0.17127 0.17191 0.20279 0.21014 0.22804
Eigenvalues --- 0.23045 0.23348 0.23885 0.24979 0.25798
Eigenvalues --- 0.28053 0.29116 0.30055 0.30927 0.31861
Eigenvalues --- 0.32666 0.34497 0.34558 0.34619 0.34765
Eigenvalues --- 0.34877 0.34942 0.34980 0.35050 0.35136
Eigenvalues --- 0.35288 0.35713 0.35800 0.36553 0.36776
Eigenvalues --- 0.36982 0.37105 0.37439 0.37758 0.40300
Eigenvalues --- 0.41767 0.44700 0.47247 0.49093 0.51531
Eigenvalues --- 0.52917 0.55630 0.56245 0.60662 0.89990
Eigenvalues --- 1.36354
En-DIIS/RFO-DIIS IScMMF= 0 using points: 20 19 18 17
RFO step: Lambda=-1.72428880D-04.
DidBck=F Rises=F RFO-DIIS coefs: 2.15516 -0.95454 -0.67743 0.47680
Iteration 1 RMS(Cart)= 0.09573401 RMS(Int)= 0.00255739
Iteration 2 RMS(Cart)= 0.00412329 RMS(Int)= 0.00005918
Iteration 3 RMS(Cart)= 0.00000794 RMS(Int)= 0.00005906
Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00005906

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.57020	0.00032	0.00144	-0.00065	0.00077	2.57097
R2	2.61981	-0.00018	-0.00109	0.00047	-0.00057	2.61924
R3	2.03254	-0.00022	-0.00020	-0.00045	-0.00065	2.03189
R4	2.62141	0.00006	0.00436	0.00059	0.00488	2.62629
R5	2.05703	0.00065	0.00466	0.00480	0.00946	2.06649
R6	2.53289	0.00137	0.00175	0.00136	0.00309	2.53597
R7	2.72151	-0.00356	-0.00835	-0.00652	-0.01487	2.70664
R8	2.52933	0.00002	-0.00019	0.00031	0.00017	2.52950
R9	2.03463	-0.00021	-0.00041	-0.00006	-0.00046	2.03417
R10	2.78200	0.00125	0.00154	0.00173	0.00327	2.78527
R11	2.06251	0.00002	-0.00074	0.00022	-0.00052	2.06199
R12	2.05788	-0.00047	0.00090	-0.00147	-0.00057	2.05730
R13	2.89584	0.00148	0.00542	0.00375	0.00917	2.90500
R14	4.59328	0.00009	-0.03792	-0.04185	-0.07977	4.51351
R15	2.50440	0.00038	-0.00009	0.00085	0.00076	2.50515
R16	2.04588	0.00020	0.00076	0.00042	0.00118	2.04705
R17	2.04544	0.00044	0.00180	0.00027	0.00207	2.04751
R18	2.06156	0.00102	-0.00038	0.00310	0.00272	2.06428
R19	2.76996	0.00030	0.00201	-0.00108	0.00100	2.77096
R20	2.76729	-0.00058	0.00100	0.00207	0.00305	2.77033
R21	2.05314	-0.00039	-0.00186	-0.00022	-0.00208	2.05106
R22	2.05224	-0.00038	-0.00319	0.00006	-0.00313	2.04911

R23	2.74449	-0.00036	-0.00039	0.00068	0.00025	2.74474
R24	2.05533	0.00009	0.00014	0.00002	0.00015	2.05548
R25	2.84166	0.00006	0.00082	-0.00009	0.00072	2.84239
R26	3.08616	-0.00045	-0.00404	-0.01393	-0.01797	3.06819
R27	2.06717	0.00000	0.00012	-0.00008	0.00004	2.06721
R28	2.06795	0.00002	0.00001	-0.00001	0.00000	2.06795
R29	2.06360	-0.00007	-0.00045	-0.00008	-0.00053	2.06306
R30	2.06915	0.00004	-0.00066	-0.00094	-0.00160	2.06755
R31	2.06277	-0.00062	-0.00114	-0.00155	-0.00268	2.06009
R32	2.87543	0.00068	0.00175	0.00272	0.00448	2.87991
R33	2.28031	0.00183	0.00229	0.00225	0.00455	2.28486
R34	2.52598	-0.00289	-0.00528	-0.00434	-0.00962	2.51636
R35	1.89949	-0.00002	0.00332	0.00096	0.00427	1.90376
A1	1.87849	0.00078	0.00378	0.00128	0.00506	1.88354
A2	2.27917	-0.00048	0.00102	-0.00217	-0.00125	2.27792
A3	2.12498	-0.00031	-0.00401	0.00059	-0.00353	2.12145
A4	1.85913	-0.00033	-0.00309	-0.00032	-0.00337	1.85577
A5	2.27754	-0.00023	-0.00211	-0.00471	-0.00673	2.27082
A6	2.13857	0.00059	0.00649	0.00441	0.01101	2.14958
A7	1.90161	-0.00022	-0.00065	-0.00036	-0.00106	1.90056
A8	2.20869	0.00074	0.00850	0.00241	0.01092	2.21961
A9	2.17269	-0.00053	-0.00803	-0.00204	-0.01005	2.16264
A10	1.89421	0.00019	0.00191	0.00038	0.00235	1.89657
A11	2.19223	-0.00011	0.00029	-0.00070	-0.00044	2.19179
A12	2.19637	-0.00007	-0.00191	0.00000	-0.00195	2.19442
A13	1.89127	-0.00042	-0.00185	-0.00096	-0.00296	1.88831
A14	2.19045	0.00036	0.00231	0.00102	0.00298	2.19343
A15	2.20067	0.00004	-0.00115	-0.00059	-0.00208	2.19860
A16	1.89171	-0.00067	-0.00462	-0.00354	-0.00819	1.88351
A17	1.85829	0.00025	0.00196	0.00052	0.00248	1.86078
A18	1.96451	0.00021	0.00346	0.00190	0.00535	1.96986
A19	1.88825	0.00000	-0.00330	0.00178	-0.00150	1.88675
A20	1.92194	0.00079	0.00705	0.00202	0.00909	1.93103
A21	1.93635	-0.00060	-0.00503	-0.00275	-0.00778	1.92857
A22	2.42389	0.00238	0.03089	0.07399	0.10488	2.52877
A23	2.14025	-0.00012	0.00695	0.00056	0.00751	2.14776
A24	1.96680	0.00030	-0.00051	0.00022	-0.00029	1.96651
A25	2.17612	-0.00019	-0.00647	-0.00075	-0.00722	2.16890
A26	2.07015	-0.00020	-0.00133	-0.00104	-0.00240	2.06774
A27	2.15440	-0.00059	0.00399	-0.00324	0.00073	2.15512
A28	2.05864	0.00078	-0.00271	0.00428	0.00154	2.06018
A29	2.05836	0.00017	0.00165	-0.00052	0.00116	2.05953
A30	2.13598	0.00000	0.00602	-0.00105	0.00494	2.14091
A31	1.97572	0.00018	-0.00091	0.00202	0.00108	1.97680

A32	2.00090	-0.00028	-0.00260	0.00351	0.00095	2.00185
A33	2.02025	-0.00006	-0.00417	-0.00110	-0.00529	2.01496
A34	2.04018	0.00016	0.00410	-0.00026	0.00376	2.04393
A35	2.13986	0.00002	-0.00249	-0.00102	-0.00342	2.13644
A36	1.94262	-0.00004	-0.00070	0.00147	0.00078	1.94340
A37	2.03777	0.00030	0.00202	0.00055	0.00258	2.04034
A38	2.02450	-0.00017	-0.00179	-0.00021	-0.00202	2.02249
A39	2.06394	-0.00021	0.00686	-0.00700	-0.00016	2.06377
A40	2.38136	-0.00023	-0.03420	-0.04661	-0.08074	2.30062
A41	1.93517	-0.00004	-0.00001	-0.00053	-0.00054	1.93463
A42	1.91657	-0.00016	-0.00102	-0.00189	-0.00291	1.91366
A43	1.93397	0.00007	0.00059	0.00112	0.00171	1.93568
A44	1.88252	0.00005	-0.00036	-0.00015	-0.00051	1.88202
A45	1.90052	0.00002	0.00078	0.00097	0.00174	1.90227
A46	1.89386	0.00006	0.00000	0.00049	0.00050	1.89435
A47	1.87116	0.00103	0.00024	0.00712	0.00734	1.87850
A48	1.94439	0.00019	0.00236	-0.00200	0.00031	1.94469
A49	1.98000	-0.00042	-0.00881	0.00124	-0.00759	1.97241
A50	1.88076	-0.00021	0.00481	0.00004	0.00486	1.88563
A51	1.90275	-0.00049	0.00258	-0.00411	-0.00148	1.90127
A52	1.88219	-0.00011	-0.00048	-0.00240	-0.00288	1.87931
A53	2.14805	0.00015	-0.00004	0.00043	0.00043	2.14848
A54	1.95311	-0.00110	-0.00194	-0.00072	-0.00263	1.95048
A55	2.18185	0.00095	0.00172	0.00037	0.00213	2.18397
A56	1.92419	0.00169	0.01015	0.00238	0.01253	1.93671
A57	2.89597	-0.00227	-0.00494	0.00529	0.00035	2.89633
D1	0.00838	-0.00027	0.00523	-0.01187	-0.00665	0.00173
D2	3.01456	-0.00001	0.01905	-0.01668	0.00231	3.01687
D3	-3.09729	-0.00003	-0.01526	-0.00212	-0.01738	-3.11467
D4	-0.09111	0.00024	-0.00144	-0.00694	-0.00842	-0.09953
D5	-0.00406	0.00022	-0.01300	0.01980	0.00683	0.00277
D6	-3.10503	0.00055	0.00960	0.03376	0.04342	-3.06161
D7	3.10545	0.00000	0.00545	0.01103	0.01644	3.12189
D8	0.00447	0.00032	0.02805	0.02499	0.05303	0.05751
D9	-0.00986	0.00024	0.00432	-0.00010	0.00421	-0.00565
D10	3.11090	-0.00001	-0.00449	0.00031	-0.00425	3.10664
D11	-3.02938	0.00007	-0.00742	0.00507	-0.00238	-3.03176
D12	0.09137	-0.00017	-0.01624	0.00549	-0.01084	0.08054
D13	-1.41291	-0.00037	-0.01072	-0.01900	-0.02972	-1.44263
D14	1.57456	-0.00014	0.00425	-0.02494	-0.02069	1.55387
D15	0.00746	-0.00010	-0.01251	0.01253	0.00003	0.00749
D16	3.12114	-0.00005	-0.00175	0.00048	-0.00121	3.11993
D17	-3.11382	0.00012	-0.00411	0.01206	0.00785	-3.10597
D18	-0.00015	0.00017	0.00665	0.00001	0.00661	0.00646

D19	-0.42037	0.00048	0.07036	0.04577	0.11611	-0.30426
D20	2.72645	0.00042	0.07753	0.03907	0.11660	2.84304
D21	2.69731	0.00020	0.06034	0.04628	0.10662	2.80393
D22	-0.43905	0.00015	0.06751	0.03958	0.10710	-0.33195
D23	-0.00214	-0.00008	0.01573	-0.01991	-0.00420	-0.00635
D24	3.09853	-0.00040	-0.00695	-0.03393	-0.04079	3.05775
D25	-3.11574	-0.00012	0.00487	-0.00781	-0.00299	-3.11872
D26	-0.01506	-0.00044	-0.01781	-0.02182	-0.03957	-0.05463
D27	-2.44452	0.00011	-0.01149	-0.00381	-0.01533	-2.45985
D28	-0.41667	-0.00009	-0.01658	-0.00322	-0.01983	-0.43650
D29	1.70858	-0.00055	-0.01945	-0.00513	-0.02458	1.68400
D30	0.74478	0.00050	0.01504	0.01258	0.02763	0.77241
D31	2.77263	0.00030	0.00995	0.01317	0.02313	2.79576
D32	-1.38531	-0.00016	0.00708	0.01126	0.01838	-1.36692
D33	-3.03365	0.00017	-0.00444	0.01299	0.00859	-3.02505
D34	1.19579	-0.00030	-0.01171	0.00974	-0.00196	1.19382
D35	-0.93208	0.00000	-0.00643	0.01349	0.00707	-0.92501
D36	1.13665	0.00034	-0.00585	0.01480	0.00895	1.14560
D37	-0.91710	-0.00013	-0.01312	0.01155	-0.00160	-0.91871
D38	-3.04497	0.00017	-0.00784	0.01530	0.00743	-3.03754
D39	-0.95332	0.00021	-0.00310	0.01303	0.00995	-0.94337
D40	-3.00707	-0.00026	-0.01038	0.00978	-0.00061	-3.00768
D41	1.14824	0.00004	-0.00510	0.01353	0.00843	1.15667
D42	3.14077	-0.00021	0.00440	-0.01369	-0.00930	3.13147
D43	-0.00140	-0.00081	-0.02294	-0.00385	-0.02679	-0.02819
D44	-0.00669	-0.00015	-0.00365	-0.00616	-0.00981	-0.01650
D45	3.13433	-0.00075	-0.03099	0.00368	-0.02731	3.10702
D46	-2.75528	-0.00013	-0.00509	0.00509	0.00000	-2.75528
D47	-0.04644	-0.00016	-0.00591	0.00116	-0.00475	-0.05119
D48	-0.01989	0.00019	0.00375	-0.00270	0.00106	-0.01883
D49	2.68895	0.00015	0.00293	-0.00664	-0.00369	2.68525
D50	0.34978	-0.00024	-0.04443	-0.05128	-0.09568	0.25410
D51	-2.02006	-0.00003	-0.03413	-0.05560	-0.08972	-2.10979
D52	2.60578	-0.00024	-0.02899	-0.00521	-0.03427	2.57151
D53	0.22619	-0.00025	-0.02761	-0.00714	-0.03483	0.19136
D54	2.56111	-0.00005	-0.00456	-0.00288	-0.00744	2.55367
D55	-1.64342	-0.00012	-0.00565	-0.00460	-0.01026	-1.65368
D56	0.44854	-0.00010	-0.00593	-0.00450	-0.01044	0.43810
D57	1.33447	0.00008	-0.00490	-0.00401	-0.00890	1.32557
D58	-2.87006	0.00001	-0.00600	-0.00573	-0.01172	-2.88178
D59	-0.77810	0.00003	-0.00628	-0.00563	-0.01190	-0.79000
D60	-1.00965	-0.00001	-0.00402	-0.00679	-0.01081	-1.02046
D61	1.06900	-0.00008	-0.00512	-0.00851	-0.01363	1.05537
D62	-3.12222	-0.00006	-0.00540	-0.00841	-0.01381	-3.13603

D63	1.46201	-0.00053	-0.00558	-0.00181	-0.00715	1.45485
D64	2.77995	-0.00031	-0.00800	-0.02318	-0.03141	2.74854
D65	2.31009	-0.00020	-0.02306	-0.01373	-0.03676	2.27333
D66	-0.81161	-0.00031	-0.01557	-0.01799	-0.03357	-0.84518
D67	-1.88951	0.00049	-0.02663	-0.00678	-0.03336	-1.92287
D68	1.27198	0.00038	-0.01913	-0.01104	-0.03017	1.24181
D69	0.14793	-0.00008	-0.01970	-0.01024	-0.02996	0.11797
D70	-2.97376	-0.00019	-0.01221	-0.01450	-0.02677	-3.00054
D71	2.98142	-0.00083	-0.01162	-0.00966	-0.02135	2.96007
D72	-0.13982	-0.00093	-0.00411	-0.01402	-0.01806	-0.15788
D73	-1.95600	-0.00071	0.01676	-0.00994	0.00682	-1.94918

Item	Value	Threshold	Converged?
Maximum Force	0.003557	0.000450	NO
RMS Force	0.000627	0.000300	NO
Maximum Displacement	0.442087	0.001800	NO
RMS Displacement	0.096501	0.001200	NO

Predicted change in Energy=-4.425378D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.949224	1.639532	1.561686
2	6	0	-1.662406	0.481990	1.610995
3	7	0	-2.477746	0.477182	0.485533
4	6	0	-2.262514	1.603371	-0.211808
5	7	0	-1.331018	2.327374	0.420537
6	6	0	-0.735332	3.585233	-0.064579
7	1	0	-0.193199	2.022907	2.223175
8	1	0	-1.576155	-0.370211	2.290808
9	1	0	-1.541258	4.211300	-0.450775
10	1	0	-0.307442	4.082443	0.804279
11	35	0	-0.398094	-2.398389	2.741743
12	1	0	-2.739179	1.865673	-1.140624
13	6	0	-3.383837	-0.554372	0.077664
14	6	0	-3.326106	-1.793747	0.544589
15	1	0	-4.107918	-0.210111	-0.650780
16	1	0	-4.055451	-2.513156	0.191778
17	1	0	-2.570675	-2.135101	1.255977
18	6	0	2.705096	-0.691580	1.284884
19	6	0	4.122177	-0.314831	1.292973
20	8	0	3.115005	0.664482	1.661995

21	1	0	2.194696	-0.734600	0.327973
22	1	0	2.247412	-1.265061	2.083284
23	1	0	4.711460	-0.620720	2.154540
24	6	0	4.894187	-0.053879	0.028733
25	1	0	5.644887	0.726303	0.185041
26	1	0	5.416770	-0.965130	-0.277936
27	1	0	4.226722	0.252074	-0.779195
28	6	0	0.339731	3.361145	-1.140311
29	1	0	0.805201	4.328781	-1.350243
30	1	0	-0.096187	2.988046	-2.067244
31	6	0	1.419421	2.376522	-0.707515
32	8	0	1.773057	1.442681	-1.389275
33	8	0	1.888508	2.660417	0.505960
34	1	0	2.472481	1.915144	0.850127

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.360501	0.000000			
3	N	2.201259	1.389773	0.000000		
4	C	2.207107	2.222665	1.341980	0.000000	
5	N	1.386043	2.220912	2.177709	1.338554	0.000000
6	C	2.544846	3.646524	3.605358	2.506339	1.473903
7	H	1.075229	2.215346	3.260033	3.222920	2.153330
8	H	2.227942	1.093540	2.188598	3.260246	3.291652
9	H	3.318810	4.263019	3.961984	2.716360	2.086280
10	H	2.636923	3.930646	4.220156	3.316705	2.067663
11	Br	4.242768	3.342702	4.205276	5.311649	5.347072
12	H	3.249240	3.262733	2.154214	1.076435	2.152513
13	C	3.597621	2.527543	1.432292	2.448880	3.554727
14	C	4.297844	3.013984	2.424938	3.639200	4.580328
15	H	4.277094	3.402228	2.102627	2.624296	3.911230
16	H	5.363777	4.087999	3.393754	4.508137	5.559280
17	H	4.119517	2.792876	2.725114	4.028093	4.706208
18	C	4.343358	4.534169	5.372785	5.673098	5.113843
19	C	5.441585	5.847859	6.696135	6.834336	6.122069
20	O	4.180758	4.781167	5.718217	5.771513	4.906480
21	H	4.128291	4.243050	4.829592	5.062035	4.670644
22	H	4.350541	4.308354	5.283496	5.816767	5.336241
23	H	6.124014	6.491346	7.461611	7.693016	6.943310
24	C	6.273997	6.766064	7.405139	7.350014	6.676605
25	H	6.797900	7.449132	8.132006	7.965785	7.161155
26	H	7.119997	7.468396	8.061422	8.097714	7.540629
27	H	5.847665	6.359850	6.826426	6.652677	6.052660

28	C	3.453426	4.457328	4.347273	3.274686	2.509250
29	H	4.334674	5.445716	5.383551	4.258494	3.421217
30	H	3.964252	4.718347	4.300340	3.170636	2.854881
31	C	3.361980	4.296789	4.496527	3.794750	2.973185
32	O	4.019669	4.661218	4.745146	4.206909	3.700457
33	O	3.195230	4.309947	4.881711	4.343216	3.237833
34	H	3.505759	4.441863	5.167728	4.862622	3.849816

		6	7	8	9	10
6	C	0.000000				
7	H	2.822869	0.000000			
8	H	4.679783	2.764807	0.000000		
9	H	1.091158	3.708954	5.339265	0.000000	
10	H	1.088679	2.503598	4.862667	1.764672	0.000000
11	Br	6.617621	4.456316	2.388446	7.428795	6.764848
12	H	2.851345	4.221597	4.257526	2.722660	3.822311
13	C	4.916415	4.628796	2.863500	5.136728	5.611793
14	C	6.001385	5.215324	2.852730	6.343267	6.611307
15	H	5.111027	5.345185	3.884378	5.116309	5.914966
16	H	6.948327	6.294396	3.891663	7.207798	7.610824
17	H	6.150982	4.886399	2.274815	6.652031	6.632052
18	C	5.652320	4.080312	4.409566	6.714333	5.665479
19	C	6.375644	4.995274	5.785303	7.456609	6.260700
20	O	5.131952	3.620008	4.844892	6.222901	4.912359
21	H	5.234512	4.110679	4.266710	6.247058	5.448987
22	H	6.085674	4.097180	3.932364	7.125027	6.062914
23	H	7.230634	5.572177	6.294078	8.320611	7.009444
24	C	6.703978	5.916935	6.861660	7.735415	6.690857
25	H	6.995926	6.318103	7.601319	8.011876	6.861294
26	H	7.655043	6.830496	7.473511	8.674068	7.708163
27	H	6.020183	5.629012	6.594357	7.003779	6.143106
28	C	1.537262	3.658953	5.419061	2.176315	2.172679
29	H	2.139868	4.368429	6.403799	2.515694	2.437338
30	H	2.185361	4.398704	5.697439	2.489488	3.080255
31	C	2.552901	3.363708	5.050540	3.492556	2.859674
32	O	3.554906	4.153627	5.295924	4.419357	4.013538
33	O	2.839953	2.772860	4.937032	3.883797	2.633125
34	H	3.730408	3.000454	4.867224	4.803622	3.525231

		11	12	13	14	15
11	Br	0.000000				
12	H	6.223799	0.000000			
13	C	4.405948	2.785036	0.000000		
14	C	3.710301	4.071336	1.325671	0.000000	
15	H	5.482751	2.534220	1.083254	2.132613	0.000000
16	H	4.460016	4.762563	2.073866	1.083497	2.452891

17	H	2.645170	4.666721	2.132689	1.092371	3.115193
18	C	3.829546	6.485581	6.208970	6.175614	7.098997
19	C	5.183918	7.599684	7.607536	7.630478	8.457163
20	O	4.784235	6.600682	6.799313	6.984225	7.634425
21	H	3.913699	5.767263	5.587054	5.625653	6.399687
22	H	2.952406	6.712761	6.019846	5.806134	6.998445
23	H	5.441733	8.517762	8.357729	8.280725	9.263900
24	C	6.392605	7.957409	8.293285	8.418223	9.029067
25	H	7.267603	8.564352	9.119732	9.325163	9.833243
26	H	6.707111	8.676242	8.817361	8.820490	9.561838
27	H	6.388340	7.159477	7.700985	7.936183	8.348433
28	C	6.984767	3.422883	5.538925	6.546004	5.724953
29	H	7.965368	4.321282	6.590307	7.625185	6.725290
30	H	7.227114	3.017242	5.287532	6.334003	5.322458
31	C	6.164456	4.212185	5.681367	6.440414	6.102897
32	O	6.044256	4.538835	5.721336	6.341590	6.153288
33	O	5.984881	4.975776	6.189986	6.858082	6.747970
34	H	5.515885	5.579152	6.402474	6.890055	7.076092

		16	17	18	19	20
16	H	0.000000				
17	H	1.865477	0.000000			
18	C	7.086467	5.469767	0.000000		
19	C	8.539254	6.936066	1.466330	0.000000	
20	O	7.979621	6.350549	1.465996	1.452456	0.000000
21	H	6.499704	5.052856	1.085374	2.196045	2.141031
22	H	6.697881	4.965417	1.084342	2.245501	2.157160
23	H	9.181093	7.492012	2.187880	1.087713	2.107845
24	C	9.282815	7.846132	2.603209	1.504127	2.519738
25	H	10.226959	8.765273	3.444186	2.151772	2.930106
26	H	9.609369	8.217116	3.141721	2.136964	3.423024
27	H	8.785424	7.486330	2.732444	2.150859	2.713928
28	C	7.456507	6.664937	5.282149	5.808663	4.777767
29	H	8.533221	7.744075	5.979759	6.289042	5.275970
30	H	7.144380	6.588894	5.711707	6.324133	5.442235
31	C	7.395397	6.334896	3.877611	4.306998	3.379447
32	O	7.219410	6.218190	3.546110	3.975132	3.422962
33	O	7.886395	6.591194	3.536867	3.802732	2.612368
34	H	7.915628	6.480944	2.652948	2.808986	1.623614

		21	22	23	24	25
21	H	0.000000				
22	H	1.834471	0.000000			
23	H	3.111818	2.547898	0.000000		
24	C	2.800032	3.562803	2.207658	0.000000	
25	H	3.749465	4.371693	2.562164	1.093922	0.000000

26	H	3.286644	3.963603	2.555978	1.094312	1.768426
27	H	2.515647	3.796466	3.098958	1.091726	1.779280
28	C	4.729893	5.952528	6.769291	5.811379	6.069896
29	H	5.512254	6.720130	7.213870	6.150536	6.225553
30	H	4.984306	6.388134	7.345755	6.208886	6.568730
31	C	3.369328	4.662108	5.292668	4.303825	4.623251
32	O	2.804867	4.428944	5.044845	3.740574	4.240606
33	O	3.413441	4.245721	4.631709	4.077898	4.237236
34	H	2.714951	3.418339	3.625621	3.227445	3.452513

		26	27	28	29	30
26	H	0.000000				
27	H	1.774559	0.000000			
28	C	6.725821	4.990533	0.000000		
29	H	7.102246	5.352797	1.094099	0.000000	
30	H	7.015833	5.275619	1.090152	1.767530	0.000000
31	C	5.227808	3.521272	1.523983	2.145153	2.126003
32	O	4.506581	2.794676	2.407677	3.044313	2.518306
33	O	5.119347	3.594299	2.366419	2.720750	3.266149
34	H	4.270520	2.915108	3.255977	3.667028	4.032397

		31	32	33	34
31	C	0.000000			
32	O	1.209096	0.000000		
33	O	1.331601	2.255687	0.000000	
34	H	1.935989	2.393186	1.007426	0.000000

Stoichiometry C11H17BrN2O3
Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.393814	1.343216	1.274316
2	6	0	-1.590184	0.957772	0.753648
3	7	0	-1.922257	1.906228	-0.206366
4	6	0	-0.954974	2.835301	-0.252152
5	7	0	-0.008529	2.512562	0.637684
6	6	0	1.271682	3.216197	0.833510
7	1	0	0.223871	0.880376	2.022888
8	1	0	-2.166622	0.042583	0.914827
9	1	0	1.069557	4.288461	0.828687

10	1	0	1.628160	2.943620	1.825400
11	35	0	-2.427646	-2.241592	0.267461
12	1	0	-0.931375	3.682716	-0.915509
13	6	0	-3.075340	1.910681	-1.055980
14	6	0	-3.818559	0.834407	-1.271994
15	1	0	-3.263328	2.880846	-1.499691
16	1	0	-4.681012	0.924122	-1.921681
17	1	0	-3.599110	-0.145614	-0.842257
18	6	0	1.371226	-2.338743	-0.206415
19	6	0	2.700362	-2.935488	-0.040833
20	8	0	2.308423	-1.809748	0.789059
21	1	0	1.214346	-1.668937	-1.045930
22	1	0	0.473817	-2.784442	0.208083
23	1	0	2.762898	-3.852910	0.540154
24	6	0	3.816718	-2.702011	-1.021463
25	1	0	4.784582	-2.682279	-0.512036
26	1	0	3.839708	-3.515352	-1.753218
27	1	0	3.676418	-1.759550	-1.554331
28	6	0	2.319578	2.857510	-0.232526
29	1	0	3.263496	3.327490	0.059348
30	1	0	2.038966	3.243858	-1.212538
31	6	0	2.537352	1.355648	-0.372201
32	8	0	2.520681	0.782224	-1.436541
33	8	0	2.715321	0.770646	0.810703
34	1	0	2.689070	-0.232717	0.724217

Rotational constants (GHZ): 0.3232312 0.2620959 0.1608072

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 538 symmetry adapted cartesian basis functions of A symmetry.

There are 519 symmetry adapted basis functions of A symmetry.

519 basis functions, 823 primitive gaussians, 538 cartesian basis functions

78 alpha electrons 78 beta electrons

nuclear repulsion energy 1574.2211132834 Hartrees.

NAtoms= 34 NActive= 34 NUniq= 34 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 519 RedAO= T EigKep= 4.21D-06 NBF= 519

NBsUse= 519 1.00D-06 EigRej= -1.00D+00 NBFU= 519

Initial guess from the checkpoint file: "./coohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.996407 -0.003503 -0.000642 0.084615 Ang= -9.72 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3338.90348429 A.U. after 13 cycles

NFock= 13 Conv=0.44D-08 -V/T= 2.0019

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000168610	-0.000048544	-0.000102124
2	6	-0.000681475	0.000412092	-0.000390636
3	7	0.000429017	-0.000064802	0.000469365
4	6	0.001227432	0.000107414	-0.000715136
5	7	-0.000596905	-0.000131756	0.000324631
6	6	0.000380761	0.000839552	-0.000194372
7	1	0.000447378	-0.000442735	0.000099866
8	1	0.000640086	0.000185227	-0.001146446
9	1	0.000094487	0.000265578	-0.000292152
10	1	-0.000127728	-0.000354336	-0.000024505
11	35	-0.000536663	-0.000002888	0.000153300
12	1	-0.000221211	-0.000073191	0.000104424
13	6	-0.000032898	0.000649466	0.000398280
14	6	-0.000419379	-0.001400005	0.000743834
15	1	0.000150992	-0.000159106	0.000041610
16	1	0.000418687	0.000344997	-0.000186771
17	1	0.000101078	0.000373799	-0.000133773
18	6	0.000332201	0.000947557	-0.000283007
19	6	-0.000035979	-0.000481998	0.000127573

20	8	-0.000755998	-0.000357906	-0.000473604
21	1	-0.000082090	-0.000093735	-0.000147513
22	1	0.000047398	0.000027872	0.000632100
23	1	-0.000091683	-0.000054248	0.000045524
24	6	0.000049479	-0.000015435	-0.000159344
25	1	0.000069062	0.000002467	-0.000001773
26	1	0.000039381	-0.000021909	0.000138648
27	1	0.000038148	0.000070116	0.000069103
28	6	-0.001251811	-0.000819305	0.001274988
29	1	0.000201068	0.000157777	-0.000235680
30	1	-0.000004176	0.000095287	-0.000330663
31	6	0.000311411	-0.000764353	0.000451841
32	8	-0.000315066	0.000930742	-0.000085061
33	8	-0.000472839	-0.000024642	0.000030300
34	1	0.000816447	-0.000099049	-0.000202829

Cartesian Forces: Max 0.001400005 RMS 0.000453565

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.002480949 RMS 0.000498530
Search for a local minimum.
Step number 21 out of a maximum of 175
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 19 20 21
DE= -5.28D-04 DEPred=-4.43D-04 R= 1.19D+00
TightC=F SS= 1.41D+00 RLast= 3.46D-01 DXNew= 2.6298D+00 1.0391D+00
Trust test= 1.19D+00 RLast= 3.46D-01 DXMaxT set to 1.56D+00
ITU= 1 1 1 1 1 1 1 1 0 0 -1 1 1 1 0 1 0 -1 0 1
ITU= 0

Eigenvalues ---	0.00134	0.00367	0.00404	0.00576	0.00698
Eigenvalues ---	0.00709	0.00904	0.01196	0.01549	0.01767
Eigenvalues ---	0.01962	0.02088	0.02257	0.02327	0.02415
Eigenvalues ---	0.02425	0.02854	0.02975	0.03129	0.03209
Eigenvalues ---	0.03493	0.03593	0.04003	0.04186	0.04664
Eigenvalues ---	0.04836	0.05006	0.05319	0.05583	0.05769
Eigenvalues ---	0.05927	0.06383	0.06984	0.09137	0.09595
Eigenvalues ---	0.10867	0.11968	0.12551	0.12778	0.13435
Eigenvalues ---	0.14961	0.15370	0.15679	0.15976	0.15999

Eigenvalues --- 0.16001 0.16006 0.16018 0.16045 0.16443
Eigenvalues --- 0.17254 0.17293 0.19969 0.21089 0.22755
Eigenvalues --- 0.23044 0.23675 0.23887 0.24944 0.25592
Eigenvalues --- 0.28890 0.29233 0.30094 0.31816 0.32161
Eigenvalues --- 0.32640 0.34497 0.34533 0.34614 0.34765
Eigenvalues --- 0.34877 0.34943 0.34976 0.35117 0.35255
Eigenvalues --- 0.35339 0.35709 0.35869 0.36549 0.36920
Eigenvalues --- 0.36943 0.37213 0.37721 0.37981 0.40771
Eigenvalues --- 0.41838 0.44615 0.48250 0.49185 0.51669
Eigenvalues --- 0.52825 0.55564 0.56317 0.60876 0.90576
Eigenvalues --- 1.38275
En-DIIS/RFO-DIIS IScMMF= 0 using points: 21 20 19 18 17
RFO step: Lambda=-8.09067462D-05.
DidBck=F Rises=F RFO-DIIS coefs: 0.89920 0.53353 -0.36939 -0.27760 0.21426
Iteration 1 RMS(Cart)= 0.03740734 RMS(Int)= 0.00032378
Iteration 2 RMS(Cart)= 0.00050812 RMS(Int)= 0.00004214
Iteration 3 RMS(Cart)= 0.00000014 RMS(Int)= 0.00004214

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.57097	-0.00073	0.00050	-0.00146	-0.00097	2.57000
R2	2.61924	0.00007	-0.00046	0.00048	0.00006	2.61930
R3	2.03189	0.00022	-0.00004	0.00045	0.00041	2.03230
R4	2.62629	-0.00163	0.00110	-0.00230	-0.00123	2.62506
R5	2.06649	-0.00075	0.00063	0.00082	0.00145	2.06794
R6	2.53597	0.00032	0.00047	0.00060	0.00106	2.53703
R7	2.70664	-0.00024	-0.00191	-0.00186	-0.00377	2.70287
R8	2.52950	-0.00005	-0.00009	0.00027	0.00020	2.52970
R9	2.03417	-0.00001	-0.00014	-0.00005	-0.00020	2.03397
R10	2.78527	-0.00017	0.00038	-0.00010	0.00028	2.78556
R11	2.06199	0.00019	-0.00020	0.00045	0.00025	2.06224
R12	2.05730	-0.00023	0.00032	-0.00080	-0.00049	2.05682
R13	2.90500	-0.00131	0.00112	-0.00214	-0.00102	2.90398
R14	4.51351	-0.00023	-0.00224	-0.03129	-0.03353	4.47997
R15	2.50515	0.00080	-0.00006	0.00105	0.00099	2.50615
R16	2.04705	-0.00018	0.00017	-0.00025	-0.00008	2.04697
R17	2.04751	-0.00045	0.00050	-0.00085	-0.00035	2.04717
R18	2.06428	-0.00013	-0.00029	0.00064	0.00036	2.06464
R19	2.77096	-0.00024	0.00072	-0.00090	-0.00007	2.77089
R20	2.77033	-0.00074	-0.00010	-0.00013	-0.00027	2.77007
R21	2.05106	0.00017	-0.00052	0.00019	-0.00033	2.05073
R22	2.04911	0.00043	-0.00090	0.00063	-0.00027	2.04884
R23	2.74474	0.00033	-0.00030	0.00139	0.00103	2.74577
R24	2.05548	0.00000	0.00005	-0.00005	0.00001	2.05549

R25	2.84239	0.00007	0.00025	0.00019	0.00043	2.84282
R26	3.06819	-0.00022	0.00035	-0.00827	-0.00792	3.06027
R27	2.06721	0.00005	0.00005	0.00012	0.00017	2.06738
R28	2.06795	-0.00001	0.00001	-0.00003	-0.00002	2.06793
R29	2.06306	-0.00005	-0.00012	-0.00018	-0.00030	2.06277
R30	2.06755	0.00027	-0.00004	0.00033	0.00029	2.06784
R31	2.06009	0.00025	-0.00017	0.00041	0.00024	2.06032
R32	2.87991	-0.00006	0.00034	0.00052	0.00086	2.88077
R33	2.28486	-0.00076	0.00040	-0.00014	0.00026	2.28512
R34	2.51636	-0.00022	-0.00123	-0.00166	-0.00289	2.51347
R35	1.90376	0.00019	0.00074	0.00225	0.00299	1.90675
A1	1.88354	-0.00030	0.00097	-0.00073	0.00023	1.88377
A2	2.27792	-0.00023	0.00043	-0.00175	-0.00138	2.27654
A3	2.12145	0.00053	-0.00115	0.00255	0.00132	2.12278
A4	1.85577	0.00056	-0.00081	0.00122	0.00042	1.85618
A5	2.27082	0.00066	-0.00015	0.00213	0.00201	2.27283
A6	2.14958	-0.00122	0.00147	-0.00363	-0.00211	2.14747
A7	1.90056	0.00018	-0.00022	0.00025	-0.00001	1.90055
A8	2.21961	-0.00165	0.00225	-0.00368	-0.00142	2.21818
A9	2.16264	0.00146	-0.00208	0.00344	0.00136	2.16400
A10	1.89657	-0.00049	0.00054	-0.00097	-0.00043	1.89614
A11	2.19179	0.00006	0.00009	-0.00042	-0.00037	2.19143
A12	2.19442	0.00044	-0.00051	0.00164	0.00109	2.19551
A13	1.88831	0.00004	-0.00045	0.00028	-0.00027	1.88805
A14	2.19343	-0.00050	0.00067	-0.00212	-0.00165	2.19178
A15	2.19860	0.00044	-0.00028	0.00077	0.00030	2.19889
A16	1.88351	0.00109	-0.00116	0.00373	0.00255	1.88607
A17	1.86078	0.00022	0.00049	-0.00108	-0.00059	1.86018
A18	1.96986	-0.00195	0.00087	-0.00598	-0.00512	1.96474
A19	1.88675	-0.00018	-0.00106	0.00180	0.00074	1.88749
A20	1.93103	0.00024	0.00197	0.00050	0.00249	1.93352
A21	1.92857	0.00065	-0.00125	0.00132	0.00007	1.92863
A22	2.52877	0.00192	-0.00215	0.04546	0.04332	2.57209
A23	2.14776	-0.00060	0.00187	-0.00136	0.00051	2.14827
A24	1.96651	0.00039	-0.00015	0.00146	0.00131	1.96782
A25	2.16890	0.00021	-0.00174	-0.00010	-0.00184	2.16706
A26	2.06774	0.00003	-0.00031	-0.00046	-0.00084	2.06690
A27	2.15512	-0.00041	0.00115	-0.00217	-0.00109	2.15404
A28	2.06018	0.00038	-0.00085	0.00260	0.00169	2.06187
A29	2.05953	0.00045	0.00058	0.00078	0.00135	2.06088
A30	2.14091	-0.00067	0.00178	-0.00208	-0.00029	2.14062
A31	1.97680	0.00012	-0.00046	0.00180	0.00137	1.97818
A32	2.00185	-0.00045	-0.00125	0.00001	-0.00125	2.00060
A33	2.01496	0.00020	-0.00102	0.00003	-0.00100	2.01396

A34	2.04393	-0.00025	0.00119	-0.00127	-0.00004	2.04390
A35	2.13644	0.00044	-0.00058	0.00128	0.00067	2.13711
A36	1.94340	-0.00007	-0.00030	0.00006	-0.00024	1.94316
A37	2.04034	0.00030	0.00053	0.00091	0.00147	2.04181
A38	2.02249	-0.00015	-0.00051	-0.00041	-0.00093	2.02155
A39	2.06377	0.00039	0.00289	-0.00472	-0.00159	2.06218
A40	2.30062	0.00080	-0.00172	-0.01803	-0.01972	2.28090
A41	1.93463	0.00003	0.00006	-0.00027	-0.00021	1.93442
A42	1.91366	-0.00015	-0.00010	-0.00147	-0.00157	1.91208
A43	1.93568	0.00003	0.00005	0.00075	0.00080	1.93648
A44	1.88202	0.00000	-0.00009	-0.00044	-0.00053	1.88149
A45	1.90227	-0.00002	0.00009	0.00040	0.00049	1.90276
A46	1.89435	0.00011	0.00000	0.00103	0.00102	1.89538
A47	1.87850	0.00030	-0.00036	0.00245	0.00208	1.88058
A48	1.94469	0.00023	0.00095	-0.00003	0.00089	1.94559
A49	1.97241	-0.00062	-0.00205	-0.00088	-0.00293	1.96948
A50	1.88563	-0.00021	0.00105	-0.00127	-0.00021	1.88542
A51	1.90127	0.00020	0.00068	-0.00077	-0.00006	1.90121
A52	1.87931	0.00011	-0.00014	0.00042	0.00029	1.87960
A53	2.14848	-0.00059	-0.00033	-0.00309	-0.00340	2.14508
A54	1.95048	-0.00003	-0.00049	0.00168	0.00122	1.95170
A55	2.18397	0.00061	0.00071	0.00145	0.00218	2.18615
A56	1.93671	0.00070	0.00297	0.00491	0.00789	1.94460
A57	2.89633	-0.00248	-0.00254	-0.00439	-0.00692	2.88940
D1	0.00173	0.00021	0.00249	0.00622	0.00872	0.01045
D2	3.01687	0.00013	0.00804	0.00341	0.01141	3.02828
D3	-3.11467	0.00021	-0.00385	0.00272	-0.00112	-3.11579
D4	-0.09953	0.00013	0.00169	-0.00009	0.00157	-0.09796
D5	0.00277	-0.00034	-0.00571	-0.01021	-0.01591	-0.01313
D6	-3.06161	-0.00008	-0.00061	0.00416	0.00355	-3.05806
D7	3.12189	-0.00035	0.00001	-0.00716	-0.00716	3.11473
D8	0.05751	-0.00009	0.00510	0.00721	0.01230	0.06981
D9	-0.00565	-0.00001	0.00157	-0.00010	0.00147	-0.00419
D10	3.10664	-0.00005	-0.00124	0.00038	-0.00090	3.10574
D11	-3.03176	-0.00009	-0.00330	0.00198	-0.00134	-3.03310
D12	0.08054	-0.00013	-0.00611	0.00246	-0.00371	0.07683
D13	-1.44263	-0.00037	-0.00214	-0.00663	-0.00877	-1.45140
D14	1.55387	-0.00033	0.00399	-0.00946	-0.00546	1.54841
D15	0.00749	-0.00020	-0.00516	-0.00631	-0.01147	-0.00398
D16	3.11993	0.00004	-0.00046	0.00313	0.00268	3.12261
D17	-3.10597	-0.00011	-0.00246	-0.00663	-0.00914	-3.11511
D18	0.00646	0.00014	0.00224	0.00281	0.00501	0.01148
D19	-0.30426	0.00003	0.01338	0.02040	0.03377	-0.27049
D20	2.84304	0.00017	0.01619	0.02073	0.03693	2.87997

D21	2.80393	-0.00004	0.01017	0.02088	0.03104	2.83497
D22	-0.33195	0.00010	0.01298	0.02121	0.03419	-0.29775
D23	-0.00635	0.00034	0.00670	0.01016	0.01684	0.01049
D24	3.05775	0.00002	0.00158	-0.00443	-0.00283	3.05491
D25	-3.11872	0.00010	0.00196	0.00074	0.00267	-3.11605
D26	-0.05463	-0.00021	-0.00316	-0.01385	-0.01700	-0.07163
D27	-2.45985	-0.00038	-0.00102	-0.00916	-0.01019	-2.47004
D28	-0.43650	0.00006	-0.00257	-0.00580	-0.00838	-0.44488
D29	1.68400	-0.00018	-0.00328	-0.00852	-0.01179	1.67221
D30	0.77241	-0.00005	0.00496	0.00777	0.01272	0.78513
D31	2.79576	0.00039	0.00340	0.01113	0.01453	2.81029
D32	-1.36692	0.00016	0.00270	0.00841	0.01112	-1.35580
D33	-3.02505	0.00036	-0.00426	0.00814	0.00389	-3.02116
D34	1.19382	0.00030	-0.00584	0.00819	0.00235	1.19617
D35	-0.92501	0.00044	-0.00488	0.00830	0.00342	-0.92159
D36	1.14560	0.00014	-0.00475	0.00712	0.00238	1.14798
D37	-0.91871	0.00008	-0.00633	0.00718	0.00083	-0.91787
D38	-3.03754	0.00021	-0.00537	0.00728	0.00190	-3.03564
D39	-0.94337	-0.00021	-0.00392	0.00370	-0.00020	-0.94358
D40	-3.00768	-0.00027	-0.00549	0.00375	-0.00175	-3.00943
D41	1.15667	-0.00013	-0.00454	0.00386	-0.00068	1.15599
D42	3.13147	0.00036	0.00265	0.00344	0.00608	3.13755
D43	-0.02819	0.00002	-0.00694	0.00104	-0.00591	-0.03410
D44	-0.01650	0.00020	-0.00051	0.00307	0.00257	-0.01393
D45	3.10702	-0.00014	-0.01010	0.00067	-0.00942	3.09760
D46	-2.75528	-0.00003	-0.00196	0.00280	0.00083	-2.75445
D47	-0.05119	0.00004	-0.00181	0.00165	-0.00017	-0.05136
D48	-0.01883	-0.00002	0.00157	-0.00079	0.00078	-0.01805
D49	2.68525	0.00005	0.00172	-0.00194	-0.00022	2.68504
D50	0.25410	0.00026	-0.00372	-0.02019	-0.02389	0.23021
D51	-2.10979	0.00030	-0.00027	-0.02221	-0.02250	-2.13229
D52	2.57151	0.00009	-0.00703	0.00175	-0.00523	2.56628
D53	0.19136	0.00007	-0.00646	0.00132	-0.00510	0.18625
D54	2.55367	-0.00002	-0.00101	0.00015	-0.00087	2.55279
D55	-1.65368	-0.00009	-0.00115	-0.00149	-0.00265	-1.65633
D56	0.43810	-0.00003	-0.00119	-0.00068	-0.00189	0.43621
D57	1.32557	0.00009	-0.00094	-0.00051	-0.00143	1.32414
D58	-2.88178	0.00002	-0.00108	-0.00215	-0.00321	-2.88499
D59	-0.79000	0.00008	-0.00112	-0.00135	-0.00245	-0.79245
D60	-1.02046	0.00002	-0.00047	-0.00119	-0.00166	-1.02212
D61	1.05537	-0.00005	-0.00061	-0.00283	-0.00344	1.05194
D62	-3.13603	0.00001	-0.00065	-0.00203	-0.00268	-3.13871
D63	1.45485	-0.00046	-0.00538	0.01276	0.00755	1.46240
D64	2.74854	0.00008	-0.00249	0.00272	0.00007	2.74861

D65	2.27333	-0.00007	-0.00047	-0.01572	-0.01617	2.25716
D66	-0.84518	-0.00002	0.00121	-0.01749	-0.01628	-0.86146
D67	-1.92287	0.00005	-0.00177	-0.01372	-0.01546	-1.93833
D68	1.24181	0.00011	-0.00009	-0.01548	-0.01557	1.22624
D69	0.11797	-0.00003	-0.00017	-0.01540	-0.01558	0.10239
D70	-3.00054	0.00003	0.00151	-0.01716	-0.01569	-3.01622
D71	2.96007	-0.00078	-0.00175	-0.00946	-0.01124	2.94882
D72	-0.15788	-0.00070	-0.00011	-0.01119	-0.01127	-0.16915
D73	-1.94918	-0.00041	0.00553	-0.01289	-0.00735	-1.95654

Item	Value	Threshold	Converged?
Maximum Force	0.002481	0.000450	NO
RMS Force	0.000499	0.000300	NO
Maximum Displacement	0.137196	0.001800	NO
RMS Displacement	0.037362	0.001200	NO

Predicted change in Energy=-1.203839D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.917063	1.628621	1.548040
2	6	0	-1.622301	0.466577	1.591119
3	7	0	-2.444123	0.466125	0.471176
4	6	0	-2.239165	1.599353	-0.218894
5	7	0	-1.318051	2.329672	0.421571
6	6	0	-0.731850	3.595560	-0.054592
7	1	0	-0.160171	2.010153	2.209952
8	1	0	-1.529644	-0.391776	2.263542
9	1	0	-1.541551	4.222961	-0.430978
10	1	0	-0.300563	4.085195	0.816562
11	35	0	-0.414808	-2.422570	2.766767
12	1	0	-2.724810	1.866992	-1.141394
13	6	0	-3.343365	-0.567942	0.061513
14	6	0	-3.296449	-1.801825	0.545380
15	1	0	-4.052467	-0.234376	-0.686321
16	1	0	-4.017500	-2.525134	0.184162
17	1	0	-2.550567	-2.135837	1.270489
18	6	0	2.670346	-0.669022	1.325644
19	6	0	4.091569	-0.309493	1.296107
20	8	0	3.104422	0.686186	1.677385
21	1	0	2.136170	-0.718145	0.382296
22	1	0	2.224957	-1.226837	2.141707

23	1	0	4.697232	-0.612451	2.147291
24	6	0	4.837963	-0.073766	0.011421
25	1	0	5.600652	0.699806	0.140852
26	1	0	5.344169	-0.995138	-0.292427
27	1	0	4.156608	0.228341	-0.786081
28	6	0	0.338615	3.379982	-1.135860
29	1	0	0.805061	4.348301	-1.341229
30	1	0	-0.099969	3.013093	-2.064160
31	6	0	1.418225	2.391138	-0.710962
32	8	0	1.755550	1.452789	-1.395037
33	8	0	1.904200	2.677063	0.493682
34	1	0	2.481750	1.928114	0.845266

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.359985	0.000000			
3	N	2.200669	1.389124	0.000000		
4	C	2.207004	2.222578	1.342539	0.000000	
5	N	1.386073	2.220706	2.177913	1.338660	0.000000
6	C	2.543930	3.645792	3.605783	2.506757	1.474053
7	H	1.075444	2.214363	3.259417	3.223394	2.154318
8	H	2.229171	1.094307	2.187429	3.260446	3.293009
9	H	3.322213	4.266827	3.967660	2.723042	2.088381
10	H	2.636265	3.929545	4.220404	3.318096	2.067163
11	Br	4.260247	3.344751	4.210988	5.330883	5.375834
12	H	3.249281	3.262410	2.154436	1.076331	2.153115
13	C	3.594661	2.524280	1.430299	2.448480	3.553548
14	C	4.293572	3.006991	2.423957	3.642799	4.582429
15	H	4.277135	3.403495	2.101730	2.620899	3.908810
16	H	5.359715	4.082505	3.391979	4.509581	5.559903
17	H	4.112969	2.781554	2.724049	4.033222	4.709621
18	C	4.265926	4.448244	5.308151	5.624448	5.071175
19	C	5.376445	5.773874	6.633051	6.783592	6.082269
20	O	4.132464	4.732608	5.682405	5.743142	4.882252
21	H	4.023494	4.122005	4.731753	4.987563	4.606775
22	H	4.287000	4.239362	5.239953	5.786897	5.306649
23	H	6.074687	6.435070	7.414287	7.655359	6.915044
24	C	6.195131	6.672512	7.316532	7.275858	6.621272
25	H	6.732272	7.370802	8.054944	7.899452	7.113629
26	H	7.033809	7.363156	7.960897	8.015220	7.479928
27	H	5.757694	6.253289	6.723607	6.565614	5.987145
28	C	3.441993	4.446295	4.337829	3.264417	2.504653
29	H	4.325535	5.436776	5.377109	4.252489	3.419054

30	H	3.953783	4.707792	4.290692	3.159086	2.851253
31	C	3.337378	4.271804	4.474467	3.774329	2.962029
32	O	3.979382	4.615151	4.700374	4.166838	3.676412
33	O	3.189111	4.304280	4.878183	4.340127	3.241725
34	H	3.483607	4.419911	5.151852	4.850521	3.844379

		6	7	8	9	10
6	C	0.000000				
7	H	2.822851	0.000000			
8	H	4.680712	2.765428	0.000000		
9	H	1.091290	3.712040	5.343817	0.000000	
10	H	1.088421	2.503407	4.862886	1.765046	0.000000
11	Br	6.654206	4.474809	2.370700	7.460442	6.794657
12	H	2.853240	4.222487	4.257235	2.730455	3.825048
13	C	4.916120	4.625482	2.858243	5.142162	5.610742
14	C	6.005739	5.209435	2.839352	6.350668	6.611043
15	H	5.108227	5.345678	3.884727	5.122280	5.915584
16	H	6.950927	6.289009	3.881297	7.214257	7.609993
17	H	6.157311	4.877071	2.251708	6.659385	6.630974
18	C	5.627312	3.996474	4.312358	6.690088	5.629213
19	C	6.351315	4.928810	5.704449	7.433572	6.231699
20	O	5.116756	3.562877	4.793762	6.207982	4.887557
21	H	5.198506	4.007134	4.133255	6.213017	5.403549
22	H	6.068109	4.021392	3.848272	7.106728	6.029258
23	H	7.213223	5.520539	6.231870	8.303680	6.986894
24	C	6.670167	5.844451	6.761627	7.704270	6.659554
25	H	6.965930	6.259814	7.519208	7.984402	6.836797
26	H	7.618995	6.752144	7.358419	8.640653	7.674806
27	H	5.980824	5.548482	6.482145	6.967933	6.108205
28	C	1.536721	3.649614	5.410406	2.177727	2.172056
29	H	2.141064	4.359989	6.396371	2.520091	2.438790
30	H	2.185614	4.390621	5.689122	2.491831	3.080292
31	C	2.550348	3.341890	5.028143	3.492025	2.856115
32	O	3.546184	4.120266	5.251678	4.412951	4.006037
33	O	2.844820	2.766222	4.933707	3.888187	2.635919
34	H	3.730595	2.974701	4.846100	4.804380	3.520666

		11	12	13	14	15
11	Br	0.000000				
12	H	6.245812	0.000000			
13	C	4.397100	2.785408	0.000000		
14	C	3.691035	4.078259	1.326197	0.000000	
15	H	5.472163	2.526957	1.083211	2.132029	0.000000
16	H	4.433932	4.766436	2.073669	1.083313	2.450823
17	H	2.623458	4.676557	2.132709	1.092559	3.114540
18	C	3.830136	6.451771	6.145971	6.123291	7.030870

19	C	5.189930	7.559201	7.541172	7.574527	8.382183
20	O	4.820383	6.581776	6.764455	6.960086	7.593129
21	H	3.885647	5.712591	5.490972	5.542050	6.298825
22	H	2.964597	6.697068	5.980599	5.776227	6.956204
23	H	5.458318	8.488216	8.306844	8.238912	9.204865
24	C	6.379687	7.892469	8.196392	8.333064	8.919214
25	H	7.268453	8.504105	9.033766	9.250957	9.733427
26	H	6.675481	8.603543	8.705230	8.718541	9.435607
27	H	6.367723	7.082749	7.589603	7.838522	8.222710
28	C	7.033332	3.416686	5.529628	6.549152	5.705022
29	H	8.013015	4.319354	6.583811	7.629269	6.710098
30	H	7.278970	3.009126	5.278439	6.341185	5.297805
31	C	6.215013	4.198183	5.659118	6.433311	6.068146
32	O	6.086827	4.506609	5.674842	6.315096	6.089488
33	O	6.045740	4.975684	6.184963	6.863663	6.734298
34	H	5.568722	5.573044	6.385650	6.884037	7.051107

		16	17	18	19	20
16	H	0.000000				
17	H	1.866427	0.000000			
18	C	7.033876	5.423331	0.000000		
19	C	8.479534	6.888699	1.466291	0.000000	
20	O	7.953871	6.333111	1.465855	1.453000	0.000000
21	H	6.416550	4.976369	1.085201	2.196733	2.141709
22	H	6.669769	4.938718	1.084199	2.245173	2.156087
23	H	9.135578	7.457887	2.187824	1.087716	2.108154
24	C	9.190118	7.773530	2.603857	1.504356	2.521532
25	H	10.144504	8.703983	3.444432	2.151890	2.931260
26	H	9.497835	8.128393	3.142266	2.136014	3.423956
27	H	8.679806	7.403041	2.733791	2.151511	2.717606
28	C	7.455776	6.675489	5.281137	5.797530	4.777089
29	H	8.533934	7.754055	5.980387	6.281060	5.273536
30	H	7.146605	6.605816	5.720436	6.316642	5.448099
31	C	7.383636	6.338057	3.883317	4.297500	3.384424
32	O	7.186505	6.206925	3.569458	3.975535	3.441935
33	O	7.888294	6.603968	3.532056	3.787873	2.608693
34	H	7.906246	6.482340	2.647914	2.793146	1.619423

		21	22	23	24	25
21	H	0.000000				
22	H	1.833625	0.000000			
23	H	3.112141	2.547478	0.000000		
24	C	2.802223	3.563073	2.207244	0.000000	
25	H	3.751202	4.371578	2.562028	1.094011	0.000000
26	H	3.289868	3.963355	2.552881	1.094301	1.768148
27	H	2.518553	3.797467	3.099012	1.091569	1.779535

28	C	4.725532	5.960161	6.761372	5.786948	6.041719
29	H	5.514641	6.725259	7.206097	6.135848	6.205302
30	H	4.990752	6.408713	7.341256	6.182225	6.535324
31	C	3.373174	4.677423	5.286119	4.276938	4.591175
32	O	2.831385	4.461983	5.046464	3.716149	4.208413
33	O	3.404946	4.249624	4.621294	4.050506	4.206874
34	H	2.708590	3.420588	3.613600	3.202275	3.425273

		26	27	28	29	30
26	H	0.000000				
27	H	1.775076	0.000000			
28	C	6.701390	4.963090	0.000000		
29	H	7.089134	5.339955	1.094253	0.000000	
30	H	6.988819	5.244690	1.090277	1.767622	0.000000
31	C	5.201449	3.490283	1.524437	2.145622	2.126708
32	O	4.481772	2.763183	2.406024	3.048001	2.515000
33	O	5.092781	3.564740	2.366551	2.714414	3.266828
34	H	4.246551	2.890618	3.259725	3.667335	4.038218

		31	32	33	34
31	C	0.000000			
32	O	1.209233	0.000000		
33	O	1.330073	2.255704	0.000000	
34	H	1.940959	2.402552	1.009009	0.000000

Stoichiometry C11H17BrN2O3
Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.258251	1.345505	1.259985
2	6	0	-1.476876	1.052170	0.732283
3	7	0	-1.738457	2.032525	-0.216476
4	6	0	-0.706685	2.890835	-0.250554
5	7	0	0.205998	2.498599	0.646760
6	6	0	1.532898	3.105959	0.854807
7	1	0	0.321504	0.830476	2.005109
8	1	0	-2.120091	0.179523	0.881514
9	1	0	1.411056	4.190390	0.863578
10	1	0	1.865657	2.794247	1.843123
11	35	0	-2.627369	-2.054524	0.271661

12	1	0	-0.622786	3.743172	-0.902453
13	6	0	-2.884670	2.125972	-1.066898
14	6	0	-3.721279	1.116760	-1.267836
15	1	0	-2.984914	3.100449	-1.529165
16	1	0	-4.568353	1.272181	-1.925010
17	1	0	-3.586569	0.126490	-0.826357
18	6	0	1.159918	-2.414263	-0.172169
19	6	0	2.442916	-3.113990	-0.052552
20	8	0	2.163195	-1.971538	0.800540
21	1	0	1.029547	-1.724373	-0.999646
22	1	0	0.243468	-2.794181	0.265174
23	1	0	2.450859	-4.040636	0.517001
24	6	0	3.545293	-2.956981	-1.064086
25	1	0	4.526106	-3.017510	-0.583250
26	1	0	3.483688	-3.763508	-1.801117
27	1	0	3.463203	-2.001662	-1.585765
28	6	0	2.550738	2.680263	-0.214910
29	1	0	3.529013	3.071010	0.081207
30	1	0	2.302084	3.097624	-1.190966
31	6	0	2.648805	1.166858	-0.369495
32	8	0	2.571058	0.609457	-1.439778
33	8	0	2.798416	0.558632	0.803864
34	1	0	2.683458	-0.440160	0.718444

Rotational constants (GHZ): 0.3264294 0.2602966 0.1610590

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 538 symmetry adapted cartesian basis functions of A symmetry.

There are 519 symmetry adapted basis functions of A symmetry.

519 basis functions, 823 primitive gaussians, 538 cartesian basis functions

78 alpha electrons 78 beta electrons

nuclear repulsion energy 1575.5731972912 Hartrees.

NAtoms= 34 NActive= 34 NUniq= 34 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 519 RedAO= T EigKep= 4.04D-06 NBF= 519

NBsUse= 519 1.00D-06 EigRej= -1.00D+00 NBFU= 519

Initial guess from the checkpoint file: "./coohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999206 -0.001050 -0.000627 0.039830 Ang= -4.57 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3338.90360779 A.U. after 12 cycles
NFock= 12 Conv=0.60D-08 -V/T= 2.0019
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000982645	0.000760965	0.000938586
2	6	-0.000620615	0.000043293	-0.000286334
3	7	0.001299366	0.000716911	-0.000349327
4	6	-0.000221617	0.000399986	0.000641315
5	7	0.000616092	-0.000713732	-0.000821636
6	6	0.000417877	0.000279535	-0.000374798
7	1	0.000239771	-0.000268055	0.000037779
8	1	0.000779779	0.000210258	-0.000795996
9	1	0.000081615	0.000034525	-0.000236675
10	1	-0.000074472	-0.000228808	0.000124792
11	35	-0.000105857	-0.000142346	0.000278992
12	1	-0.000201278	0.000034019	0.000061704
13	6	-0.000650206	-0.000530249	0.000081969
14	6	0.000005411	-0.000865550	0.000002317
15	1	0.000059358	0.000054533	0.000148421
16	1	0.000265414	0.000249669	0.000031887
17	1	-0.000306403	0.000186999	0.000032683
18	6	0.000240887	0.000928577	-0.000094201
19	6	0.000103154	-0.000697485	0.000153137
20	8	-0.000442814	-0.000016878	-0.000782648
21	1	-0.000043436	-0.000163472	-0.000244548

22	1	0.000176959	-0.000251321	0.000499046
23	1	-0.000173441	-0.000035745	0.000083465
24	6	0.000012709	0.000006404	0.000130934
25	1	-0.000012915	-0.000003758	0.000001113
26	1	0.000011070	-0.000010454	0.000049668
27	1	0.000045347	0.000074562	-0.000021232
28	6	-0.000662993	-0.000262837	0.001141485
29	1	0.000085320	0.000137336	-0.000163205
30	1	-0.000028136	0.000033300	-0.000159754
31	6	-0.000014101	-0.000769260	-0.000741493
32	8	-0.000024460	0.000417211	0.000203818
33	8	-0.000187238	0.000107110	0.001244421
34	1	0.000312499	0.000284756	-0.000815687

Cartesian Forces: Max 0.001299366 RMS 0.000439515

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.001677766 RMS 0.000304186

Search for a local minimum.

Step number 22 out of a maximum of 175

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 20 21 22

DE= -1.24D-04 DEPred=-1.20D-04 R= 1.03D+00

TightC=F SS= 1.41D+00 RLast= 1.19D-01 DXNew= 2.6298D+00 3.5583D-01

Trust test= 1.03D+00 RLast= 1.19D-01 DXMaxT set to 1.56D+00

ITU= 1 1 1 1 1 1 1 1 1 0 0 -1 1 1 1 0 1 0 -1 0

ITU= 1 0

Eigenvalues ---	0.00147	0.00337	0.00427	0.00617	0.00692
Eigenvalues ---	0.00702	0.00872	0.01237	0.01542	0.01755
Eigenvalues ---	0.01982	0.02082	0.02265	0.02328	0.02399
Eigenvalues ---	0.02418	0.02882	0.03098	0.03206	0.03337
Eigenvalues ---	0.03538	0.03622	0.04193	0.04578	0.04670
Eigenvalues ---	0.04955	0.05164	0.05359	0.05616	0.05760
Eigenvalues ---	0.05926	0.06338	0.06680	0.09034	0.09553
Eigenvalues ---	0.10736	0.11933	0.12532	0.12776	0.13377
Eigenvalues ---	0.14264	0.15326	0.15581	0.15975	0.16001
Eigenvalues ---	0.16005	0.16010	0.16024	0.16046	0.16235
Eigenvalues ---	0.16939	0.17474	0.19790	0.21287	0.22579
Eigenvalues ---	0.23055	0.23626	0.23879	0.25154	0.25401

Eigenvalues --- 0.28862 0.29205 0.30172 0.31704 0.31982
Eigenvalues --- 0.32744 0.34498 0.34542 0.34618 0.34766
Eigenvalues --- 0.34877 0.34942 0.34980 0.35113 0.35229
Eigenvalues --- 0.35347 0.35710 0.35831 0.36553 0.36865
Eigenvalues --- 0.36950 0.37216 0.37724 0.37883 0.40974
Eigenvalues --- 0.43073 0.45314 0.48455 0.49165 0.51661
Eigenvalues --- 0.52804 0.55688 0.56249 0.60713 0.90575
Eigenvalues --- 1.37313
En-DIIS/RFO-DIIS IScMMF= 0 using points: 22 21 20 19 18
RFO step: Lambda=-3.51182456D-05.
DidBck=F Rises=F RFO-DIIS coefs: 1.01822 0.05598 -0.32515 0.08988 0.16106
Iteration 1 RMS(Cart)= 0.03884274 RMS(Int)= 0.00051654
Iteration 2 RMS(Cart)= 0.00100428 RMS(Int)= 0.00006466
Iteration 3 RMS(Cart)= 0.00000051 RMS(Int)= 0.00006466

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.57000	-0.00038	-0.00004	-0.00045	-0.00049	2.56951
R2	2.61930	-0.00003	-0.00030	0.00008	-0.00023	2.61906
R3	2.03230	0.00009	-0.00017	0.00037	0.00020	2.03249
R4	2.62506	-0.00049	-0.00096	-0.00016	-0.00111	2.62396
R5	2.06794	-0.00032	-0.00137	0.00005	-0.00132	2.06662
R6	2.53703	-0.00006	0.00052	0.00056	0.00109	2.53812
R7	2.70287	0.00097	-0.00094	0.00024	-0.00071	2.70217
R8	2.52970	-0.00015	0.00002	-0.00027	-0.00026	2.52944
R9	2.03397	0.00005	-0.00014	0.00012	-0.00002	2.03395
R10	2.78556	-0.00020	0.00080	0.00006	0.00086	2.78642
R11	2.06224	0.00004	0.00026	-0.00013	0.00013	2.06237
R12	2.05682	-0.00003	-0.00076	0.00033	-0.00043	2.05639
R13	2.90398	-0.00077	-0.00042	-0.00141	-0.00183	2.90215
R14	4.47997	0.00013	0.03001	-0.00059	0.02942	4.50940
R15	2.50615	0.00041	0.00042	0.00069	0.00111	2.50726
R16	2.04697	-0.00012	-0.00008	0.00004	-0.00005	2.04692
R17	2.04717	-0.00035	-0.00006	-0.00062	-0.00069	2.04648
R18	2.06464	-0.00025	0.00106	-0.00139	-0.00033	2.06431
R19	2.77089	-0.00037	0.00018	-0.00002	0.00030	2.77119
R20	2.77007	-0.00029	-0.00128	-0.00107	-0.00239	2.76768
R21	2.05073	0.00024	0.00007	0.00029	0.00036	2.05109
R22	2.04884	0.00044	0.00042	0.00054	0.00096	2.04980
R23	2.74577	0.00037	-0.00072	0.00079	-0.00002	2.74575
R24	2.05549	-0.00002	0.00009	0.00001	0.00010	2.05559
R25	2.84282	-0.00012	-0.00007	-0.00003	-0.00009	2.84273
R26	3.06027	0.00001	0.00114	-0.00383	-0.00269	3.05758
R27	2.06738	-0.00001	0.00002	-0.00002	0.00000	2.06738

R28	2.06793	0.00000	0.00004	-0.00005	-0.00001	2.06792
R29	2.06277	0.00000	0.00002	-0.00019	-0.00017	2.06260
R30	2.06784	0.00019	0.00024	0.00010	0.00034	2.06818
R31	2.06032	0.00013	-0.00017	0.00010	-0.00007	2.06026
R32	2.88077	0.00001	0.00095	0.00016	0.00111	2.88188
R33	2.28512	-0.00045	-0.00017	0.00053	0.00036	2.28548
R34	2.51347	0.00029	-0.00067	-0.00064	-0.00131	2.51216
R35	1.90675	-0.00030	-0.00122	0.00035	-0.00088	1.90587
A1	1.88377	-0.00018	-0.00017	0.00008	-0.00009	1.88368
A2	2.27654	-0.00014	-0.00080	-0.00103	-0.00178	2.27476
A3	2.12278	0.00031	0.00073	0.00085	0.00163	2.12441
A4	1.85618	0.00026	0.00058	0.00030	0.00086	1.85705
A5	2.27283	-0.00034	-0.00010	-0.00110	-0.00121	2.27162
A6	2.14747	0.00009	0.00000	0.00149	0.00149	2.14896
A7	1.90055	-0.00002	-0.00042	-0.00035	-0.00076	1.89979
A8	2.21818	-0.00044	-0.00036	0.00069	0.00033	2.21851
A9	2.16400	0.00047	0.00076	-0.00021	0.00054	2.16453
A10	1.89614	-0.00011	0.00011	0.00012	0.00022	1.89636
A11	2.19143	-0.00002	-0.00048	-0.00060	-0.00108	2.19035
A12	2.19551	0.00013	0.00038	0.00050	0.00089	2.19640
A13	1.88805	0.00006	-0.00011	-0.00006	-0.00016	1.88789
A14	2.19178	-0.00045	0.00045	-0.00111	-0.00060	2.19118
A15	2.19889	0.00040	-0.00039	0.00095	0.00063	2.19952
A16	1.88607	0.00041	-0.00160	0.00297	0.00137	1.88744
A17	1.86018	-0.00020	0.00006	-0.00193	-0.00186	1.85832
A18	1.96474	-0.00037	0.00085	-0.00284	-0.00199	1.96276
A19	1.88749	0.00004	0.00083	0.00061	0.00143	1.88892
A20	1.93352	-0.00018	0.00012	-0.00021	-0.00009	1.93343
A21	1.92863	0.00033	-0.00029	0.00149	0.00121	1.92984
A22	2.57209	0.00136	-0.02100	0.01440	-0.00659	2.56550
A23	2.14827	0.00024	-0.00113	0.00335	0.00222	2.15048
A24	1.96782	-0.00020	0.00039	-0.00107	-0.00068	1.96714
A25	2.16706	-0.00004	0.00075	-0.00231	-0.00156	2.16550
A26	2.06690	-0.00004	-0.00004	-0.00087	-0.00090	2.06600
A27	2.15404	-0.00002	-0.00280	0.00157	-0.00122	2.15282
A28	2.06187	0.00007	0.00282	-0.00086	0.00196	2.06383
A29	2.06088	0.00050	0.00019	0.00191	0.00205	2.06293
A30	2.14062	-0.00081	-0.00097	-0.00333	-0.00424	2.13639
A31	1.97818	0.00003	0.00047	0.00123	0.00180	1.97997
A32	2.00060	-0.00016	-0.00061	-0.00113	-0.00180	1.99880
A33	2.01396	0.00020	0.00068	0.00089	0.00157	2.01553
A34	2.04390	-0.00032	-0.00045	-0.00090	-0.00113	2.04277
A35	2.13711	0.00040	0.00039	0.00201	0.00219	2.13930
A36	1.94316	0.00002	0.00043	-0.00081	-0.00041	1.94275

A37	2.04181	0.00001	0.00005	0.00053	0.00065	2.04247
A38	2.02155	-0.00004	-0.00003	-0.00055	-0.00059	2.02097
A39	2.06218	0.00059	0.00199	0.00433	0.00694	2.06912
A40	2.28090	0.00110	0.02044	0.00540	0.02574	2.30663
A41	1.93442	-0.00004	0.00004	-0.00060	-0.00056	1.93386
A42	1.91208	-0.00007	-0.00013	-0.00072	-0.00084	1.91124
A43	1.93648	0.00010	0.00000	0.00095	0.00095	1.93742
A44	1.88149	0.00002	-0.00001	-0.00026	-0.00027	1.88122
A45	1.90276	-0.00004	-0.00021	-0.00015	-0.00036	1.90240
A46	1.89538	0.00003	0.00031	0.00077	0.00108	1.89646
A47	1.88058	-0.00010	0.00223	0.00203	0.00424	1.88482
A48	1.94559	-0.00004	-0.00018	0.00055	0.00040	1.94598
A49	1.96948	0.00039	0.00493	-0.00138	0.00357	1.97306
A50	1.88542	-0.00002	-0.00229	-0.00110	-0.00337	1.88205
A51	1.90121	-0.00003	-0.00366	0.00036	-0.00327	1.89794
A52	1.87960	-0.00022	-0.00158	-0.00048	-0.00201	1.87760
A53	2.14508	0.00001	-0.00119	0.00046	-0.00069	2.14439
A54	1.95170	0.00001	0.00011	0.00000	0.00015	1.95184
A55	2.18615	-0.00002	0.00110	-0.00050	0.00063	2.18679
A56	1.94460	-0.00051	0.00141	-0.00026	0.00115	1.94576
A57	2.88940	-0.00168	-0.00318	-0.01350	-0.01668	2.87272
D1	0.01045	-0.00028	-0.00178	-0.00426	-0.00604	0.00441
D2	3.02828	-0.00024	0.00288	0.00221	0.00506	3.03333
D3	-3.11579	0.00016	0.00355	0.00329	0.00687	-3.10892
D4	-0.09796	0.00020	0.00821	0.00977	0.01797	-0.07999
D5	-0.01313	0.00044	0.00176	0.00586	0.00762	-0.00552
D6	-3.05806	0.00030	0.00069	0.00822	0.00892	-3.04914
D7	3.11473	0.00004	-0.00307	-0.00091	-0.00398	3.11075
D8	0.06981	-0.00010	-0.00414	0.00145	-0.00268	0.06712
D9	-0.00419	0.00002	0.00120	0.00120	0.00240	-0.00178
D10	3.10574	0.00012	0.00065	0.00554	0.00620	3.11194
D11	-3.03310	0.00002	-0.00298	-0.00447	-0.00749	-3.04059
D12	0.07683	0.00013	-0.00354	-0.00014	-0.00369	0.07314
D13	-1.45140	-0.00002	-0.00821	-0.01803	-0.02625	-1.47765
D14	1.54841	0.00003	-0.00288	-0.01073	-0.01361	1.53480
D15	-0.00398	0.00026	-0.00012	0.00245	0.00233	-0.00165
D16	3.12261	0.00003	0.00116	0.00359	0.00476	3.12737
D17	-3.11511	0.00018	0.00043	-0.00174	-0.00132	-3.11643
D18	0.01148	-0.00005	0.00170	-0.00060	0.00111	0.01258
D19	-0.27049	-0.00001	-0.00791	0.02108	0.01317	-0.25732
D20	2.87997	0.00002	-0.00869	0.02426	0.01556	2.89553
D21	2.83497	0.00010	-0.00855	0.02603	0.01748	2.85245
D22	-0.29775	0.00013	-0.00934	0.02921	0.01988	-0.27788
D23	0.01049	-0.00043	-0.00101	-0.00510	-0.00610	0.00439

D24	3.05491	-0.00035	0.00010	-0.00762	-0.00749	3.04742
D25	-3.11605	-0.00020	-0.00228	-0.00623	-0.00851	-3.12457
D26	-0.07163	-0.00012	-0.00117	-0.00875	-0.00991	-0.08154
D27	-2.47004	0.00002	0.01161	-0.00077	0.01084	-2.45920
D28	-0.44488	0.00016	0.01183	0.00041	0.01223	-0.43265
D29	1.67221	0.00020	0.01203	-0.00073	0.01130	1.68351
D30	0.78513	-0.00012	0.01035	0.00208	0.01243	0.79756
D31	2.81029	0.00002	0.01056	0.00326	0.01382	2.82411
D32	-1.35580	0.00006	0.01077	0.00212	0.01289	-1.34292
D33	-3.02116	0.00014	-0.00789	-0.00137	-0.00924	-3.03040
D34	1.19617	0.00025	-0.00637	-0.00160	-0.00798	1.18819
D35	-0.92159	0.00028	-0.00783	-0.00039	-0.00823	-0.92982
D36	1.14798	0.00000	-0.00651	-0.00306	-0.00955	1.13842
D37	-0.91787	0.00011	-0.00499	-0.00330	-0.00830	-0.92617
D38	-3.03564	0.00014	-0.00645	-0.00209	-0.00854	-3.04418
D39	-0.94358	-0.00014	-0.00743	-0.00466	-0.01208	-0.95565
D40	-3.00943	-0.00003	-0.00592	-0.00489	-0.01082	-3.02025
D41	1.15599	0.00000	-0.00738	-0.00369	-0.01107	1.14493
D42	3.13755	0.00009	-0.00141	0.00571	0.00430	-3.14133
D43	-0.03410	0.00024	-0.00089	-0.00078	-0.00166	-0.03576
D44	-0.01393	0.00006	-0.00053	0.00217	0.00164	-0.01229
D45	3.09760	0.00020	0.00000	-0.00431	-0.00432	3.09328
D46	-2.75445	0.00005	0.00103	0.00000	0.00100	-2.75345
D47	-0.05136	0.00014	0.00078	0.00129	0.00203	-0.04934
D48	-0.01805	-0.00019	0.00093	-0.00124	-0.00032	-0.01837
D49	2.68504	-0.00011	0.00067	0.00005	0.00070	2.68574
D50	0.23021	0.00041	0.02351	0.00314	0.02664	0.25685
D51	-2.13229	0.00024	0.02261	0.00164	0.02421	-2.10808
D52	2.56628	0.00015	0.00388	-0.00311	0.00101	2.56729
D53	0.18625	0.00018	0.00338	-0.00190	0.00168	0.18794
D54	2.55279	0.00001	0.00011	-0.00014	-0.00007	2.55273
D55	-1.65633	-0.00003	0.00005	-0.00128	-0.00127	-1.65760
D56	0.43621	0.00002	0.00035	-0.00019	0.00013	0.43633
D57	1.32414	0.00002	0.00049	-0.00030	0.00022	1.32436
D58	-2.88499	-0.00002	0.00043	-0.00143	-0.00098	-2.88597
D59	-0.79245	0.00003	0.00073	-0.00034	0.00042	-0.79203
D60	-1.02212	0.00002	-0.00024	0.00104	0.00081	-1.02131
D61	1.05194	-0.00002	-0.00030	-0.00010	-0.00039	1.05155
D62	-3.13871	0.00003	0.00000	0.00100	0.00100	-3.13771
D63	1.46240	-0.00014	-0.02168	0.03708	0.01541	1.47781
D64	2.74861	0.00040	-0.01245	0.04201	0.02956	2.77816
D65	2.25716	0.00005	0.02802	-0.00311	0.02490	2.28205
D66	-0.86146	0.00006	0.02192	-0.00122	0.02067	-0.84079
D67	-1.93833	0.00015	0.03143	-0.00119	0.03027	-1.90806

D68	1.22624	0.00017	0.02532	0.00070	0.02604	1.25229
D69	0.10239	-0.00001	0.02603	-0.00256	0.02347	0.12586
D70	-3.01622	0.00001	0.01993	-0.00067	0.01925	-2.99698
D71	2.94882	-0.00007	0.00241	-0.00658	-0.00418	2.94464
D72	-0.16915	-0.00006	-0.00385	-0.00466	-0.00850	-0.17765
D73	-1.95654	0.00020	-0.00045	0.00015	-0.00031	-1.95685

Item	Value	Threshold	Converged?
Maximum Force	0.001678	0.000450	NO
RMS Force	0.000304	0.000300	NO
Maximum Displacement	0.172106	0.001800	NO
RMS Displacement	0.038959	0.001200	NO

Predicted change in Energy=-5.924014D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.919196	1.637511	1.555201
2	6	0	-1.615305	0.470170	1.595232
3	7	0	-2.443319	0.469031	0.480587
4	6	0	-2.248484	1.606905	-0.205884
5	7	0	-1.325961	2.338429	0.430875
6	6	0	-0.741983	3.605065	-0.047437
7	1	0	-0.157669	2.016830	2.213229
8	1	0	-1.517690	-0.386401	2.268089
9	1	0	-1.553772	4.238048	-0.409924
10	1	0	-0.296469	4.086729	0.820710
11	35	0	-0.393547	-2.435716	2.748606
12	1	0	-2.744344	1.876666	-1.122297
13	6	0	-3.341738	-0.566551	0.074266
14	6	0	-3.300087	-1.798640	0.564752
15	1	0	-4.045821	-0.237147	-0.680089
16	1	0	-4.018941	-2.522102	0.200564
17	1	0	-2.556905	-2.130030	1.293562
18	6	0	2.663342	-0.679591	1.271502
19	6	0	4.084916	-0.321053	1.303907
20	8	0	3.081513	0.675465	1.637537
21	1	0	2.169847	-0.733300	0.306280
22	1	0	2.185481	-1.234825	2.071473
23	1	0	4.650904	-0.621826	2.182792
24	6	0	4.890206	-0.088602	0.054741
25	1	0	5.646492	0.684786	0.218324

26	1	0	5.409830	-1.011053	-0.221951
27	1	0	4.247683	0.212485	-0.774620
28	6	0	0.311118	3.388371	-1.144048
29	1	0	0.775424	4.355030	-1.362609
30	1	0	-0.141089	3.019354	-2.064898
31	6	0	1.400997	2.401725	-0.738583
32	8	0	1.744840	1.478719	-1.440390
33	8	0	1.890428	2.673698	0.467127
34	1	0	2.472372	1.923536	0.807364

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.359726	0.000000			
3	N	2.200702	1.388539	0.000000		
4	C	2.206664	2.221959	1.343115	0.000000	
5	N	1.385948	2.220324	2.178442	1.338521	0.000000
6	C	2.543840	3.645356	3.606669	2.507448	1.474510
7	H	1.075550	2.213319	3.259129	3.223609	2.155253
8	H	2.227694	1.093608	2.187170	3.260041	3.291931
9	H	3.320722	4.268646	3.973637	2.728950	2.089831
10	H	2.631717	3.926667	4.220472	3.318703	2.066005
11	Br	4.276880	3.356656	4.216993	5.339718	5.388296
12	H	3.249208	3.261583	2.154365	1.076318	2.153457
13	C	3.594408	2.523628	1.429925	2.449000	3.553792
14	C	4.296133	3.007969	2.425586	3.646571	4.585895
15	H	4.276289	3.403643	2.100921	2.618361	3.907105
16	H	5.361514	4.083657	3.392326	4.510921	5.561470
17	H	4.116420	2.781844	2.725610	4.038334	4.714507
18	C	4.275983	4.442249	5.293663	5.615761	5.072439
19	C	5.379615	5.762242	6.627212	6.790321	6.092013
20	O	4.115578	4.701493	5.648443	5.716175	4.862850
21	H	4.089345	4.175778	4.770460	5.025985	4.655290
22	H	4.260971	4.192826	5.182647	5.737755	5.271616
23	H	6.043549	6.387727	7.376684	7.633778	6.896030
24	C	6.243397	6.708727	7.367013	7.341905	6.683763
25	H	6.767806	7.394298	8.096936	7.959957	7.169018
26	H	7.087294	7.405991	8.022228	8.093438	7.550900
27	H	5.844262	6.329078	6.812552	6.668437	6.085915
28	C	3.444580	4.441920	4.330000	3.256584	2.502556
29	H	4.332466	5.436594	5.372026	4.246673	3.420393
30	H	3.952221	4.697680	4.275968	3.145164	2.845428
31	C	3.350935	4.275006	4.472185	3.772826	2.967817
32	O	4.011966	4.639262	4.717022	4.181756	3.697372

33	O	3.186154	4.291657	4.862314	4.326845	3.234019
34	H	3.484796	4.409321	5.136768	4.838741	3.839429

		6	7	8	9	10
6	C	0.000000				
7	H	2.823920	0.000000			
8	H	4.679229	2.761917	0.000000		
9	H	1.091359	3.709965	5.344023	0.000000	
10	H	1.088193	2.498571	4.857486	1.765834	0.000000
11	Br	6.665606	4.490816	2.386271	7.474059	6.802095
12	H	2.855194	4.223300	4.256861	2.738807	3.827760
13	C	4.916902	4.624643	2.858752	5.149314	5.611048
14	C	6.009883	5.210573	2.841252	6.359340	6.612473
15	H	5.106680	5.345037	3.886576	5.129392	5.916582
16	H	6.952850	6.289844	3.884859	7.221452	7.610389
17	H	6.163079	4.878378	2.251647	6.667875	6.631836
18	C	5.629753	4.014429	4.308153	6.692863	5.628632
19	C	6.367063	4.928701	5.685343	7.451001	6.233663
20	O	5.103021	3.552883	4.762124	6.194349	4.869773
21	H	5.236916	4.076396	4.191297	6.252407	5.438753
22	H	6.040229	4.010450	3.804203	7.077548	6.003617
23	H	7.205814	5.485053	6.173674	8.296900	6.964356
24	C	6.736110	5.879877	6.785921	7.775646	6.702365
25	H	7.029316	6.280309	7.528246	8.053830	6.874218
26	H	7.693101	6.789346	7.387897	8.722393	7.722459
27	H	6.077431	5.620500	6.546470	7.070717	6.180951
28	C	1.535752	3.656801	5.407043	2.176857	2.171898
29	H	2.143514	4.373152	6.396992	2.519216	2.447003
30	H	2.185012	4.394052	5.680578	2.493958	3.080611
31	C	2.553052	3.360175	5.033136	3.494389	2.855174
32	O	3.556116	4.154280	5.279734	4.422285	4.010142
33	O	2.839333	2.770388	4.921680	3.883159	2.627583
34	H	3.726970	2.983668	4.836334	4.800895	3.513696

		11	12	13	14	15
11	Br	0.000000				
12	H	6.253540	0.000000			
13	C	4.397465	2.785310	0.000000		
14	C	3.690942	4.082016	1.326783	0.000000	
15	H	5.470718	2.521427	1.083186	2.131668	0.000000
16	H	4.432094	4.766940	2.073338	1.082950	2.448937
17	H	2.625017	4.682427	2.132396	1.092384	3.113708
18	C	3.822353	6.442654	6.124307	6.108539	7.001238
19	C	5.159030	7.573323	7.531765	7.567555	8.369717
20	O	4.794785	6.557452	6.726409	6.927978	7.550042
21	H	3.928634	5.744739	5.518986	5.578704	6.312972

22	H	2.924386	6.647158	5.914861	5.716603	6.884444
23	H	5.390438	8.476777	8.266272	8.198853	9.163901
24	C	6.378393	7.970825	8.245831	8.382436	8.967420
25	H	7.254098	8.580441	9.076061	9.291324	9.777425
26	H	6.673309	8.697131	8.767854	8.780765	9.498323
27	H	6.400555	7.195750	7.676380	7.925110	8.306221
28	C	7.040546	3.409043	5.519878	6.547204	5.687051
29	H	8.023890	4.311474	6.575531	7.628379	6.693155
30	H	7.279515	2.995191	5.261074	6.333040	5.269670
31	C	6.227496	4.196042	5.653753	6.437541	6.052676
32	O	6.119084	4.518000	5.687759	6.341369	6.087200
33	O	6.043823	4.964135	6.166775	6.852210	6.710303
34	H	5.566416	5.562366	6.367248	6.872753	7.026230

		16	17	18	19	20
16	H	0.000000				
17	H	1.867060	0.000000			
18	C	7.013890	5.418047	0.000000		
19	C	8.469621	6.883770	1.466449	0.000000	
20	O	7.918697	6.307208	1.464591	1.452988	0.000000
21	H	6.442987	5.026705	1.085392	2.198340	2.141962
22	H	6.606983	4.888431	1.084707	2.243210	2.154154
23	H	9.094310	7.417406	2.187278	1.087771	2.107903
24	C	9.236671	7.820586	2.605513	1.504307	2.521986
25	H	10.183567	8.739282	3.445272	2.151446	2.931446
26	H	9.558426	8.186437	3.143798	2.135355	3.423901
27	H	8.761621	7.487801	2.737252	2.152075	2.718971
28	C	7.449233	6.679839	5.283574	5.830425	4.772019
29	H	8.527860	7.759876	5.987503	6.318924	5.278080
30	H	7.132867	6.605420	5.716519	6.353446	5.439393
31	C	7.382533	6.350701	3.889533	4.334594	3.383793
32	O	7.205586	6.245204	3.585569	4.030670	3.450442
33	O	7.873248	6.598300	3.533973	3.805852	2.604128
34	H	7.891074	6.477763	2.651069	2.808030	1.617999

		21	22	23	24	25
21	H	0.000000				
22	H	1.835123	0.000000			
23	H	3.112774	2.542925	0.000000		
24	C	2.807002	3.563225	2.206851	0.000000	
25	H	3.755765	4.370088	2.560775	1.094010	0.000000
26	H	3.294490	3.963116	2.551520	1.094296	1.767971
27	H	2.525916	3.801003	3.099184	1.091480	1.779234
28	C	4.748315	5.935213	6.781097	5.873200	6.134464
29	H	5.533599	6.710265	7.235904	6.219822	6.300583
30	H	5.004530	6.373423	7.366427	6.282212	6.645254

31	C	3.392824	4.662223	5.313961	4.359550	4.678438
32	O	2.850354	4.459895	5.097542	3.819063	4.313299
33	O	3.422219	4.235273	4.628630	4.098663	4.257428
34	H	2.720549	3.414018	3.621694	3.234356	3.457819

		26	27	28	29	30
26	H	0.000000				
27	H	1.775689	0.000000			
28	C	6.797209	5.071417	0.000000		
29	H	7.181481	5.437186	1.094431	0.000000	
30	H	7.103051	5.366996	1.090242	1.765570	0.000000
31	C	5.290057	3.591336	1.525027	2.143863	2.125701
32	O	4.595183	2.882849	2.406273	3.036278	2.514020
33	O	5.141830	3.627142	2.366614	2.723609	3.264611
34	H	4.277845	2.929522	3.259566	3.674314	4.034958

		31	32	33	34
31	C	0.000000			
32	O	1.209423	0.000000		
33	O	1.329379	2.255614	0.000000	
34	H	1.940738	2.404073	1.008545	0.000000

Stoichiometry C11H17BrN2O3
Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.253454	1.357451	1.269898
2	6	0	-1.468526	1.059292	0.737399
3	7	0	-1.730812	2.037230	-0.212803
4	6	0	-0.700420	2.898159	-0.245293
5	7	0	0.212369	2.507463	0.652377
6	6	0	1.541790	3.111707	0.856608
7	1	0	0.326340	0.840600	2.013882
8	1	0	-2.111908	0.188626	0.892249
9	1	0	1.423008	4.196444	0.873937
10	1	0	1.878978	2.790466	1.840108
11	35	0	-2.627273	-2.055500	0.265681
12	1	0	-0.619759	3.752119	-0.895451
13	6	0	-2.877163	2.129112	-1.062580
14	6	0	-3.723966	1.125362	-1.251697

15	1	0	-2.968449	3.097935	-1.538333
16	1	0	-4.567172	1.281102	-1.913157
17	1	0	-3.596555	0.138994	-0.799871
18	6	0	1.150317	-2.403699	-0.202247
19	6	0	2.409393	-3.134146	-0.024347
20	8	0	2.138653	-1.955730	0.781390
21	1	0	1.058907	-1.739546	-1.055840
22	1	0	0.213942	-2.746758	0.224487
23	1	0	2.374807	-4.040309	0.576417
24	6	0	3.544057	-3.043766	-1.007865
25	1	0	4.508373	-3.115694	-0.496221
26	1	0	3.479452	-3.874195	-1.717581
27	1	0	3.505991	-2.105360	-1.563989
28	6	0	2.549506	2.691199	-0.223306
29	1	0	3.531253	3.083832	0.059168
30	1	0	2.290096	3.109142	-1.196270
31	6	0	2.654759	1.178436	-0.385099
32	8	0	2.594401	0.627593	-1.460102
33	8	0	2.794241	0.564521	0.785756
34	1	0	2.680208	-0.433478	0.695433

Rotational constants (GHZ): 0.3243674 0.2608176 0.1605694

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 538 symmetry adapted cartesian basis functions of A symmetry.

There are 519 symmetry adapted basis functions of A symmetry.

519 basis functions, 823 primitive gaussians, 538 cartesian basis functions

78 alpha electrons 78 beta electrons

nuclear repulsion energy 1574.2797723816 Hartrees.

NAtoms= 34 NActive= 34 NUniq= 34 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 519 RedAO= T EigKep= 3.94D-06 NBF= 519

NBsUse= 519 1.00D-06 EigRej= -1.00D+00 NBFU= 519

Initial guess from the checkpoint file: "./coohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999998 0.001097 0.000422 0.001453 Ang= 0.21 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3338.90368102 A.U. after 13 cycles
NFock= 13 Conv=0.16D-08 -V/T= 2.0019
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000030771	0.000284061	0.000467041
2	6	-0.000939001	0.000187957	0.000620510
3	7	0.001145054	0.001073137	-0.000326876
4	6	-0.000240690	-0.000222476	0.000480498
5	7	0.000301873	-0.000369758	-0.000473259
6	6	0.000260257	0.000120001	-0.000284406
7	1	0.000124243	-0.000104719	-0.000049240
8	1	0.000862559	-0.000141596	-0.001032819
9	1	0.000030313	-0.000019631	-0.000130296
10	1	-0.000022955	0.000020542	0.000101183
11	35	-0.000357709	0.000182709	0.000236111
12	1	-0.000030504	0.000008664	-0.000034913
13	6	-0.000862611	-0.001061967	-0.000061863
14	6	0.000434911	0.000136507	-0.000224845
15	1	0.000023793	0.000104266	0.000159876
16	1	0.000105321	0.000066048	0.000114910
17	1	-0.000311560	-0.000022609	0.000062326
18	6	0.000281826	0.000255610	0.000295827
19	6	-0.000044105	-0.000480078	0.000094525
20	8	-0.000062139	0.000247855	-0.000668798
21	1	0.000071273	0.000036149	-0.000330589
22	1	0.000033182	-0.000317986	0.000260448
23	1	-0.000192684	-0.000046556	0.000023599
24	6	0.000002559	0.000035659	0.000515764

25	1	-0.000038027	0.000016839	-0.000064203
26	1	-0.000046628	0.000019948	-0.000116514
27	1	-0.000074804	0.000059716	-0.000183981
28	6	-0.000110683	-0.000467489	0.000689411
29	1	-0.000126537	0.000253057	0.000125414
30	1	-0.000163394	0.000034989	-0.000209735
31	6	-0.000021290	-0.001071420	-0.001538811
32	8	-0.000146675	0.000623297	0.000631937
33	8	-0.000135361	0.000279645	0.001667178
34	1	0.000280965	0.000279629	-0.000815409

Cartesian Forces: Max 0.001667178 RMS 0.000443645

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.001681170 RMS 0.000275569
Search for a local minimum.
Step number 23 out of a maximum of 175
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 20 21 22 23
DE= -7.32D-05 DEPred=-5.92D-05 R= 1.24D+00
TightC=F SS= 1.41D+00 RLast= 1.14D-01 DXNew= 2.6298D+00 3.4098D-01
Trust test= 1.24D+00 RLast= 1.14D-01 DXMaxT set to 1.56D+00
ITU= 1 1 1 1 1 1 1 1 1 1 0 0 -1 1 1 1 0 1 0 -1
ITU= 0 1 0

Eigenvalues ---	0.00150	0.00330	0.00429	0.00600	0.00698
Eigenvalues ---	0.00758	0.00953	0.01241	0.01535	0.01677
Eigenvalues ---	0.01993	0.02096	0.02255	0.02317	0.02397
Eigenvalues ---	0.02422	0.02815	0.03076	0.03131	0.03355
Eigenvalues ---	0.03518	0.03597	0.04196	0.04415	0.04675
Eigenvalues ---	0.04884	0.04960	0.05338	0.05577	0.05738
Eigenvalues ---	0.05965	0.06138	0.06604	0.09250	0.09524
Eigenvalues ---	0.09990	0.11816	0.12569	0.12620	0.13073
Eigenvalues ---	0.13455	0.15319	0.15519	0.15941	0.15994
Eigenvalues ---	0.16002	0.16010	0.16015	0.16035	0.16125
Eigenvalues ---	0.16907	0.17597	0.20320	0.21871	0.22202
Eigenvalues ---	0.23062	0.23586	0.23958	0.24835	0.25562
Eigenvalues ---	0.28938	0.29576	0.30282	0.31583	0.32195
Eigenvalues ---	0.33078	0.34498	0.34571	0.34629	0.34812
Eigenvalues ---	0.34877	0.34943	0.34986	0.35094	0.35180

Eigenvalues --- 0.35291 0.35723 0.35825 0.36559 0.36846
Eigenvalues --- 0.36954 0.37190 0.37727 0.38027 0.40617
Eigenvalues --- 0.43985 0.45392 0.49034 0.49686 0.51755
Eigenvalues --- 0.52990 0.56050 0.56477 0.61091 0.91058
Eigenvalues --- 1.40130
En-DIIS/RFO-DIIS IScMMF= 0 using points: 23 22 21 20 19
RFO step: Lambda=-2.93455943D-05.
DidBck=F Rises=F RFO-DIIS coefs: 1.32591 0.01915 -0.27905 -0.37289 0.30688
Iteration 1 RMS(Cart)= 0.02970660 RMS(Int)= 0.00032096
Iteration 2 RMS(Cart)= 0.00048926 RMS(Int)= 0.00004591
Iteration 3 RMS(Cart)= 0.00000027 RMS(Int)= 0.00004591

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56951	-0.00013	-0.00086	0.00022	-0.00065	2.56886
R2	2.61906	0.00005	0.00006	0.00032	0.00037	2.61944
R3	2.03249	0.00002	0.00023	0.00003	0.00026	2.03275
R4	2.62396	-0.00026	-0.00146	0.00022	-0.00124	2.62272
R5	2.06662	-0.00048	-0.00039	0.00052	0.00013	2.06675
R6	2.53812	-0.00049	0.00055	-0.00050	0.00005	2.53817
R7	2.70217	0.00094	-0.00041	0.00180	0.00139	2.70356
R8	2.52944	-0.00003	0.00007	-0.00017	-0.00010	2.52934
R9	2.03395	0.00005	-0.00004	0.00011	0.00007	2.03402
R10	2.78642	-0.00022	0.00008	0.00037	0.00045	2.78687
R11	2.06237	0.00001	0.00029	-0.00027	0.00003	2.06240
R12	2.05639	0.00008	-0.00053	0.00035	-0.00018	2.05621
R13	2.90215	-0.00060	-0.00183	-0.00015	-0.00198	2.90017
R14	4.50940	-0.00028	-0.00261	-0.02936	-0.03198	4.47742
R15	2.50726	-0.00018	0.00080	-0.00027	0.00053	2.50779
R16	2.04692	-0.00009	-0.00015	-0.00002	-0.00017	2.04675
R17	2.04648	-0.00015	-0.00063	-0.00007	-0.00069	2.04579
R18	2.06431	-0.00017	0.00031	-0.00036	-0.00004	2.06426
R19	2.77119	-0.00044	-0.00053	-0.00021	-0.00092	2.77027
R20	2.76768	0.00017	-0.00062	-0.00069	-0.00124	2.76643
R21	2.05109	0.00026	0.00031	0.00038	0.00069	2.05178
R22	2.04980	0.00034	0.00073	0.00072	0.00145	2.05125
R23	2.74575	0.00006	0.00054	0.00070	0.00134	2.74709
R24	2.05559	-0.00007	0.00000	-0.00011	-0.00011	2.05548
R25	2.84273	-0.00020	-0.00001	-0.00065	-0.00066	2.84206
R26	3.05758	0.00003	-0.00538	-0.00426	-0.00964	3.04794
R27	2.06738	-0.00002	0.00003	-0.00008	-0.00005	2.06733
R28	2.06792	-0.00001	-0.00001	-0.00003	-0.00004	2.06788
R29	2.06260	0.00020	-0.00008	0.00041	0.00033	2.06293
R30	2.06818	0.00015	0.00035	0.00010	0.00045	2.06863

R31	2.06026	0.00023	0.00033	-0.00012	0.00021	2.06047
R32	2.88188	-0.00008	0.00026	0.00019	0.00045	2.88234
R33	2.28548	-0.00089	-0.00010	0.00024	0.00014	2.28562
R34	2.51216	0.00076	-0.00099	0.00051	-0.00047	2.51169
R35	1.90587	-0.00028	0.00064	-0.00018	0.00046	1.90634
A1	1.88368	-0.00029	-0.00046	0.00025	-0.00022	1.88347
A2	2.27476	0.00010	-0.00140	-0.00046	-0.00185	2.27291
A3	2.12441	0.00019	0.00167	0.00005	0.00172	2.12612
A4	1.85705	0.00015	0.00091	-0.00029	0.00063	1.85767
A5	2.27162	0.00005	0.00027	-0.00144	-0.00116	2.27046
A6	2.14896	-0.00020	-0.00097	0.00113	0.00016	2.14912
A7	1.89979	0.00012	-0.00016	-0.00002	-0.00018	1.89961
A8	2.21851	-0.00044	-0.00160	0.00026	-0.00135	2.21717
A9	2.16453	0.00032	0.00179	-0.00013	0.00166	2.16619
A10	1.89636	-0.00008	-0.00044	0.00056	0.00012	1.89648
A11	2.19035	0.00004	-0.00057	-0.00020	-0.00077	2.18959
A12	2.19640	0.00005	0.00102	-0.00035	0.00068	2.19707
A13	1.88789	0.00011	0.00012	-0.00050	-0.00035	1.88754
A14	2.19118	-0.00026	-0.00135	-0.00038	-0.00169	2.18949
A15	2.19952	0.00016	0.00064	0.00057	0.00123	2.20075
A16	1.88744	0.00006	0.00260	-0.00098	0.00163	1.88907
A17	1.85832	-0.00022	-0.00150	0.00004	-0.00147	1.85685
A18	1.96276	0.00027	-0.00367	0.00087	-0.00280	1.95995
A19	1.88892	0.00006	0.00140	0.00010	0.00149	1.89042
A20	1.93343	-0.00025	0.00019	-0.00056	-0.00038	1.93305
A21	1.92984	0.00007	0.00114	0.00051	0.00163	1.93147
A22	2.56550	0.00168	0.01607	0.03121	0.04729	2.61278
A23	2.15048	-0.00012	-0.00004	0.00116	0.00113	2.15161
A24	1.96714	-0.00005	0.00013	-0.00100	-0.00087	1.96628
A25	2.16550	0.00017	-0.00010	-0.00017	-0.00027	2.16523
A26	2.06600	-0.00002	-0.00062	-0.00087	-0.00147	2.06453
A27	2.15282	0.00017	-0.00142	0.00203	0.00063	2.15345
A28	2.06383	-0.00014	0.00187	-0.00094	0.00095	2.06478
A29	2.06293	0.00004	0.00083	0.00049	0.00134	2.06427
A30	2.13639	-0.00029	-0.00259	-0.00211	-0.00473	2.13166
A31	1.97997	-0.00024	0.00114	-0.00040	0.00070	1.98067
A32	1.99880	0.00022	-0.00014	-0.00107	-0.00120	1.99760
A33	2.01553	0.00017	0.00079	0.00170	0.00251	2.01804
A34	2.04277	-0.00019	-0.00117	-0.00111	-0.00232	2.04045
A35	2.13930	0.00004	0.00134	0.00168	0.00304	2.14234
A36	1.94275	0.00014	0.00003	-0.00114	-0.00111	1.94164
A37	2.04247	-0.00038	0.00029	-0.00106	-0.00081	2.04165
A38	2.02097	0.00016	-0.00019	0.00064	0.00046	2.02143
A39	2.06912	0.00035	-0.00204	0.00149	-0.00087	2.06825

A40	2.30663	0.00051	0.00345	-0.00328	0.00006	2.30669
A41	1.93386	0.00004	-0.00034	0.00014	-0.00020	1.93366
A42	1.91124	0.00010	-0.00072	0.00029	-0.00043	1.91081
A43	1.93742	0.00003	0.00054	0.00045	0.00098	1.93841
A44	1.88122	-0.00002	-0.00020	0.00006	-0.00014	1.88108
A45	1.90240	-0.00006	-0.00002	-0.00040	-0.00043	1.90197
A46	1.89646	-0.00009	0.00076	-0.00057	0.00019	1.89664
A47	1.88482	-0.00050	0.00259	-0.00050	0.00209	1.88691
A48	1.94598	-0.00006	0.00018	-0.00025	-0.00006	1.94592
A49	1.97306	0.00058	0.00119	-0.00007	0.00112	1.97418
A50	1.88205	0.00011	-0.00209	0.00019	-0.00189	1.88015
A51	1.89794	0.00006	-0.00143	0.00073	-0.00072	1.89723
A52	1.87760	-0.00020	-0.00068	-0.00006	-0.00074	1.87686
A53	2.14439	0.00011	-0.00186	0.00314	0.00128	2.14567
A54	1.95184	0.00017	0.00080	-0.00206	-0.00126	1.95058
A55	2.18679	-0.00028	0.00112	-0.00109	0.00002	2.18681
A56	1.94576	-0.00130	0.00131	-0.00230	-0.00099	1.94476
A57	2.87272	-0.00068	-0.00622	-0.00820	-0.01443	2.85830
D1	0.00441	0.00005	-0.00137	-0.00010	-0.00148	0.00293
D2	3.03333	-0.00002	0.00089	-0.00600	-0.00507	3.02826
D3	-3.10892	0.00009	0.00376	0.00658	0.01031	-3.09861
D4	-0.07999	0.00002	0.00602	0.00068	0.00671	-0.07328
D5	-0.00552	0.00003	0.00136	0.00109	0.00245	-0.00307
D6	-3.04914	-0.00010	0.00621	0.00441	0.01058	-3.03856
D7	3.11075	-0.00001	-0.00330	-0.00490	-0.00821	3.10254
D8	0.06712	-0.00014	0.00155	-0.00159	-0.00007	0.06705
D9	-0.00178	-0.00011	0.00093	-0.00093	0.00000	-0.00179
D10	3.11194	-0.00002	0.00272	0.00322	0.00595	3.11790
D11	-3.04059	-0.00006	-0.00128	0.00465	0.00339	-3.03720
D12	0.07314	0.00003	0.00052	0.00880	0.00935	0.08248
D13	-1.47765	-0.00001	-0.00904	-0.00307	-0.01211	-1.48976
D14	1.53480	-0.00006	-0.00628	-0.00995	-0.01623	1.51857
D15	-0.00165	0.00013	-0.00010	0.00164	0.00154	-0.00011
D16	3.12737	0.00006	0.00240	0.00218	0.00455	3.13192
D17	-3.11643	0.00005	-0.00182	-0.00237	-0.00415	-3.12058
D18	0.01258	-0.00001	0.00069	-0.00182	-0.00113	0.01145
D19	-0.25732	-0.00008	-0.00174	0.01739	0.01566	-0.24166
D20	2.89553	-0.00007	-0.00134	0.01761	0.01627	2.91180
D21	2.85245	0.00002	0.00029	0.02214	0.02243	2.87488
D22	-0.27788	0.00002	0.00069	0.02235	0.02304	-0.25484
D23	0.00439	-0.00009	-0.00077	-0.00168	-0.00245	0.00194
D24	3.04742	0.00000	-0.00571	-0.00509	-0.01086	3.03656
D25	-3.12457	-0.00003	-0.00325	-0.00223	-0.00547	-3.13004
D26	-0.08154	0.00007	-0.00819	-0.00564	-0.01388	-0.09541

D27	-2.45920	0.00010	0.00206	-0.00378	-0.00172	-2.46092
D28	-0.43265	0.00008	0.00419	-0.00412	0.00007	-0.43258
D29	1.68351	0.00019	0.00239	-0.00295	-0.00055	1.68296
D30	0.79756	-0.00005	0.00779	0.00019	0.00798	0.80554
D31	2.82411	-0.00006	0.00993	-0.00015	0.00977	2.83388
D32	-1.34292	0.00005	0.00813	0.00102	0.00915	-1.33377
D33	-3.03040	0.00001	-0.00088	0.00870	0.00781	-3.02258
D34	1.18819	0.00023	-0.00006	0.00892	0.00886	1.19705
D35	-0.92982	0.00012	-0.00017	0.00923	0.00905	-0.92076
D36	1.13842	-0.00007	-0.00184	0.00976	0.00792	1.14635
D37	-0.92617	0.00014	-0.00102	0.00998	0.00897	-0.91720
D38	-3.04418	0.00003	-0.00113	0.01029	0.00916	-3.03502
D39	-0.95565	-0.00004	-0.00444	0.00967	0.00523	-0.95043
D40	-3.02025	0.00018	-0.00361	0.00988	0.00627	-3.01398
D41	1.14493	0.00007	-0.00373	0.01019	0.00647	1.15139
D42	-3.14133	-0.00003	0.00204	0.00025	0.00229	-3.13904
D43	-0.03576	0.00020	-0.00116	0.00747	0.00631	-0.02945
D44	-0.01229	-0.00003	0.00161	0.00001	0.00162	-0.01067
D45	3.09328	0.00019	-0.00158	0.00722	0.00564	3.09892
D46	-2.75345	0.00004	0.00170	-0.00156	0.00016	-2.75329
D47	-0.04934	0.00013	0.00153	0.00171	0.00325	-0.04608
D48	-0.01837	-0.00013	-0.00079	-0.00091	-0.00171	-0.02008
D49	2.68574	-0.00004	-0.00095	0.00235	0.00138	2.68712
D50	0.25685	0.00024	0.00399	-0.00526	-0.00127	0.25558
D51	-2.10808	0.00001	0.00165	-0.00629	-0.00460	-2.11268
D52	2.56729	0.00014	0.00633	-0.00240	0.00388	2.57117
D53	0.18794	0.00013	0.00629	-0.00093	0.00533	0.19326
D54	2.55273	-0.00002	0.00041	-0.00099	-0.00056	2.55216
D55	-1.65760	0.00004	-0.00051	-0.00064	-0.00113	-1.65873
D56	0.43633	0.00001	0.00031	-0.00088	-0.00055	0.43578
D57	1.32436	-0.00003	0.00017	-0.00051	-0.00037	1.32399
D58	-2.88597	0.00003	-0.00074	-0.00016	-0.00093	-2.88690
D59	-0.79203	0.00000	0.00007	-0.00040	-0.00035	-0.79239
D60	-1.02131	-0.00001	0.00002	0.00183	0.00184	-1.01947
D61	1.05155	0.00005	-0.00090	0.00218	0.00128	1.05283
D62	-3.13771	0.00002	-0.00008	0.00194	0.00186	-3.13585
D63	1.47781	0.00009	0.00681	0.03351	0.04003	1.51784
D64	2.77816	0.00021	0.00501	0.03353	0.03881	2.81698
D65	2.28205	0.00022	0.00715	-0.00654	0.00061	2.28266
D66	-0.84079	0.00024	0.00377	-0.00562	-0.00185	-0.84264
D67	-1.90806	0.00001	0.01020	-0.00672	0.00347	-1.90458
D68	1.25229	0.00003	0.00682	-0.00580	0.00101	1.25330
D69	0.12586	0.00006	0.00661	-0.00614	0.00048	0.12634
D70	-2.99698	0.00008	0.00323	-0.00522	-0.00199	-2.99897

D71	2.94464	0.00027	-0.00240	-0.00268	-0.00507	2.93957
D72	-0.17765	0.00029	-0.00582	-0.00179	-0.00762	-0.18527
D73	-1.95685	0.00036	-0.01027	-0.00258	-0.01285	-1.96970

Item	Value	Threshold	Converged?
Maximum Force	0.001681	0.000450	NO
RMS Force	0.000276	0.000300	YES
Maximum Displacement	0.107378	0.001800	NO
RMS Displacement	0.029588	0.001200	NO

Predicted change in Energy=-5.925712D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.905413	1.647222	1.555675
2	6	0	-1.587261	0.471746	1.591179
3	7	0	-2.419228	0.466630	0.480312
4	6	0	-2.240894	1.610681	-0.200403
5	7	0	-1.323489	2.348995	0.435797
6	6	0	-0.745995	3.618786	-0.042757
7	1	0	-0.140092	2.026440	2.209570
8	1	0	-1.474035	-0.388289	2.257249
9	1	0	-1.560566	4.251380	-0.399680
10	1	0	-0.296092	4.097635	0.824564
11	35	0	-0.402248	-2.431594	2.795761
12	1	0	-2.746902	1.880586	-1.111255
13	6	0	-3.311400	-0.576418	0.076743
14	6	0	-3.269669	-1.804644	0.577558
15	1	0	-4.010651	-0.255659	-0.685660
16	1	0	-3.982733	-2.532411	0.211659
17	1	0	-2.534635	-2.126947	1.318571
18	6	0	2.631815	-0.687504	1.234523
19	6	0	4.053241	-0.335599	1.303549
20	8	0	3.045188	0.663414	1.618250
21	1	0	2.160504	-0.734633	0.257531
22	1	0	2.136514	-1.246607	2.022140
23	1	0	4.594082	-0.644386	2.195324
24	6	0	4.892387	-0.095816	0.078714
25	1	0	5.646850	0.673113	0.269333
26	1	0	5.415980	-1.018005	-0.191206
27	1	0	4.274236	0.215025	-0.765668
28	6	0	0.299205	3.403987	-1.145814

29	1	0	0.768374	4.368959	-1.362639
30	1	0	-0.160146	3.043822	-2.066763
31	6	0	1.386511	2.408390	-0.754672
32	8	0	1.722554	1.488855	-1.464893
33	8	0	1.885335	2.671156	0.448952
34	1	0	2.461744	1.913400	0.782445

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.359383	0.000000			
3	N	2.200418	1.387884	0.000000		
4	C	2.206504	2.221301	1.343141	0.000000	
5	N	1.386146	2.220034	2.178514	1.338466	0.000000
6	C	2.543121	3.644357	3.606854	2.508399	1.474748
7	H	1.075686	2.212189	3.258497	3.224004	2.156558
8	H	2.226846	1.093676	2.186728	3.259449	3.291364
9	H	3.321789	4.271987	3.979449	2.734200	2.091243
10	H	2.628749	3.924524	4.220239	3.319301	2.065049
11	Br	4.292753	3.359264	4.222465	5.357014	5.410374
12	H	3.249317	3.260790	2.154003	1.076357	2.153807
13	C	3.594522	2.522860	1.430660	2.450754	3.555103
14	C	4.296719	3.006639	2.427219	3.650759	4.589165
15	H	4.276335	3.403812	2.100909	2.617391	3.906754
16	H	5.361493	4.082440	3.392782	4.513203	5.563267
17	H	4.117637	2.779395	2.728120	4.045173	4.720193
18	C	4.250420	4.389951	5.235829	5.575300	5.050022
19	C	5.346344	5.705243	6.573747	6.757664	6.072007
20	O	4.071736	4.636491	5.585111	5.669874	4.829567
21	H	4.093685	4.156887	4.739896	5.008244	4.656045
22	H	4.224352	4.123707	5.105605	5.680273	5.236073
23	H	5.992083	6.310288	7.304939	7.585626	6.861043
24	C	6.231699	6.677987	7.344204	7.339873	6.688925
25	H	6.748015	7.356642	8.071478	7.957147	7.170907
26	H	7.079197	7.378458	8.002847	8.095542	7.559779
27	H	5.853938	6.322799	6.813093	6.686875	6.109982
28	C	3.440257	4.432598	4.319980	3.249900	2.499527
29	H	4.327351	5.427921	5.365206	4.244359	3.419139
30	H	3.953223	4.693908	4.270007	3.141131	2.845866
31	C	3.342154	4.254048	4.447389	3.755212	2.960548
32	O	4.006884	4.618329	4.688617	4.162055	3.691997
33	O	3.171995	4.266264	4.836340	4.309529	3.224982
34	H	3.465037	4.373426	5.099835	4.813776	3.825950

	6	7	8	9	10

6	C	0.000000				
7	H	2.824121	0.000000			
8	H	4.677256	2.759093	0.000000		
9	H	1.091373	3.711643	5.347269	0.000000	
10	H	1.088097	2.496483	4.854241	1.766722	0.000000
11	Br	6.691969	4.504044	2.369350	7.497645	6.821123
12	H	2.857736	4.224289	4.256149	2.744885	3.830036
13	C	4.918874	4.623961	2.857605	5.157522	5.612316
14	C	6.013927	5.209119	2.837556	6.368002	6.613628
15	H	5.107115	5.345237	3.887508	5.137908	5.918606
16	H	6.955460	6.288136	3.882687	7.229138	7.610814
17	H	6.169756	4.876304	2.242525	6.677144	6.633290
18	C	5.620070	3.999960	4.241875	6.681262	5.624790
19	C	6.362576	4.897361	5.609198	7.446892	6.228939
20	O	5.085886	3.514756	4.683778	6.177258	4.856744
21	H	5.243107	4.089832	4.162776	6.256087	5.450432
22	H	6.020358	3.991353	3.718609	7.054182	5.992719
23	H	7.190275	5.435615	6.073834	8.281441	6.948348
24	C	6.753101	5.862624	6.735197	7.795356	6.712796
25	H	7.045769	6.251776	7.468962	8.074554	6.881438
26	H	7.713093	6.775124	7.339195	8.745403	7.734942
27	H	6.108266	5.623127	6.522625	7.104297	6.204143
28	C	1.534703	3.653658	5.395051	2.175670	2.172076
29	H	2.144332	4.367308	6.384621	2.522910	2.447562
30	H	2.184125	4.395735	5.674748	2.489687	3.080385
31	C	2.553324	3.356059	5.007575	3.493980	2.859840
32	O	3.557079	4.154531	5.253208	4.420985	4.015256
33	O	2.839661	2.760034	4.890349	3.884780	2.633353
34	H	3.725438	2.969683	4.791991	4.800266	3.518283

		11	12	13	14	15
11	Br	0.000000				
12	H	6.273522	0.000000			
13	C	4.392937	2.786910	0.000000		
14	C	3.679075	4.087334	1.327063	0.000000	
15	H	5.465853	2.518280	1.083096	2.131696	0.000000
16	H	4.416743	4.769897	2.072389	1.082583	2.447357
17	H	2.611891	4.691421	2.132988	1.092361	3.114045
18	C	3.832082	6.405339	6.055956	6.042112	6.927911
19	C	5.145025	7.548821	7.470006	7.504010	8.306004
20	O	4.780211	6.517669	6.657299	6.859429	7.479141
21	H	3.986225	5.726743	5.477176	5.543837	6.261165
22	H	2.906544	6.591302	5.823529	5.623615	6.789830
23	H	5.340220	8.437949	8.184720	8.111839	9.082543
24	C	6.393071	7.980033	8.217852	8.353927	8.937219

25	H	7.253525	8.591804	9.047025	9.259514	9.748946
26	H	6.691187	8.710968	8.742652	8.755016	9.470323
27	H	6.446540	7.224258	7.673195	7.924256	8.298632
28	C	7.076867	3.405982	5.511328	6.544976	5.672707
29	H	8.056684	4.314204	6.570626	7.627813	6.684644
30	H	7.326863	2.992894	5.256534	6.337916	5.255512
31	C	6.263440	4.182204	5.627672	6.419074	6.019242
32	O	6.167485	4.500506	5.655324	6.319892	6.043192
33	O	6.064537	4.951451	6.139327	6.828132	6.679539
34	H	5.579863	5.542307	6.326642	6.834832	6.982267

		16	17	18	19	20
16	H	0.000000				
17	H	1.867255	0.000000			
18	C	6.942779	5.363886	0.000000		
19	C	8.402088	6.827099	1.465965	0.000000	
20	O	7.847513	6.245826	1.463934	1.453697	0.000000
21	H	6.401052	5.010856	1.085757	2.199053	2.142138
22	H	6.509710	4.805169	1.085477	2.240570	2.153368
23	H	9.003405	7.333846	2.185289	1.087713	2.107706
24	C	9.204478	7.798935	2.606947	1.503955	2.521655
25	H	10.149264	8.710794	3.445766	2.150974	2.930583
26	H	9.528459	8.168321	3.145395	2.134719	3.423734
27	H	8.756775	7.495974	2.740962	2.152600	2.719316
28	C	7.444363	6.685437	5.277061	5.837523	4.763530
29	H	8.525276	7.765020	5.982097	6.327067	5.272632
30	H	7.134265	6.620840	5.711070	6.366484	5.433215
31	C	7.360305	6.343737	3.884873	4.344790	3.380372
32	O	7.178558	6.240621	3.584709	4.052777	3.454921
33	O	7.846505	6.581350	3.529158	3.804042	2.596834
34	H	7.849988	6.447918	2.645374	2.803999	1.612899

		21	22	23	24	25
21	H	0.000000				
22	H	1.837536	0.000000			
23	H	3.112151	2.536198	0.000000		
24	C	2.811271	3.563153	2.206797	0.000000	
25	H	3.759853	4.368079	2.559993	1.093984	0.000000
26	H	3.298452	3.963087	2.551594	1.094276	1.767845
27	H	2.533111	3.805010	3.099736	1.091656	1.779084
28	C	4.749946	5.919431	6.782219	5.903000	6.169086
29	H	5.532597	6.697993	7.240771	6.246534	6.334204
30	H	5.006444	6.356221	7.373665	6.323644	6.693191
31	C	3.391492	4.651042	5.320754	4.388251	4.712777
32	O	2.846479	4.451237	5.117965	3.865454	4.367273
33	O	3.422245	4.229288	4.623845	4.103117	4.263031

34	H	2.716314	3.410024	3.617369	3.231131	3.456370
		26	27	28	29	30
26	H	0.000000				
27	H	1.775936	0.000000			
28	C	6.829837	5.110270	0.000000		
29	H	7.210539	5.468328	1.094670	0.000000	
30	H	7.149079	5.418365	1.090353	1.764633	0.000000
31	C	5.319239	3.626283	1.525267	2.143723	2.125442
32	O	4.641984	2.936433	2.407378	3.035773	2.514902
33	O	5.146374	3.635208	2.365613	2.722498	3.263693
34	H	4.274183	2.926818	3.258313	3.674052	4.033627
		31	32	33	34	
31	C	0.000000				
32	O	1.209498	0.000000			
33	O	1.329128	2.255468	0.000000		
34	H	1.940069	2.403574	1.008791	0.000000	

Stoichiometry C11H17BrN2O3
Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.164381	1.362673	1.269688
2	6	0	-1.384379	1.121948	0.720527
3	7	0	-1.591003	2.114267	-0.227541
4	6	0	-0.522926	2.928514	-0.243007
5	7	0	0.361112	2.492510	0.662460
6	6	0	1.718873	3.026244	0.878087
7	1	0	0.384293	0.810839	2.012343
8	1	0	-2.066022	0.278334	0.861260
9	1	0	1.657779	4.115643	0.902029
10	1	0	2.032526	2.679730	1.860688
11	35	0	-2.757530	-1.912016	0.279881
12	1	0	-0.398604	3.783115	-0.885459
13	6	0	-2.725911	2.263125	-1.085803
14	6	0	-3.628357	1.308110	-1.271905
15	1	0	-2.757987	3.230887	-1.571092
16	1	0	-4.455026	1.506933	-1.942034
17	1	0	-3.564566	0.321920	-0.806488

18	6	0	1.002599	-2.434017	-0.243381
19	6	0	2.200024	-3.252637	-0.031044
20	8	0	1.996397	-2.050712	0.760883
21	1	0	0.978446	-1.771337	-1.103114
22	1	0	0.035048	-2.709598	0.164248
23	1	0	2.082880	-4.148403	0.574763
24	6	0	3.364343	-3.253335	-0.983011
25	1	0	4.306289	-3.392431	-0.444317
26	1	0	3.257786	-4.082357	-1.689275
27	1	0	3.411766	-2.318960	-1.545511
28	6	0	2.705791	2.560451	-0.200962
29	1	0	3.708240	2.890862	0.089258
30	1	0	2.477327	3.004996	-1.170010
31	6	0	2.723429	1.046152	-0.382693
32	8	0	2.638303	0.512626	-1.464816
33	8	0	2.821857	0.411353	0.780889
34	1	0	2.645529	-0.576545	0.677804

Rotational constants (GHZ): 0.3259504 0.2598048 0.1607084

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 538 symmetry adapted cartesian basis functions of A symmetry.

There are 519 symmetry adapted basis functions of A symmetry.

519 basis functions, 823 primitive gaussians, 538 cartesian basis functions

78 alpha electrons 78 beta electrons

nuclear repulsion energy 1575.0558010356 Hartrees.

NAtoms= 34 NActive= 34 NUniq= 34 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 519 RedAO= T EigKep= 3.81D-06 NBF= 519

NBsUse= 519 1.00D-06 EigRej= -1.00D+00 NBFU= 519

Initial guess from the checkpoint file: "./coohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999597 0.000088 0.000874 0.028369 Ang= 3.25 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid=

0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3338.90370697 A.U. after 11 cycles

NFock= 11 Conv=0.70D-08 -V/T= 2.0019

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000460547	0.000074095	0.000156029
2	6	-0.000674375	0.000366856	0.000615147
3	7	0.000419086	0.000945501	-0.000310740
4	6	-0.000490889	-0.000478057	0.000259428
5	7	0.000348902	-0.000151532	-0.000182923
6	6	-0.000073486	-0.000215969	-0.000079082
7	1	-0.000112609	0.000116830	-0.000104736
8	1	0.000658085	-0.000523727	-0.000402960
9	1	-0.000018133	-0.000038630	0.000018126
10	1	0.000006240	0.000226143	0.000048976
11	35	-0.000020231	-0.000013926	0.000339587
12	1	0.000087308	0.000041378	-0.000067094
13	6	-0.000545344	-0.000853807	-0.000165244
14	6	0.000365430	0.000899319	-0.000204854
15	1	0.000040571	0.000088908	0.000050605
16	1	-0.000050915	-0.000167909	0.000109318
17	1	-0.000249382	-0.000238587	-0.000050567
18	6	-0.000038988	-0.000424486	0.000505920
19	6	0.000071868	-0.000046799	0.000350444
20	8	0.000303852	0.000030834	-0.000663332
21	1	0.000153142	0.000128435	-0.000238607
22	1	-0.000130743	-0.000122462	-0.000055194
23	1	-0.000080033	-0.000028359	-0.000055335
24	6	-0.000024066	-0.000044521	0.000381615
25	1	-0.000054045	0.000023037	-0.000059593
26	1	-0.000037631	0.000035095	-0.000214954
27	1	-0.000066486	-0.000058861	-0.000101475

28	6	0.000383217	-0.000477071	-0.000232051
29	1	-0.000205381	0.000177041	0.000288256
30	1	-0.000246914	-0.000005378	-0.000145967
31	6	0.000074134	-0.000589310	-0.001526107
32	8	-0.000336669	0.000595249	0.000712729
33	8	-0.000140648	0.000194107	0.001458442
34	1	0.000224585	0.000536566	-0.000433806

Cartesian Forces: Max 0.001526107 RMS 0.000382939

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.001284088 RMS 0.000252128
Search for a local minimum.
Step number 24 out of a maximum of 175
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 20 21 22 23 24
DE= -2.59D-05 DEPred=-5.93D-05 R= 4.38D-01
Trust test= 4.38D-01 RLast= 1.04D-01 DXMaxT set to 1.56D+00
ITU= 0 1 1 1 1 1 1 1 1 1 1 0 0 -1 1 1 1 0 1 0
ITU= -1 0 1 0

Eigenvalues ---	0.00154	0.00322	0.00416	0.00577	0.00694
Eigenvalues ---	0.00716	0.00968	0.01233	0.01513	0.01653
Eigenvalues ---	0.02005	0.02074	0.02259	0.02270	0.02369
Eigenvalues ---	0.02422	0.02674	0.03006	0.03115	0.03387
Eigenvalues ---	0.03505	0.03584	0.04005	0.04208	0.04817
Eigenvalues ---	0.04831	0.04968	0.05338	0.05576	0.05725
Eigenvalues ---	0.05990	0.06134	0.06527	0.09050	0.09484
Eigenvalues ---	0.09584	0.11779	0.12578	0.12687	0.13148
Eigenvalues ---	0.13560	0.15351	0.15537	0.15907	0.15985
Eigenvalues ---	0.16007	0.16012	0.16016	0.16038	0.16295
Eigenvalues ---	0.16914	0.17632	0.20284	0.21647	0.22132
Eigenvalues ---	0.23094	0.23837	0.24046	0.25390	0.25500
Eigenvalues ---	0.29006	0.29483	0.30173	0.31728	0.32616
Eigenvalues ---	0.33395	0.34498	0.34577	0.34635	0.34811
Eigenvalues ---	0.34884	0.34947	0.34987	0.35039	0.35148
Eigenvalues ---	0.35281	0.35720	0.35894	0.36577	0.36942
Eigenvalues ---	0.37007	0.37302	0.37732	0.38090	0.40301
Eigenvalues ---	0.42950	0.45031	0.49048	0.51466	0.51688
Eigenvalues ---	0.54145	0.55881	0.57558	0.62917	0.91190

Eigenvalues --- 1.39539

En-DIIS/RFO-DIIS IScMMF= 0 using points: 24 23 22 21 20

RFO step: Lambda=-2.15761724D-05.

DidBck=F Rises=F RFO-DIIS coefs: 1.34270 -0.13665 -0.08457 -0.13073 0.00926

Iteration 1 RMS(Cart)= 0.02813540 RMS(Int)= 0.00024356

Iteration 2 RMS(Cart)= 0.00038024 RMS(Int)= 0.00000659

Iteration 3 RMS(Cart)= 0.00000024 RMS(Int)= 0.00000659

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56886	0.00023	-0.00045	0.00026	-0.00019	2.56867
R2	2.61944	-0.00001	0.00009	0.00009	0.00019	2.61963
R3	2.03275	-0.00011	0.00019	-0.00024	-0.00006	2.03270
R4	2.62272	0.00060	-0.00085	0.00095	0.00010	2.62282
R5	2.06675	0.00045	-0.00014	0.00184	0.00170	2.06845
R6	2.53817	-0.00058	0.00034	-0.00075	-0.00042	2.53775
R7	2.70356	0.00056	0.00001	0.00083	0.00084	2.70439
R8	2.52934	-0.00002	-0.00007	-0.00015	-0.00021	2.52912
R9	2.03402	0.00003	0.00000	0.00009	0.00009	2.03411
R10	2.78687	-0.00020	0.00034	-0.00037	-0.00003	2.78684
R11	2.06240	-0.00002	0.00007	-0.00004	0.00003	2.06243
R12	2.05621	0.00015	-0.00020	0.00028	0.00008	2.05629
R13	2.90017	-0.00013	-0.00127	-0.00057	-0.00183	2.89834
R14	4.47742	0.00008	-0.00823	-0.00188	-0.01011	4.46731
R15	2.50779	-0.00053	0.00052	-0.00059	-0.00007	2.50771
R16	2.04675	-0.00003	-0.00009	-0.00007	-0.00016	2.04659
R17	2.04579	0.00011	-0.00044	0.00016	-0.00028	2.04551
R18	2.06426	-0.00014	-0.00006	-0.00056	-0.00063	2.06364
R19	2.77027	-0.00018	-0.00027	-0.00022	-0.00050	2.76977
R20	2.76643	0.00041	-0.00098	0.00084	-0.00013	2.76630
R21	2.05178	0.00014	0.00029	0.00044	0.00073	2.05252
R22	2.05125	0.00009	0.00069	0.00050	0.00119	2.05245
R23	2.74709	-0.00001	0.00058	0.00031	0.00089	2.74798
R24	2.05548	-0.00007	-0.00002	-0.00019	-0.00021	2.05527
R25	2.84206	-0.00014	-0.00020	-0.00045	-0.00065	2.84141
R26	3.04794	0.00039	-0.00465	-0.00128	-0.00594	3.04200
R27	2.06733	-0.00003	0.00000	-0.00009	-0.00008	2.06725
R28	2.06788	0.00001	-0.00002	0.00001	-0.00001	2.06787
R29	2.06293	0.00009	0.00005	0.00018	0.00023	2.06316
R30	2.06863	0.00002	0.00027	0.00000	0.00028	2.06891
R31	2.06047	0.00022	0.00011	0.00052	0.00063	2.06110
R32	2.88234	-0.00016	0.00045	-0.00020	0.00025	2.88259
R33	2.28562	-0.00097	0.00011	-0.00070	-0.00059	2.28503
R34	2.51169	0.00094	-0.00069	0.00133	0.00063	2.51232

R35	1.90634	0.00000	0.00030	0.00063	0.00093	1.90727
A1	1.88347	-0.00011	-0.00011	-0.00007	-0.00019	1.88328
A2	2.27291	0.00020	-0.00116	0.00036	-0.00082	2.27208
A3	2.12612	-0.00009	0.00112	-0.00033	0.00076	2.12688
A4	1.85767	-0.00021	0.00047	-0.00051	-0.00003	1.85764
A5	2.27046	-0.00030	-0.00034	-0.00256	-0.00290	2.26756
A6	2.14912	0.00051	0.00000	0.00259	0.00259	2.15171
A7	1.89961	0.00011	-0.00021	0.00037	0.00016	1.89977
A8	2.21717	0.00046	-0.00067	0.00155	0.00087	2.21804
A9	2.16619	-0.00057	0.00094	-0.00187	-0.00094	2.16525
A10	1.89648	0.00005	0.00001	-0.00011	-0.00010	1.89638
A11	2.18959	0.00006	-0.00052	0.00031	-0.00023	2.18936
A12	2.19707	-0.00011	0.00056	-0.00021	0.00035	2.19742
A13	1.88754	0.00017	-0.00016	0.00032	0.00016	1.88770
A14	2.18949	-0.00003	-0.00093	0.00004	-0.00091	2.18858
A15	2.20075	-0.00013	0.00061	-0.00037	0.00021	2.20096
A16	1.88907	-0.00010	0.00123	-0.00031	0.00092	1.88999
A17	1.85685	-0.00005	-0.00098	0.00081	-0.00017	1.85668
A18	1.95995	0.00028	-0.00204	0.00012	-0.00192	1.95804
A19	1.89042	-0.00001	0.00091	-0.00058	0.00033	1.89075
A20	1.93305	-0.00006	0.00007	-0.00038	-0.00031	1.93274
A21	1.93147	-0.00007	0.00089	0.00034	0.00122	1.93269
A22	2.61278	0.00128	0.01914	0.02313	0.04227	2.65506
A23	2.15161	0.00020	0.00083	0.00133	0.00217	2.15378
A24	1.96628	-0.00020	-0.00027	-0.00119	-0.00147	1.96481
A25	2.16523	0.00001	-0.00057	-0.00015	-0.00072	2.16451
A26	2.06453	-0.00002	-0.00077	-0.00050	-0.00127	2.06326
A27	2.15345	0.00034	-0.00017	0.00222	0.00204	2.15549
A28	2.06478	-0.00032	0.00092	-0.00164	-0.00072	2.06405
A29	2.06427	-0.00007	0.00103	-0.00151	-0.00047	2.06380
A30	2.13166	0.00000	-0.00258	0.00038	-0.00220	2.12945
A31	1.98067	-0.00024	0.00077	-0.00075	0.00001	1.98068
A32	1.99760	0.00026	-0.00094	0.00083	-0.00011	1.99749
A33	2.01804	0.00005	0.00111	0.00083	0.00193	2.01997
A34	2.04045	0.00000	-0.00107	-0.00040	-0.00147	2.03898
A35	2.14234	-0.00021	0.00161	-0.00058	0.00103	2.14337
A36	1.94164	0.00015	-0.00050	0.00024	-0.00026	1.94138
A37	2.04165	-0.00037	0.00001	-0.00069	-0.00068	2.04097
A38	2.02143	0.00019	-0.00006	0.00083	0.00077	2.02220
A39	2.06825	0.00023	0.00094	0.00066	0.00158	2.06983
A40	2.30669	0.00040	0.00367	0.00372	0.00739	2.31408
A41	1.93366	0.00003	-0.00020	0.00024	0.00004	1.93370
A42	1.91081	0.00024	-0.00049	0.00126	0.00077	1.91158
A43	1.93841	-0.00008	0.00061	-0.00057	0.00004	1.93845

A44	1.88108	-0.00004	-0.00016	0.00041	0.00025	1.88133
A45	1.90197	0.00000	-0.00018	-0.00018	-0.00036	1.90161
A46	1.89664	-0.00015	0.00041	-0.00116	-0.00076	1.89589
A47	1.88691	-0.00039	0.00178	-0.00208	-0.00030	1.88661
A48	1.94592	-0.00002	0.00017	-0.00032	-0.00015	1.94578
A49	1.97418	0.00003	0.00084	-0.00029	0.00054	1.97472
A50	1.88015	0.00011	-0.00141	0.00035	-0.00107	1.87908
A51	1.89723	0.00023	-0.00091	0.00086	-0.00006	1.89717
A52	1.87686	0.00005	-0.00060	0.00155	0.00095	1.87781
A53	2.14567	-0.00010	-0.00012	-0.00015	-0.00027	2.14540
A54	1.95058	0.00042	-0.00023	0.00132	0.00108	1.95167
A55	2.18681	-0.00033	0.00038	-0.00121	-0.00083	2.18598
A56	1.94476	-0.00109	0.00074	-0.00347	-0.00273	1.94204
A57	2.85830	-0.00058	-0.00922	-0.00785	-0.01708	2.84122
D1	0.00293	0.00004	-0.00063	0.00070	0.00007	0.00300
D2	3.02826	0.00004	0.00067	-0.00370	-0.00302	3.02524
D3	-3.09861	-0.00005	0.00497	0.00202	0.00697	-3.09164
D4	-0.07328	-0.00004	0.00627	-0.00237	0.00388	-0.06940
D5	-0.00307	-0.00002	0.00041	0.00072	0.00114	-0.00193
D6	-3.03856	-0.00012	0.00549	0.00082	0.00631	-3.03225
D7	3.10254	0.00006	-0.00465	-0.00045	-0.00512	3.09743
D8	0.06705	-0.00004	0.00043	-0.00035	0.00005	0.06710
D9	-0.00179	-0.00004	0.00063	-0.00188	-0.00125	-0.00303
D10	3.11790	0.00000	0.00325	0.00054	0.00379	3.12168
D11	-3.03720	0.00002	-0.00052	0.00254	0.00202	-3.03518
D12	0.08248	0.00006	0.00209	0.00496	0.00706	0.08954
D13	-1.48976	0.00019	-0.01035	-0.00697	-0.01732	-1.50709
D14	1.51857	0.00014	-0.00884	-0.01226	-0.02110	1.49747
D15	-0.00011	0.00003	-0.00039	0.00237	0.00198	0.00187
D16	3.13192	0.00002	0.00288	0.00165	0.00452	3.13644
D17	-3.12058	-0.00003	-0.00288	-0.00002	-0.00289	-3.12347
D18	0.01145	-0.00004	0.00039	-0.00073	-0.00035	0.01110
D19	-0.24166	-0.00003	0.01111	0.00584	0.01695	-0.22471
D20	2.91180	-0.00005	0.01219	0.00615	0.01833	2.93013
D21	2.87488	0.00003	0.01407	0.00864	0.02272	2.89760
D22	-0.25484	0.00001	0.01515	0.00895	0.02410	-0.23074
D23	0.00194	0.00000	-0.00001	-0.00191	-0.00192	0.00002
D24	3.03656	0.00010	-0.00523	-0.00198	-0.00723	3.02934
D25	-3.13004	0.00000	-0.00328	-0.00120	-0.00447	-3.13451
D26	-0.09541	0.00011	-0.00850	-0.00127	-0.00978	-0.10519
D27	-2.46092	0.00011	0.00055	-0.00326	-0.00271	-2.46363
D28	-0.43258	0.00002	0.00171	-0.00367	-0.00196	-0.43454
D29	1.68296	0.00007	0.00093	-0.00265	-0.00171	1.68125
D30	0.80554	-0.00003	0.00659	-0.00319	0.00339	0.80893

D31	2.83388	-0.00011	0.00775	-0.00360	0.00414	2.83802
D32	-1.33377	-0.00006	0.00697	-0.00258	0.00440	-1.32937
D33	-3.02258	-0.00002	0.00117	0.00480	0.00596	-3.01662
D34	1.19705	0.00010	0.00170	0.00584	0.00754	1.20459
D35	-0.92076	0.00003	0.00176	0.00427	0.00603	-0.91474
D36	1.14635	-0.00004	0.00095	0.00538	0.00633	1.15268
D37	-0.91720	0.00007	0.00148	0.00642	0.00791	-0.90930
D38	-3.03502	0.00000	0.00154	0.00485	0.00639	-3.02862
D39	-0.95043	0.00006	-0.00081	0.00613	0.00531	-0.94512
D40	-3.01398	0.00017	-0.00029	0.00717	0.00689	-3.00709
D41	1.15139	0.00010	-0.00022	0.00560	0.00537	1.15676
D42	-3.13904	-0.00006	0.00250	-0.00047	0.00203	-3.13701
D43	-0.02945	0.00003	0.00135	0.00238	0.00373	-0.02572
D44	-0.01067	-0.00004	0.00130	-0.00082	0.00048	-0.01019
D45	3.09892	0.00005	0.00015	0.00203	0.00218	3.10110
D46	-2.75329	-0.00002	0.00036	0.00043	0.00080	-2.75249
D47	-0.04608	-0.00002	0.00156	0.00027	0.00183	-0.04425
D48	-0.02008	-0.00004	-0.00057	-0.00025	-0.00082	-0.02090
D49	2.68712	-0.00004	0.00063	-0.00042	0.00021	2.68733
D50	0.25558	0.00033	0.00304	0.00553	0.00857	0.26415
D51	-2.11268	0.00023	0.00151	0.00417	0.00569	-2.10700
D52	2.57117	-0.00001	0.00122	0.00124	0.00246	2.57364
D53	0.19326	-0.00007	0.00187	0.00043	0.00230	0.19556
D54	2.55216	-0.00003	-0.00024	-0.00138	-0.00163	2.55054
D55	-1.65873	0.00008	-0.00087	0.00007	-0.00081	-1.65954
D56	0.43578	0.00000	-0.00030	-0.00092	-0.00122	0.43456
D57	1.32399	-0.00005	-0.00017	-0.00126	-0.00144	1.32256
D58	-2.88690	0.00007	-0.00080	0.00018	-0.00062	-2.88752
D59	-0.79239	-0.00001	-0.00022	-0.00081	-0.00103	-0.79342
D60	-1.01947	-0.00008	0.00070	-0.00182	-0.00112	-1.02059
D61	1.05283	0.00004	0.00007	-0.00037	-0.00030	1.05252
D62	-3.13585	-0.00004	0.00065	-0.00136	-0.00072	-3.13657
D63	1.51784	-0.00009	0.01788	-0.00551	0.01235	1.53020
D64	2.81698	0.00000	0.01969	-0.00430	0.01541	2.83238
D65	2.28266	0.00006	0.00372	-0.00041	0.00331	2.28597
D66	-0.84264	0.00027	0.00196	0.00243	0.00439	-0.83825
D67	-1.90458	-0.00025	0.00586	-0.00262	0.00324	-1.90135
D68	1.25330	-0.00004	0.00410	0.00021	0.00431	1.25761
D69	0.12634	0.00002	0.00338	-0.00093	0.00246	0.12879
D70	-2.99897	0.00023	0.00163	0.00190	0.00353	-2.99543
D71	2.93957	-0.00003	-0.00377	0.00026	-0.00350	2.93607
D72	-0.18527	0.00018	-0.00557	0.00316	-0.00240	-0.18768
D73	-1.96970	0.00008	-0.00542	-0.00642	-0.01184	-1.98154

Item	Value	Threshold	Converged?

Maximum Force	0.001284	0.000450	NO
RMS Force	0.000252	0.000300	YES
Maximum Displacement	0.098111	0.001800	NO
RMS Displacement	0.028211	0.001200	NO

Predicted change in Energy=-4.135728D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.887609	1.654038	1.554411
2	6	0	-1.555163	0.470408	1.586683
3	7	0	-2.391390	0.460862	0.478981
4	6	0	-2.230715	1.610747	-0.195843
5	7	0	-1.318702	2.356173	0.439582
6	6	0	-0.752682	3.631335	-0.038351
7	1	0	-0.120353	2.036043	2.204354
8	1	0	-1.424880	-0.391703	2.248412
9	1	0	-1.572811	4.259531	-0.390331
10	1	0	-0.301815	4.110858	0.828150
11	35	0	-0.393803	-2.435160	2.839723
12	1	0	-2.746872	1.880585	-1.101057
13	6	0	-3.276420	-0.588661	0.074902
14	6	0	-3.236875	-1.813852	0.583172
15	1	0	-3.968420	-0.274915	-0.696856
16	1	0	-3.944093	-2.544725	0.212588
17	1	0	-2.511481	-2.131290	1.335211
18	6	0	2.596445	-0.683501	1.215339
19	6	0	4.020381	-0.347889	1.305061
20	8	0	3.018824	0.664059	1.600787
21	1	0	2.140096	-0.729027	0.230766
22	1	0	2.084596	-1.235331	1.998363
23	1	0	4.542480	-0.660583	2.206458
24	6	0	4.881632	-0.120369	0.093731
25	1	0	5.640714	0.641341	0.294471
26	1	0	5.399800	-1.048478	-0.166157
27	1	0	4.280595	0.194697	-0.761525
28	6	0	0.287067	3.424247	-1.146671
29	1	0	0.753771	4.391336	-1.360101
30	1	0	-0.176515	3.069942	-2.068168
31	6	0	1.377943	2.427992	-0.766786
32	8	0	1.713845	1.515475	-1.485547

33	8	0	1.879665	2.680183	0.438266
34	1	0	2.455818	1.917346	0.761970

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.359282	0.000000			
3	N	2.200358	1.387938	0.000000		
4	C	2.206625	2.221293	1.342921	0.000000	
5	N	1.386247	2.219879	2.178168	1.338355	0.000000
6	C	2.542597	3.643648	3.606230	2.508418	1.474733
7	H	1.075656	2.211654	3.258177	3.224197	2.157068
8	H	2.226062	1.094575	2.189040	3.260914	3.291499
9	H	3.322668	4.273915	3.981917	2.736188	2.091913
10	H	2.628037	3.924172	4.220274	3.319604	2.064937
11	Br	4.314789	3.370637	4.236791	5.381288	5.438105
12	H	3.249568	3.260785	2.153718	1.076403	2.153932
13	C	3.595144	2.523853	1.431103	2.450346	3.554954
14	C	4.299839	3.008826	2.428997	3.653368	4.592289
15	H	4.275565	3.404977	2.100234	2.612729	3.903219
16	H	5.363971	4.084869	3.393436	4.513360	5.564441
17	H	4.124769	2.783274	2.732546	4.052875	4.728869
18	C	4.209238	4.324957	5.170134	5.527791	5.016950
19	C	5.306435	5.642306	6.515158	6.720503	6.047049
20	O	4.030190	4.578107	5.529028	5.628655	4.798518
21	H	4.074068	4.114863	4.691675	4.975995	4.639541
22	H	4.168879	4.040653	5.021956	5.615746	5.187594
23	H	5.938730	6.232537	7.233282	7.536987	6.824670
24	C	6.210173	6.634023	7.306373	7.325715	6.685582
25	H	6.725475	7.312981	8.036250	7.946040	7.169043
26	H	7.056590	7.331506	7.962220	8.080663	7.556245
27	H	5.848382	6.296521	6.791545	6.687478	6.121010
28	C	3.436474	4.426082	4.312601	3.245318	2.497093
29	H	4.322188	5.421106	5.359373	4.241973	3.417000
30	H	3.953925	4.692141	4.266256	3.139203	2.846554
31	C	3.334619	4.239583	4.430508	3.743832	2.955059
32	O	4.003512	4.606211	4.671673	4.151141	3.689069
33	O	3.155402	4.242643	4.813414	4.294300	3.214737
34	H	3.446128	4.343012	5.069206	4.793224	3.813594

		6	7	8	9	10
6	C	0.000000				
7	H	2.823919	0.000000			
8	H	4.676107	2.756390	0.000000		
9	H	1.091390	3.712940	5.349657	0.000000	

10	H	1.088139	2.496341	4.852987	1.766983	0.000000
11	Br	6.724170	4.524393	2.363997	7.526101	6.848740
12	H	2.858542	4.224750	4.257922	2.746441	3.830700
13	C	4.918379	4.624327	2.862017	5.159815	5.612587
14	C	6.017273	5.211779	2.842333	6.372033	6.616402
15	H	5.102292	5.344639	3.893307	5.137519	5.916472
16	H	6.956421	6.290593	3.889282	7.230795	7.611957
17	H	6.179636	4.882579	2.245173	6.685895	6.641095
18	C	5.604123	3.969264	4.162144	6.662915	5.615666
19	C	6.357759	4.861845	5.526545	7.442208	6.228101
20	O	5.071071	3.478659	4.613086	6.162393	4.848096
21	H	5.239594	4.080477	4.110200	6.249572	5.453832
22	H	5.990224	3.950459	3.618101	7.019686	5.970435
23	H	7.176244	5.386447	5.973563	8.267263	6.937837
24	C	6.770393	5.841634	6.669960	7.815221	6.731328
25	H	7.065858	6.227579	7.403222	8.099087	6.901885
26	H	7.731107	6.753198	7.268959	8.765987	7.753439
27	H	6.137373	5.617414	6.477348	7.136038	6.233929
28	C	1.533733	3.649995	5.386913	2.174603	2.172127
29	H	2.143368	4.360829	6.375371	2.524046	2.445684
30	H	2.183413	4.396197	5.672237	2.485941	3.080238
31	C	2.553079	3.350549	4.989782	3.493308	2.863118
32	O	3.557386	4.153389	5.237497	4.419440	4.018966
33	O	2.839209	2.744823	4.861393	3.885937	2.637745
34	H	3.724613	2.954863	4.754055	4.800362	3.524261

		11	12	13	14	15
11	Br	0.000000				
12	H	6.300185	0.000000			
13	C	4.400372	2.785763	0.000000		
14	C	3.682541	4.089694	1.327025	0.000000	
15	H	5.472837	2.510326	1.083011	2.131187	0.000000
16	H	4.417964	4.768896	2.071456	1.082435	2.445346
17	H	2.615426	4.699570	2.133827	1.092029	3.114178
18	C	3.827338	6.363274	5.983321	5.975362	6.849882
19	C	5.118291	7.520054	7.403686	7.438947	8.236136
20	O	4.773484	6.482526	6.597555	6.805098	7.415013
21	H	4.017237	5.697919	5.420576	5.496623	6.195214
22	H	2.879225	6.531341	5.732223	5.536742	6.695193
23	H	5.283658	8.398324	8.104561	8.030160	9.000745
24	C	6.381923	7.976553	8.171503	8.307683	8.886638
25	H	7.235922	8.592719	9.004243	9.215363	9.703490
26	H	6.672633	8.707566	8.691739	8.702842	9.415073
27	H	6.460273	7.234832	7.643411	7.896508	8.262625
28	C	7.119520	3.404374	5.504009	6.545855	5.656439

29	H	8.096696	4.315724	6.565215	7.629281	6.671797
30	H	7.378398	2.992759	5.252384	6.344041	5.238999
31	C	6.308426	4.174385	5.609967	6.411878	5.991176
32	O	6.225565	4.492119	5.636056	6.314559	6.009631
33	O	6.091173	4.941024	6.115766	6.811486	6.649903
34	H	5.601938	5.526319	6.293702	6.808859	6.942983

		16	17	18	19	20
16	H	0.000000				
17	H	1.866438	0.000000			
18	C	6.873740	5.310496	0.000000		
19	C	8.333813	6.771015	1.465701	0.000000	
20	O	7.791381	6.202321	1.463863	1.454169	0.000000
21	H	6.349366	4.982300	1.086144	2.198828	2.142384
22	H	6.422507	4.729317	1.086109	2.239528	2.153725
23	H	8.918937	7.258128	2.184010	1.087604	2.107853
24	C	9.153417	7.761649	2.607144	1.503609	2.521229
25	H	10.100805	8.673460	3.445400	2.150662	2.929383
26	H	9.470509	8.124959	3.146513	2.134973	3.424022
27	H	8.723464	7.479226	2.741457	2.152415	2.718987
28	C	7.441702	6.697433	5.271234	5.846163	4.757064
29	H	8.523627	7.776325	5.981831	6.343034	5.271614
30	H	7.135894	6.639870	5.706054	6.377631	5.427679
31	C	7.349228	6.350832	3.885222	4.356666	3.377774
32	O	7.168064	6.253715	3.592946	4.071821	3.457360
33	O	7.827308	6.575481	3.525902	3.808309	2.591118
34	H	7.821174	6.433826	2.643809	2.806082	1.609757

		21	22	23	24	25
21	H	0.000000				
22	H	1.839517	0.000000			
23	H	3.111188	2.532752	0.000000		
24	C	2.811629	3.562888	2.206914	0.000000	
25	H	3.759826	4.367050	2.560629	1.093940	0.000000
26	H	3.299283	3.963665	2.552404	1.094270	1.767967
27	H	2.533702	3.805834	3.099841	1.091776	1.778916
28	C	4.751919	5.902035	6.785120	5.934048	6.203466
29	H	5.538129	6.686536	7.252348	6.285567	6.378267
30	H	5.008388	6.339138	7.379578	6.358989	6.732037
31	C	3.397463	4.643850	5.328581	4.417066	4.742321
32	O	2.857483	4.454438	5.134911	3.899356	4.399191
33	O	3.425433	4.219852	4.623614	4.119903	4.280543
34	H	2.717563	3.406735	3.617517	3.237808	3.462703

		26	27	28	29	30
26	H	0.000000				
27	H	1.775546	0.000000			

28	C	6.863433	5.150398	0.000000		
29	H	7.252770	5.514396	1.094817	0.000000	
30	H	7.188485	5.462617	1.090687	1.764334	0.000000
31	C	5.349947	3.662380	1.525400	2.143906	2.126508
32	O	4.679841	2.976050	2.407061	3.034478	2.515805
33	O	5.163293	3.658088	2.366859	2.725767	3.265272
34	H	4.280720	2.935707	3.258395	3.677061	4.033279

		31	32	33	34
31	C	0.000000			
32	O	1.209188	0.000000		
33	O	1.329464	2.255016	0.000000	
34	H	1.938986	2.400700	1.009285	0.000000

Stoichiometry C11H17BrN2O3
Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.057142	1.362847	1.267071
2	6	0	-1.283270	1.194622	0.704970
3	7	0	-1.422696	2.200208	-0.241459
4	6	0	-0.310241	2.952458	-0.242324
5	7	0	0.538530	2.462544	0.669139
6	6	0	1.925048	2.911211	0.895193
7	1	0	0.452880	0.774227	2.008987
8	1	0	-2.011363	0.387893	0.835983
9	1	0	1.931714	4.002222	0.923162
10	1	0	2.210693	2.541902	1.878079
11	35	0	-2.898100	-1.735228	0.293265
12	1	0	-0.132446	3.803068	-0.877537
13	6	0	-2.539945	2.420599	-1.108199
14	6	0	-3.508283	1.532072	-1.292149
15	1	0	-2.498512	3.382865	-1.603417
16	1	0	-4.312479	1.784745	-1.971184
17	1	0	-3.522878	0.549273	-0.816313
18	6	0	0.818596	-2.458800	-0.264524
19	6	0	1.938154	-3.377516	-0.039067
20	8	0	1.835273	-2.156824	0.744473
21	1	0	0.858348	-1.802410	-1.128978

22	1	0	-0.172012	-2.648668	0.138313
23	1	0	1.737561	-4.255255	0.571030
24	6	0	3.105225	-3.486116	-0.980868
25	1	0	4.027226	-3.702574	-0.433358
26	1	0	2.933001	-4.307119	-1.683520
27	1	0	3.238383	-2.563229	-1.548779
28	6	0	2.885317	2.389663	-0.181008
29	1	0	3.905586	2.650629	0.118281
30	1	0	2.694098	2.857378	-1.147588
31	6	0	2.804074	0.878932	-0.375778
32	8	0	2.694462	0.361439	-1.463124
33	8	0	2.847117	0.228254	0.782773
34	1	0	2.602841	-0.744029	0.665938

Rotational constants (GHZ): 0.3274903 0.2585337 0.1607717

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 538 symmetry adapted cartesian basis functions of A symmetry.

There are 519 symmetry adapted basis functions of A symmetry.

519 basis functions, 823 primitive gaussians, 538 cartesian basis functions

78 alpha electrons 78 beta electrons

nuclear repulsion energy 1575.3799303983 Hartrees.

NAtoms= 34 NActive= 34 NUniq= 34 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 519 RedAO= T EigKep= 3.69D-06 NBF= 519

NBsUse= 519 1.00D-06 EigRej= -1.00D+00 NBFU= 519

Initial guess from the checkpoint file: "./coohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999414 -0.000027 0.000573 0.034220 Ang= -3.92 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3338.90369953 A.U. after 11 cycles
NFock= 11 Conv=0.64D-08 -V/T= 2.0019
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000489118	-0.000151328	-0.000159102
2	6	-0.000148494	0.000209146	0.000657872
3	7	-0.000177812	0.000552665	-0.000030130
4	6	-0.000409382	-0.000524136	0.000217775
5	7	0.000384273	0.000091498	0.000128322
6	6	-0.000346830	-0.000248658	0.000158106
7	1	-0.000248041	0.000245215	-0.000081997
8	1	0.000253258	-0.000698651	-0.000400714
9	1	-0.000055690	-0.000040418	0.000090810
10	1	-0.000010308	0.000283154	-0.000021816
11	35	-0.000168558	0.000160729	0.000222342
12	1	0.000167318	0.000017964	-0.000089146
13	6	-0.000261381	-0.000533202	-0.000241939
14	6	0.000296659	0.000990145	-0.000149606
15	1	-0.000014316	0.000056919	0.000018650
16	1	-0.000125974	-0.000257655	0.000097373
17	1	-0.000059580	-0.000238323	0.000043692
18	6	-0.000185186	-0.000730733	0.000506055
19	6	-0.000094291	0.000138376	0.000505045
20	8	0.000478347	-0.000217644	-0.000632974
21	1	0.000186895	0.000161173	-0.000019600
22	1	-0.000119528	-0.000024822	-0.000272825
23	1	0.000049822	-0.000002618	-0.000039065
24	6	0.000015867	-0.000040808	0.000083321
25	1	-0.000018064	0.000010600	-0.000066573
26	1	-0.000032634	0.000023201	-0.000142277
27	1	-0.000038306	-0.000026977	-0.000038248
28	6	0.000778304	-0.000143686	-0.000690190
29	1	-0.000161759	0.000098254	0.000286539
30	1	-0.000079460	-0.000034621	0.000048682
31	6	-0.000031302	-0.000261263	-0.001131627

32	8	-0.000207898	0.000204016	0.000370222
33	8	-0.000029870	0.000043626	0.000860776
34	1	-0.000075198	0.000888861	-0.000087752

Cartesian Forces: Max 0.001131627 RMS 0.000329224

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.001172586 RMS 0.000245412
Search for a local minimum.
Step number 25 out of a maximum of 175
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 20 21 22 23 24
25
DE= 7.43D-06 DEPred=-4.14D-05 R=-1.80D-01
Trust test=-1.80D-01 RLast= 8.03D-02 DXMaxT set to 7.82D-01
ITU= -1 0 1 1 1 1 1 1 1 1 1 1 0 0 -1 1 1 1 0 1
ITU= 0 -1 0 1 0

Eigenvalues ---	0.00145	0.00283	0.00417	0.00571	0.00692
Eigenvalues ---	0.00700	0.00963	0.01250	0.01594	0.01639
Eigenvalues ---	0.02004	0.02121	0.02266	0.02291	0.02406
Eigenvalues ---	0.02456	0.02614	0.02955	0.03119	0.03389
Eigenvalues ---	0.03460	0.03552	0.03792	0.04217	0.04821
Eigenvalues ---	0.04870	0.04973	0.05361	0.05635	0.05734
Eigenvalues ---	0.05981	0.06169	0.06976	0.08734	0.09354
Eigenvalues ---	0.09519	0.11779	0.12580	0.12741	0.13153
Eigenvalues ---	0.13593	0.15373	0.15504	0.15851	0.15984
Eigenvalues ---	0.16007	0.16013	0.16032	0.16041	0.16271
Eigenvalues ---	0.16961	0.17557	0.20390	0.21278	0.22364
Eigenvalues ---	0.23089	0.23922	0.24211	0.25306	0.25652
Eigenvalues ---	0.29017	0.29394	0.30750	0.31948	0.32891
Eigenvalues ---	0.33557	0.34499	0.34549	0.34621	0.34799
Eigenvalues ---	0.34885	0.34948	0.34988	0.35131	0.35266
Eigenvalues ---	0.35320	0.35714	0.36093	0.36586	0.36933
Eigenvalues ---	0.37059	0.37348	0.37727	0.38551	0.39923
Eigenvalues ---	0.42254	0.45019	0.49032	0.51169	0.51585
Eigenvalues ---	0.53404	0.55685	0.56830	0.61900	0.89992
Eigenvalues ---	1.48322				

En-DIIS/RFO-DIIS IScMMF= 0 using points: 25 24 23 22 21
RFO step: Lambda=-1.70406621D-05.

DidBck=F Rises=F RFO-DIIS coefs: 1.35646 -0.10466 -0.45614 0.24649 -0.04215

Iteration 1 RMS(Cart)= 0.02481191 RMS(Int)= 0.00023547

Iteration 2 RMS(Cart)= 0.00029650 RMS(Int)= 0.00000475

Iteration 3 RMS(Cart)= 0.00000007 RMS(Int)= 0.00000475

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56867	0.00045	-0.00017	0.00045	0.00027	2.56894
R2	2.61963	0.00006	0.00021	0.00004	0.00025	2.61988
R3	2.03270	-0.00014	0.00002	-0.00025	-0.00023	2.03247
R4	2.62282	0.00037	-0.00010	0.00009	-0.00001	2.62281
R5	2.06845	0.00033	0.00097	0.00085	0.00182	2.07027
R6	2.53775	-0.00048	-0.00031	-0.00071	-0.00102	2.53673
R7	2.70439	0.00017	0.00063	0.00051	0.00114	2.70553
R8	2.52912	0.00016	-0.00004	0.00012	0.00008	2.52921
R9	2.03411	0.00000	0.00005	0.00003	0.00008	2.03418
R10	2.78684	0.00016	-0.00006	0.00039	0.00032	2.78717
R11	2.06243	-0.00001	0.00000	0.00006	0.00006	2.06249
R12	2.05629	0.00011	0.00005	0.00011	0.00016	2.05644
R13	2.89834	0.00058	-0.00082	0.00036	-0.00046	2.89787
R14	4.46731	-0.00015	-0.01908	-0.01119	-0.03027	4.43704
R15	2.50771	-0.00046	-0.00008	-0.00016	-0.00024	2.50748
R16	2.04659	0.00002	-0.00009	-0.00010	-0.00019	2.04640
R17	2.04551	0.00023	-0.00015	0.00018	0.00003	2.04553
R18	2.06364	0.00005	-0.00015	-0.00003	-0.00019	2.06345
R19	2.76977	-0.00006	-0.00047	0.00018	-0.00029	2.76949
R20	2.76630	0.00048	0.00012	0.00037	0.00048	2.76678
R21	2.05252	-0.00007	0.00035	0.00002	0.00037	2.05288
R22	2.05245	-0.00013	0.00058	0.00020	0.00079	2.05323
R23	2.74798	-0.00011	0.00070	-0.00002	0.00068	2.74866
R24	2.05527	-0.00001	-0.00012	-0.00001	-0.00013	2.05514
R25	2.84141	0.00008	-0.00036	0.00023	-0.00014	2.84127
R26	3.04200	0.00057	-0.00433	0.00596	0.00163	3.04363
R27	2.06725	-0.00001	-0.00003	-0.00002	-0.00005	2.06719
R28	2.06787	0.00000	-0.00001	0.00000	-0.00002	2.06785
R29	2.06316	0.00004	0.00019	-0.00005	0.00014	2.06329
R30	2.06891	-0.00004	0.00016	0.00020	0.00036	2.06926
R31	2.06110	0.00000	0.00030	0.00006	0.00036	2.06146
R32	2.88259	-0.00021	0.00001	-0.00045	-0.00044	2.88215
R33	2.28503	-0.00044	-0.00024	-0.00062	-0.00085	2.28418
R34	2.51232	0.00070	0.00025	0.00103	0.00129	2.51361
R35	1.90727	-0.00011	0.00075	-0.00034	0.00042	1.90769
A1	1.88328	-0.00002	-0.00010	-0.00022	-0.00030	1.88297
A2	2.27208	0.00025	-0.00045	0.00067	0.00022	2.27230

A3	2.12688	-0.00022	0.00043	-0.00048	-0.00005	2.12683
A4	1.85764	-0.00020	-0.00001	-0.00006	-0.00007	1.85757
A5	2.26756	0.00029	-0.00099	0.00058	-0.00042	2.26714
A6	2.15171	-0.00008	0.00057	-0.00029	0.00028	2.15198
A7	1.89977	0.00009	0.00017	0.00011	0.00028	1.90005
A8	2.21804	0.00018	-0.00015	-0.00016	-0.00032	2.21772
A9	2.16525	-0.00027	0.00003	0.00006	0.00009	2.16534
A10	1.89638	0.00019	-0.00007	0.00018	0.00011	1.89650
A11	2.18936	0.00001	-0.00007	0.00019	0.00011	2.18947
A12	2.19742	-0.00020	0.00016	-0.00036	-0.00021	2.19721
A13	1.88770	-0.00006	-0.00001	0.00000	-0.00002	1.88768
A14	2.18858	0.00046	-0.00070	0.00135	0.00063	2.18921
A15	2.20096	-0.00038	0.00027	-0.00063	-0.00038	2.20058
A16	1.88999	-0.00052	0.00057	-0.00081	-0.00025	1.88974
A17	1.85668	-0.00016	-0.00008	0.00026	0.00019	1.85687
A18	1.95804	0.00112	-0.00120	0.00198	0.00078	1.95882
A19	1.89075	0.00007	0.00023	-0.00090	-0.00067	1.89008
A20	1.93274	-0.00024	-0.00008	-0.00058	-0.00066	1.93208
A21	1.93269	-0.00029	0.00060	-0.00002	0.00058	1.93327
A22	2.65506	0.00117	0.03015	0.01493	0.04507	2.70013
A23	2.15378	-0.00020	0.00062	-0.00029	0.00033	2.15411
A24	1.96481	0.00005	-0.00055	-0.00007	-0.00061	1.96420
A25	2.16451	0.00015	-0.00008	0.00037	0.00028	2.16480
A26	2.06326	0.00008	-0.00067	0.00020	-0.00048	2.06278
A27	2.15549	0.00021	0.00109	0.00098	0.00206	2.15755
A28	2.06405	-0.00029	-0.00035	-0.00116	-0.00151	2.06254
A29	2.06380	-0.00013	-0.00019	-0.00130	-0.00149	2.06230
A30	2.12945	0.00017	-0.00112	0.00009	-0.00103	2.12842
A31	1.98068	-0.00026	-0.00013	-0.00036	-0.00049	1.98019
A32	1.99749	0.00033	-0.00003	0.00107	0.00104	1.99852
A33	2.01997	-0.00002	0.00096	0.00066	0.00162	2.02159
A34	2.03898	0.00006	-0.00088	-0.00023	-0.00110	2.03788
A35	2.14337	-0.00023	0.00072	-0.00047	0.00024	2.14361
A36	1.94138	0.00017	-0.00030	0.00044	0.00014	1.94152
A37	2.04097	-0.00037	-0.00052	-0.00022	-0.00073	2.04024
A38	2.02220	0.00014	0.00047	0.00040	0.00087	2.02306
A39	2.06983	0.00019	-0.00114	0.00417	0.00306	2.07289
A40	2.31408	0.00021	-0.00344	0.00810	0.00466	2.31874
A41	1.93370	0.00007	0.00007	0.00042	0.00048	1.93418
A42	1.91158	0.00016	0.00027	0.00056	0.00083	1.91241
A43	1.93845	-0.00008	0.00010	-0.00034	-0.00024	1.93821
A44	1.88133	-0.00004	0.00009	0.00012	0.00021	1.88154
A45	1.90161	-0.00002	-0.00014	-0.00037	-0.00051	1.90109
A46	1.89589	-0.00009	-0.00040	-0.00039	-0.00079	1.89510

A47	1.88661	-0.00043	-0.00036	-0.00211	-0.00246	1.88415
A48	1.94578	-0.00014	-0.00011	0.00009	-0.00002	1.94575
A49	1.97472	0.00054	-0.00038	0.00118	0.00080	1.97552
A50	1.87908	0.00019	-0.00018	0.00037	0.00019	1.87928
A51	1.89717	-0.00004	0.00047	0.00010	0.00057	1.89774
A52	1.87781	-0.00012	0.00057	0.00036	0.00094	1.87874
A53	2.14540	-0.00001	0.00022	0.00019	0.00041	2.14581
A54	1.95167	0.00015	0.00009	-0.00084	-0.00075	1.95092
A55	2.18598	-0.00014	-0.00033	0.00062	0.00030	2.18628
A56	1.94204	-0.00067	-0.00113	0.00041	-0.00072	1.94132
A57	2.84122	0.00035	-0.00660	-0.00230	-0.00890	2.83232
D1	0.00300	0.00010	0.00125	-0.00341	-0.00216	0.00084
D2	3.02524	0.00017	-0.00291	-0.00125	-0.00414	3.02110
D3	-3.09164	-0.00018	0.00363	-0.00255	0.00108	-3.09056
D4	-0.06940	-0.00011	-0.00053	-0.00039	-0.00091	-0.07031
D5	-0.00193	-0.00015	-0.00121	0.00407	0.00287	0.00094
D6	-3.03225	-0.00030	0.00324	-0.00250	0.00073	-3.03152
D7	3.09743	0.00012	-0.00338	0.00334	-0.00003	3.09739
D8	0.06710	-0.00004	0.00107	-0.00323	-0.00217	0.06494
D9	-0.00303	-0.00001	-0.00087	0.00158	0.00070	-0.00233
D10	3.12168	0.00001	0.00154	0.00287	0.00441	3.12610
D11	-3.03518	-0.00011	0.00305	-0.00048	0.00258	-3.03259
D12	0.08954	-0.00009	0.00547	0.00082	0.00629	0.09584
D13	-1.50709	0.00003	-0.00423	-0.00590	-0.01013	-1.51722
D14	1.49747	0.00011	-0.00906	-0.00339	-0.01244	1.48502
D15	0.00187	-0.00008	0.00013	0.00095	0.00108	0.00296
D16	3.13644	0.00002	0.00190	0.00105	0.00294	3.13939
D17	-3.12347	-0.00010	-0.00219	-0.00029	-0.00248	-3.12595
D18	0.01110	0.00000	-0.00043	-0.00020	-0.00063	0.01047
D19	-0.22471	0.00001	0.00872	0.00802	0.01674	-0.20797
D20	2.93013	-0.00005	0.00901	0.00726	0.01627	2.94640
D21	2.89760	0.00004	0.01148	0.00950	0.02098	2.91858
D22	-0.23074	-0.00002	0.01177	0.00874	0.02051	-0.21023
D23	0.00002	0.00014	0.00065	-0.00308	-0.00242	-0.00241
D24	3.02934	0.00036	-0.00390	0.00371	-0.00019	3.02915
D25	-3.13451	0.00004	-0.00112	-0.00318	-0.00430	-3.13881
D26	-0.10519	0.00026	-0.00567	0.00361	-0.00206	-0.10725
D27	-2.46363	0.00023	-0.00405	0.00336	-0.00068	-2.46431
D28	-0.43454	-0.00003	-0.00354	0.00205	-0.00149	-0.43603
D29	1.68125	0.00017	-0.00355	0.00336	-0.00019	1.68106
D30	0.80893	0.00002	0.00121	-0.00445	-0.00323	0.80570
D31	2.83802	-0.00024	0.00172	-0.00576	-0.00404	2.83398
D32	-1.32937	-0.00005	0.00171	-0.00444	-0.00274	-1.33211
D33	-3.01662	-0.00019	0.00614	0.00584	0.01199	-3.00463

D34	1.20459	-0.00007	0.00665	0.00665	0.01330	1.21789
D35	-0.91474	-0.00020	0.00625	0.00526	0.01151	-0.90322
D36	1.15268	-0.00013	0.00630	0.00593	0.01224	1.16491
D37	-0.90930	0.00000	0.00681	0.00674	0.01354	-0.89575
D38	-3.02862	-0.00014	0.00641	0.00535	0.01176	-3.01687
D39	-0.94512	0.00014	0.00567	0.00746	0.01313	-0.93199
D40	-3.00709	0.00027	0.00617	0.00827	0.01444	-2.99265
D41	1.15676	0.00013	0.00578	0.00688	0.01265	1.16942
D42	-3.13701	-0.00010	0.00068	0.00016	0.00084	-3.13617
D43	-0.02572	-0.00003	0.00301	0.00060	0.00361	-0.02212
D44	-0.01019	-0.00004	0.00035	0.00101	0.00136	-0.00883
D45	3.10110	0.00003	0.00268	0.00144	0.00413	3.10523
D46	-2.75249	-0.00003	0.00016	0.00084	0.00099	-2.75150
D47	-0.04425	-0.00006	0.00105	0.00015	0.00119	-0.04306
D48	-0.02090	0.00001	-0.00062	-0.00055	-0.00117	-0.02207
D49	2.68733	-0.00002	0.00027	-0.00124	-0.00097	2.68636
D50	0.26415	0.00023	-0.00372	0.00966	0.00594	0.27009
D51	-2.10700	0.00018	-0.00503	0.00786	0.00283	-2.10416
D52	2.57364	-0.00014	0.00143	-0.00239	-0.00095	2.57269
D53	0.19556	-0.00015	0.00160	-0.00328	-0.00167	0.19390
D54	2.55054	0.00000	-0.00074	0.00068	-0.00007	2.55047
D55	-1.65954	0.00008	-0.00042	0.00143	0.00101	-1.65853
D56	0.43456	0.00003	-0.00068	0.00110	0.00041	0.43497
D57	1.32256	-0.00004	-0.00071	0.00079	0.00008	1.32263
D58	-2.88752	0.00005	-0.00039	0.00154	0.00115	-2.88636
D59	-0.79342	-0.00001	-0.00065	0.00120	0.00056	-0.79286
D60	-1.02059	-0.00005	-0.00017	-0.00015	-0.00032	-1.02090
D61	1.05252	0.00003	0.00015	0.00061	0.00076	1.05328
D62	-3.13657	-0.00002	-0.00011	0.00027	0.00017	-3.13640
D63	1.53020	-0.00004	0.01165	-0.01720	-0.00554	1.52466
D64	2.83238	0.00003	0.00923	-0.01133	-0.00211	2.83027
D65	2.28597	0.00012	-0.00444	0.00032	-0.00411	2.28186
D66	-0.83825	0.00011	-0.00381	0.00186	-0.00196	-0.84021
D67	-1.90135	-0.00012	-0.00481	-0.00151	-0.00632	-1.90767
D68	1.25761	-0.00012	-0.00419	0.00002	-0.00416	1.25345
D69	0.12879	0.00002	-0.00446	-0.00084	-0.00530	0.12350
D70	-2.99543	0.00002	-0.00383	0.00070	-0.00314	-2.99857
D71	2.93607	0.00035	-0.00215	0.00047	-0.00167	2.93439
D72	-0.18768	0.00034	-0.00151	0.00206	0.00054	-0.18713
D73	-1.98154	0.00014	-0.00771	-0.00456	-0.01226	-1.99381

Item	Value	Threshold	Converged?
Maximum Force	0.001173	0.000450	NO
RMS Force	0.000245	0.000300	YES
Maximum Displacement	0.100622	0.001800	NO

RMS Displacement 0.024754 0.001200 NO
Predicted change in Energy=-3.081092D-05
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.875062	1.655947	1.552242
2	6	0	-1.530358	0.465193	1.579305
3	7	0	-2.366469	0.451944	0.471562
4	6	0	-2.217377	1.605483	-0.198589
5	7	0	-1.311713	2.357056	0.438764
6	6	0	-0.758386	3.639359	-0.035444
7	1	0	-0.111228	2.042828	2.203134
8	1	0	-1.389521	-0.399605	2.236947
9	1	0	-1.584747	4.259455	-0.387312
10	1	0	-0.314665	4.122244	0.832980
11	35	0	-0.411025	-2.430660	2.892970
12	1	0	-2.738164	1.874825	-1.101344
13	6	0	-3.244548	-0.603553	0.065745
14	6	0	-3.208852	-1.824175	0.584849
15	1	0	-3.927739	-0.297439	-0.716709
16	1	0	-3.909687	-2.559518	0.210956
17	1	0	-2.495216	-2.134796	1.350715
18	6	0	2.571084	-0.676148	1.220764
19	6	0	3.998641	-0.355181	1.303818
20	8	0	3.008734	0.670061	1.594698
21	1	0	2.112774	-0.724191	0.237009
22	1	0	2.056816	-1.218234	2.009566
23	1	0	4.519125	-0.667623	2.206152
24	6	0	4.858684	-0.144980	0.088598
25	1	0	5.626539	0.609882	0.281536
26	1	0	5.365778	-1.080130	-0.167837
27	1	0	4.258345	0.171170	-0.766840
28	6	0	0.284764	3.447036	-1.142889
29	1	0	0.748345	4.418808	-1.342368
30	1	0	-0.175698	3.103162	-2.070109
31	6	0	1.377607	2.449929	-0.771929
32	8	0	1.715092	1.544259	-1.497814
33	8	0	1.877309	2.692367	0.436710
34	1	0	2.453893	1.926937	0.754152

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.359426	0.000000			
3	N	2.200406	1.387930	0.000000		
4	C	2.206755	2.221073	1.342380	0.000000	
5	N	1.386381	2.219862	2.177852	1.338398	0.000000
6	C	2.543283	3.643993	3.605912	2.508370	1.474905
7	H	1.075537	2.211792	3.258123	3.224191	2.157059
8	H	2.226832	1.095538	2.190011	3.261528	3.292218
9	H	3.323218	4.273988	3.980691	2.734850	2.091906
10	H	2.629450	3.925422	4.220382	3.319418	2.065284
11	Br	4.325880	3.371140	4.242214	5.395470	5.454961
12	H	3.249704	3.260634	2.153319	1.076443	2.153890
13	C	3.595758	2.524189	1.431707	2.450468	3.555306
14	C	4.300427	3.007904	2.429642	3.655045	4.593819
15	H	4.275826	3.405983	2.100268	2.610535	3.901929
16	H	5.364526	4.084417	3.393868	4.514296	5.565435
17	H	4.127377	2.782650	2.735088	4.057983	4.733822
18	C	4.174262	4.272357	5.119895	5.490880	4.988784
19	C	5.278194	5.596314	6.469832	6.688820	6.025314
20	O	4.007199	4.543739	5.495618	5.603849	4.780000
21	H	4.040057	4.060641	4.637018	4.936329	4.611064
22	H	4.131098	3.985833	4.971961	5.578356	5.157238
23	H	5.909639	6.186474	7.188438	7.505349	6.802281
24	C	6.185584	6.588959	7.259878	7.295015	6.667579
25	H	6.706696	7.275048	7.996827	7.921412	7.156583
26	H	7.028007	7.279919	7.908460	8.044732	7.534661
27	H	5.825339	6.252994	6.745416	6.656962	6.103862
28	C	3.437576	4.426782	4.313475	3.247111	2.497683
29	H	4.318289	5.418462	5.359890	4.244824	3.415712
30	H	3.962950	4.702362	4.276509	3.148664	2.853358
31	C	3.332672	4.233644	4.422253	3.737074	2.950737
32	O	4.003026	4.600652	4.661624	4.141986	3.684091
33	O	3.145493	4.228241	4.798996	4.283851	3.206602
34	H	3.433996	4.323405	5.048896	4.778265	3.803191

		6	7	8	9	10
6	C	0.000000				
7	H	2.824705	0.000000			
8	H	4.677106	2.756928	0.000000		
9	H	1.091422	3.714176	5.350859	0.000000	
10	H	1.088222	2.498536	4.855261	1.766649	0.000000
11	Br	6.748437	4.536281	2.347979	7.542912	6.869746
12	H	2.858188	4.224759	4.258645	2.743478	3.829601

13	C	4.918693	4.624874	2.863013	5.158396	5.613023
14	C	6.019946	5.212277	2.840562	6.371293	6.617990
15	H	5.099734	5.344912	3.895777	5.134530	5.915187
16	H	6.958267	6.291156	3.888586	7.229223	7.612952
17	H	6.186992	4.884931	2.240281	6.688508	6.646307
18	C	5.593481	3.943688	4.098230	6.649588	5.612708
19	C	6.354469	4.842545	5.468545	7.438348	6.234872
20	O	5.066092	3.462491	4.571795	6.157287	4.852088
21	H	5.230522	4.058107	4.046131	6.236840	5.453034
22	H	5.975252	3.920766	3.549520	7.000792	5.960619
23	H	7.171260	5.365326	5.914801	8.261926	6.942187
24	C	6.774075	5.827332	6.612133	7.819422	6.747359
25	H	7.074283	6.218348	7.353080	8.109833	6.923777
26	H	7.732819	6.735872	7.202789	8.767505	7.767481
27	H	6.142546	5.605089	6.422376	7.141418	6.251626
28	C	1.533487	3.650271	5.387316	2.173935	2.172390
29	H	2.141455	4.353703	6.371740	2.526033	2.439278
30	H	2.183321	4.403302	5.682735	2.480774	3.079896
31	C	2.553355	3.351621	4.982989	3.492543	2.869870
32	O	3.556131	4.157047	5.231221	4.415252	4.024739
33	O	2.840178	2.737962	4.844927	3.888523	2.646947
34	H	3.724861	2.948360	4.731100	4.801479	3.534190

		11	12	13	14	15
11	Br	0.000000				
12	H	6.317224	0.000000			
13	C	4.400042	2.785836	0.000000		
14	C	3.677374	4.092358	1.326899	0.000000	
15	H	5.472448	2.506344	1.082908	2.131144	0.000000
16	H	4.410265	4.770534	2.071061	1.082449	2.444973
17	H	2.609586	4.706238	2.134795	1.091930	3.114842
18	C	3.842859	6.331490	5.929664	5.927058	6.792048
19	C	5.126224	7.492815	7.352435	7.390725	8.180058
20	O	4.795283	6.461186	6.562265	6.774908	7.375182
21	H	4.041748	5.663716	5.361417	5.445242	6.130212
22	H	2.888013	6.498970	5.679853	5.488556	6.640432
23	H	5.280758	8.370891	8.053575	7.980468	8.945930
24	C	6.392079	7.950326	8.116230	8.255368	8.824568
25	H	7.246839	8.572088	8.956293	9.169557	9.649039
26	H	6.675622	8.676237	8.626669	8.639701	9.342555
27	H	6.478175	7.208708	7.588597	7.846496	8.199639
28	C	7.163769	3.407590	5.506733	6.555616	5.652247
29	H	8.136181	4.322694	6.568872	7.638613	6.670846
30	H	7.437118	3.002258	5.264927	6.366120	5.241526
31	C	6.360098	4.168793	5.602658	6.414392	5.974761

32	O	6.292801	4.483074	5.626353	6.318945	5.986945
33	O	6.124957	4.933211	6.101977	6.803685	6.630829
34	H	5.636573	5.513895	6.272919	6.794570	6.916394

		16	17	18	19	20
16	H	0.000000				
17	H	1.865520	0.000000			
18	C	6.824016	5.273703	0.000000		
19	C	8.282215	6.733454	1.465549	0.000000	
20	O	7.759476	6.182250	1.464118	1.454527	0.000000
21	H	6.295962	4.946081	1.086338	2.197895	2.142429
22	H	6.374417	4.689901	1.086525	2.239112	2.154976
23	H	8.865943	7.217018	2.183100	1.087534	2.108212
24	C	9.095565	7.722186	2.607116	1.503536	2.520902
25	H	10.049362	8.639405	3.445552	2.150921	2.929321
26	H	9.400337	8.075491	3.146702	2.135506	3.424231
27	H	8.667727	7.443931	2.741417	2.152235	2.717955
28	C	7.450168	6.715891	5.273970	5.851163	4.756678
29	H	8.532708	7.792503	5.987537	6.352771	5.271510
30	H	7.156248	6.672211	5.714704	6.385031	5.430598
31	C	7.349565	6.365853	3.894556	4.364308	3.380743
32	O	7.169311	6.275050	3.612976	4.083089	3.464298
33	O	7.818093	6.576920	3.527458	3.813067	2.590517
34	H	7.805030	6.430182	2.647170	2.810061	1.610621

		21	22	23	24	25
21	H	0.000000				
22	H	1.840969	0.000000			
23	H	3.109863	2.530768	0.000000		
24	C	2.810255	3.562647	2.207372	0.000000	
25	H	3.758760	4.367038	2.561744	1.093912	0.000000
26	H	3.297367	3.963507	2.553979	1.094262	1.768070
27	H	2.532362	3.805996	3.100042	1.091848	1.778627
28	C	4.758664	5.902786	6.787953	5.944736	6.213935
29	H	5.550364	6.687585	7.258275	6.306403	6.398575
30	H	5.020810	6.348411	7.385567	6.368316	6.738889
31	C	3.410787	4.653328	5.334532	4.426281	4.748577
32	O	2.883337	4.477707	5.145327	3.905433	4.397563
33	O	3.430481	4.218874	4.625976	4.130414	4.291567
34	H	2.722550	3.409667	3.620114	3.243274	3.467518

		26	27	28	29	30
26	H	0.000000				
27	H	1.775096	0.000000			
28	C	6.874785	5.163531	0.000000		
29	H	7.275887	5.540195	1.095007	0.000000	
30	H	7.199065	5.473191	1.090876	1.764762	0.000000

31	C	5.360201	3.673067	1.525169	2.144261	2.127144
32	O	4.688685	2.981247	2.406735	3.036741	2.516503
33	O	5.173648	3.670736	2.366613	2.724018	3.266149
34	H	4.286210	2.941459	3.258004	3.676100	4.034192

		31	32	33	34
31	C	0.000000			
32	O	1.208737	0.000000		
33	O	1.330145	2.255405	0.000000	
34	H	1.939288	2.400755	1.009506	0.000000

Stoichiometry C11H17BrN2O3
Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.019944	1.351695	1.260960
2	6	0	-1.205354	1.237746	0.683292
3	7	0	-1.289401	2.250445	-0.262079
4	6	0	-0.145815	2.953296	-0.248069
5	7	0	0.670712	2.424345	0.671064
6	6	0	2.072987	2.811990	0.913340
7	1	0	0.495325	0.739729	2.006809
8	1	0	-1.968872	0.461167	0.802322
9	1	0	2.126849	3.901721	0.941425
10	1	0	2.330649	2.431719	1.899865
11	35	0	-3.011355	-1.584188	0.309620
12	1	0	0.075390	3.798258	-0.877224
13	6	0	-2.387899	2.523614	-1.138700
14	6	0	-3.403653	1.689216	-1.319492
15	1	0	-2.289224	3.476657	-1.643341
16	1	0	-4.187603	1.979432	-2.007164
17	1	0	-3.480095	0.715217	-0.831851
18	6	0	0.681635	-2.474835	-0.270150
19	6	0	1.745488	-3.459670	-0.055320
20	8	0	1.720007	-2.238630	0.734655
21	1	0	0.757083	-1.818486	-1.132498
22	1	0	-0.316892	-2.609152	0.136593
23	1	0	1.494891	-4.326761	0.551381
24	6	0	2.899590	-3.632467	-1.003375

25	1	0	3.809818	-3.906439	-0.462018
26	1	0	2.675851	-4.437056	-1.710472
27	1	0	3.085004	-2.715748	-1.566741
28	6	0	3.022651	2.249599	-0.151291
29	1	0	4.049159	2.456453	0.168915
30	1	0	2.872745	2.734783	-1.116763
31	6	0	2.868185	0.746727	-0.360225
32	8	0	2.746363	0.244007	-1.452689
33	8	0	2.861506	0.086066	0.794231
34	1	0	2.568618	-0.871438	0.665758

Rotational constants (GHZ): 0.3297560 0.2559854 0.1606100

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 538 symmetry adapted cartesian basis functions of A symmetry.

There are 519 symmetry adapted basis functions of A symmetry.

519 basis functions, 823 primitive gaussians, 538 cartesian basis functions

78 alpha electrons 78 beta electrons

nuclear repulsion energy 1575.0058110852 Hartrees.

NAtoms= 34 NActive= 34 NUniq= 34 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 519 RedAO= T EigKep= 3.57D-06 NBF= 519

NBsUse= 519 1.00D-06 EigRej= -1.00D+00 NBFU= 519

Initial guess from the checkpoint file: "./coohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999654 -0.000151 0.000903 0.026277 Ang= -3.01 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3338.90376014 A.U. after 11 cycles

NFock= 11 Conv=0.52D-08 -V/T= 2.0019

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000446851	-0.000501172	-0.000617831
2	6	0.000205074	0.000409973	0.000659169
3	7	-0.000559008	0.000017973	0.000119230
4	6	-0.000301176	-0.000267678	-0.000056398
5	7	0.000178596	0.000474369	0.000252932
6	6	-0.000495835	-0.000329813	0.000472056
7	1	-0.000240663	0.000242085	0.000019922
8	1	-0.000092574	-0.000591599	-0.000129367
9	1	-0.000029366	-0.000005744	0.000107227
10	1	0.000007492	0.000141304	-0.000042715
11	35	0.000078137	0.000010110	0.000229818
12	1	0.000208666	-0.000012149	-0.000119392
13	6	0.000088563	-0.000213051	-0.000143303
14	6	0.000048507	0.000773286	-0.000120297
15	1	-0.000020511	0.000039852	-0.000062226
16	1	-0.000162763	-0.000232628	0.000060302
17	1	0.000067808	-0.000124131	-0.000011709
18	6	-0.000253133	-0.000637318	0.000356795
19	6	-0.000102743	0.000299459	0.000585432
20	8	0.000493508	-0.000663828	-0.000522064
21	1	0.000117496	0.000133800	0.000145404
22	1	-0.000063101	0.000094970	-0.000442027
23	1	0.000124795	0.000047535	-0.000016183
24	6	-0.000019483	-0.000088138	-0.000085814
25	1	-0.000011646	-0.000014135	-0.000012228
26	1	-0.000016529	0.000003726	-0.000043142
27	1	-0.000040237	0.000009408	-0.000009417
28	6	0.000793404	0.000196301	-0.000950835
29	1	-0.000117016	-0.000065754	0.000141862
30	1	0.000015404	-0.000047252	0.000176282
31	6	-0.000184589	0.000286927	-0.000322238
32	8	0.000045653	-0.000261885	0.000071314
33	8	0.000222783	-0.000331338	0.000372281
34	1	-0.000432365	0.001206535	-0.000062841

Cartesian Forces: Max 0.001206535 RMS 0.000320712

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000860344 RMS 0.000204555

Search for a local minimum.

Step number 26 out of a maximum of 175

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 21 22 23 24 25 26

DE= -6.06D-05 DEPred=-3.08D-05 R= 1.97D+00

TightC=F SS= 1.41D+00 RLast= 8.25D-02 DXNew= 1.3149D+00 2.4756D-01

Trust test= 1.97D+00 RLast= 8.25D-02 DXMaxT set to 7.82D-01

ITU= 1 -1 0 1 1 1 1 1 1 1 1 1 1 0 0 -1 1 1 1 0

ITU= 1 0 -1 0 1 0

Eigenvalues --- 0.00154 0.00317 0.00416 0.00543 0.00698

Eigenvalues --- 0.00729 0.01055 0.01215 0.01514 0.01597

Eigenvalues --- 0.02021 0.02078 0.02227 0.02266 0.02368

Eigenvalues --- 0.02456 0.02577 0.02902 0.03124 0.03325

Eigenvalues --- 0.03430 0.03553 0.03759 0.04222 0.04808

Eigenvalues --- 0.04909 0.04992 0.05346 0.05636 0.05748

Eigenvalues --- 0.05954 0.06313 0.06896 0.08262 0.09322

Eigenvalues --- 0.09522 0.11802 0.12605 0.12835 0.13201

Eigenvalues --- 0.13637 0.15290 0.15556 0.15794 0.15985

Eigenvalues --- 0.16007 0.16013 0.16032 0.16101 0.16148

Eigenvalues --- 0.17016 0.17525 0.20479 0.20769 0.22460

Eigenvalues --- 0.23141 0.23912 0.24039 0.25402 0.25726

Eigenvalues --- 0.28955 0.29139 0.30872 0.31989 0.32649

Eigenvalues --- 0.33659 0.34499 0.34564 0.34622 0.34803

Eigenvalues --- 0.34887 0.34954 0.34990 0.35123 0.35262

Eigenvalues --- 0.35548 0.35721 0.36116 0.36554 0.36953

Eigenvalues --- 0.37064 0.37377 0.37782 0.39022 0.40285

Eigenvalues --- 0.42015 0.45140 0.49392 0.50948 0.51708

Eigenvalues --- 0.53648 0.55806 0.56428 0.61264 0.90405

Eigenvalues --- 1.42560

En-DIIS/RFO-DIIS IScMMF= 0 using points: 26 25 24 23 22

RFO step: Lambda=-1.32888959D-05.

DidBck=F Rises=F RFO-DIIS coefs: 1.31937 -0.07075 -0.46487 0.12131 0.09494

Iteration 1 RMS(Cart)= 0.01625300 RMS(Int)= 0.00009397
Iteration 2 RMS(Cart)= 0.00016618 RMS(Int)= 0.00000477
Iteration 3 RMS(Cart)= 0.00000002 RMS(Int)= 0.00000477

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56894	0.00019	0.00023	-0.00009	0.00013	2.56908
R2	2.61988	-0.00001	0.00007	-0.00004	0.00003	2.61991
R3	2.03247	-0.00007	-0.00016	-0.00011	-0.00027	2.03220
R4	2.62281	0.00056	0.00039	0.00024	0.00064	2.62344
R5	2.07027	0.00052	0.00110	0.00032	0.00142	2.07169
R6	2.53673	0.00000	-0.00054	-0.00003	-0.00057	2.53616
R7	2.70553	-0.00010	0.00034	0.00055	0.00089	2.70642
R8	2.52921	0.00019	0.00002	0.00034	0.00036	2.52957
R9	2.03418	-0.00001	0.00003	0.00006	0.00009	2.03427
R10	2.78717	0.00006	-0.00008	0.00024	0.00016	2.78733
R11	2.06249	-0.00002	0.00001	0.00004	0.00005	2.06254
R12	2.05644	0.00003	0.00015	-0.00015	0.00000	2.05644
R13	2.89787	0.00082	0.00000	0.00151	0.00151	2.89938
R14	4.43704	0.00009	-0.00806	0.00145	-0.00661	4.43043
R15	2.50748	-0.00040	-0.00031	-0.00028	-0.00059	2.50688
R16	2.04640	0.00007	-0.00006	0.00009	0.00002	2.04642
R17	2.04553	0.00024	0.00015	0.00029	0.00044	2.04597
R18	2.06345	0.00007	-0.00017	0.00046	0.00028	2.06373
R19	2.76949	0.00005	-0.00005	0.00035	0.00029	2.76977
R20	2.76678	0.00030	0.00062	-0.00038	0.00025	2.76703
R21	2.05288	-0.00018	0.00012	-0.00019	-0.00008	2.05281
R22	2.05323	-0.00034	0.00014	-0.00016	-0.00002	2.05322
R23	2.74866	-0.00026	0.00015	-0.00077	-0.00061	2.74805
R24	2.05514	0.00003	-0.00008	0.00009	0.00001	2.05515
R25	2.84127	0.00008	-0.00005	0.00006	0.00001	2.84128
R26	3.04363	0.00065	0.00138	0.00683	0.00821	3.05185
R27	2.06719	-0.00002	-0.00003	-0.00007	-0.00010	2.06709
R28	2.06785	0.00000	0.00000	-0.00003	-0.00003	2.06783
R29	2.06329	0.00004	0.00004	0.00019	0.00023	2.06353
R30	2.06926	-0.00013	0.00005	-0.00020	-0.00015	2.06912
R31	2.06146	-0.00015	0.00023	-0.00053	-0.00030	2.06116
R32	2.88215	-0.00017	-0.00028	-0.00037	-0.00065	2.88150
R33	2.28418	0.00016	-0.00048	0.00014	-0.00034	2.28384
R34	2.51361	0.00024	0.00080	0.00064	0.00144	2.51505
R35	1.90769	-0.00048	0.00035	-0.00200	-0.00165	1.90604
A1	1.88297	0.00027	-0.00009	0.00063	0.00056	1.88353
A2	2.27230	0.00005	0.00043	-0.00004	0.00041	2.27271
A3	2.12683	-0.00031	-0.00035	-0.00046	-0.00079	2.12604
A4	1.85757	-0.00028	-0.00025	-0.00039	-0.00064	1.85693

A5	2.26714	0.00004	-0.00049	-0.00007	-0.00055	2.26659
A6	2.15198	0.00024	0.00056	0.00034	0.00089	2.15288
A7	1.90005	0.00001	0.00024	0.00007	0.00031	1.90036
A8	2.21772	0.00036	0.00037	-0.00030	0.00008	2.21780
A9	2.16534	-0.00037	-0.00061	0.00023	-0.00038	2.16496
A10	1.89650	0.00012	-0.00004	0.00022	0.00019	1.89668
A11	2.18947	0.00003	0.00025	0.00008	0.00033	2.18980
A12	2.19721	-0.00015	-0.00021	-0.00030	-0.00051	2.19669
A13	1.88768	-0.00013	0.00012	-0.00054	-0.00042	1.88727
A14	2.18921	0.00020	0.00040	0.00040	0.00080	2.19001
A15	2.20058	-0.00007	-0.00040	0.00047	0.00008	2.20066
A16	1.88974	-0.00037	-0.00033	-0.00004	-0.00038	1.88937
A17	1.85687	-0.00016	0.00051	-0.00066	-0.00015	1.85672
A18	1.95882	0.00086	0.00057	0.00178	0.00235	1.96117
A19	1.89008	0.00006	-0.00059	-0.00036	-0.00095	1.88913
A20	1.93208	-0.00016	-0.00020	-0.00030	-0.00050	1.93158
A21	1.93327	-0.00025	0.00002	-0.00049	-0.00047	1.93281
A22	2.70013	0.00059	0.01530	0.00599	0.02130	2.72143
A23	2.15411	-0.00010	0.00019	-0.00130	-0.00111	2.15300
A24	1.96420	0.00003	-0.00031	0.00014	-0.00017	1.96404
A25	2.16480	0.00008	0.00012	0.00118	0.00130	2.16609
A26	2.06278	0.00012	-0.00007	0.00059	0.00053	2.06330
A27	2.15755	0.00003	0.00115	-0.00065	0.00050	2.15805
A28	2.06254	-0.00015	-0.00105	0.00006	-0.00099	2.06155
A29	2.06230	-0.00002	-0.00108	-0.00044	-0.00151	2.06079
A30	2.12842	0.00017	0.00055	-0.00028	0.00026	2.12868
A31	1.98019	-0.00014	-0.00047	-0.00106	-0.00154	1.97865
A32	1.99852	0.00025	0.00073	0.00089	0.00163	2.00015
A33	2.02159	-0.00011	0.00031	0.00071	0.00102	2.02261
A34	2.03788	0.00016	-0.00011	0.00032	0.00021	2.03809
A35	2.14361	-0.00026	-0.00053	-0.00074	-0.00127	2.14234
A36	1.94152	0.00014	0.00026	0.00027	0.00053	1.94206
A37	2.04024	-0.00025	-0.00029	-0.00045	-0.00074	2.03949
A38	2.02306	0.00008	0.00043	0.00043	0.00085	2.02392
A39	2.07289	0.00002	0.00090	0.00366	0.00453	2.07742
A40	2.31874	0.00016	0.00087	0.01101	0.01187	2.33061
A41	1.93418	0.00002	0.00026	0.00015	0.00041	1.93459
A42	1.91241	0.00006	0.00063	0.00018	0.00081	1.91322
A43	1.93821	-0.00006	-0.00037	-0.00014	-0.00051	1.93770
A44	1.88154	-0.00001	0.00018	0.00006	0.00024	1.88178
A45	1.90109	0.00001	-0.00013	-0.00038	-0.00051	1.90059
A46	1.89510	-0.00001	-0.00058	0.00014	-0.00044	1.89466
A47	1.88415	-0.00015	-0.00172	0.00024	-0.00148	1.88266
A48	1.94575	-0.00002	-0.00007	-0.00005	-0.00012	1.94563

A49	1.97552	0.00007	-0.00019	-0.00028	-0.00047	1.97505
A50	1.87928	0.00008	0.00053	0.00019	0.00072	1.87999
A51	1.89774	0.00005	0.00063	0.00049	0.00112	1.89886
A52	1.87874	-0.00003	0.00088	-0.00054	0.00035	1.87909
A53	2.14581	0.00009	-0.00015	0.00168	0.00154	2.14734
A54	1.95092	0.00017	0.00029	-0.00107	-0.00079	1.95013
A55	2.18628	-0.00026	-0.00018	-0.00063	-0.00081	2.18547
A56	1.94132	-0.00068	-0.00080	-0.00229	-0.00310	1.93822
A57	2.83232	0.00038	-0.00239	-0.00193	-0.00432	2.82800
D1	0.00084	0.00014	0.00022	0.00162	0.00184	0.00268
D2	3.02110	0.00020	-0.00146	0.00056	-0.00089	3.02021
D3	-3.09056	-0.00020	-0.00080	-0.00151	-0.00230	-3.09287
D4	-0.07031	-0.00013	-0.00248	-0.00256	-0.00503	-0.07534
D5	0.00094	-0.00021	-0.00005	-0.00209	-0.00215	-0.00121
D6	-3.03152	-0.00029	-0.00133	-0.00533	-0.00666	-3.03818
D7	3.09739	0.00011	0.00087	0.00073	0.00161	3.09901
D8	0.06494	0.00002	-0.00041	-0.00250	-0.00290	0.06204
D9	-0.00233	-0.00002	-0.00031	-0.00059	-0.00090	-0.00323
D10	3.12610	-0.00002	0.00048	-0.00055	-0.00007	3.12602
D11	-3.03259	-0.00007	0.00131	0.00041	0.00172	-3.03087
D12	0.09584	-0.00007	0.00209	0.00044	0.00255	0.09838
D13	-1.51722	0.00014	-0.00243	-0.00157	-0.00400	-1.52122
D14	1.48502	0.00019	-0.00442	-0.00283	-0.00725	1.47777
D15	0.00296	-0.00011	0.00029	-0.00071	-0.00043	0.00253
D16	3.13939	-0.00002	0.00063	-0.00106	-0.00043	3.13896
D17	-3.12595	-0.00011	-0.00049	-0.00074	-0.00123	-3.12719
D18	0.01047	-0.00002	-0.00015	-0.00109	-0.00123	0.00925
D19	-0.20797	0.00003	0.00492	0.00203	0.00696	-0.20102
D20	2.94640	-0.00003	0.00476	-0.00019	0.00457	2.95097
D21	2.91858	0.00003	0.00584	0.00207	0.00791	2.92649
D22	-0.21023	-0.00003	0.00567	-0.00015	0.00552	-0.20471
D23	-0.00241	0.00019	-0.00014	0.00172	0.00158	-0.00083
D24	3.02915	0.00030	0.00120	0.00498	0.00618	3.03533
D25	-3.13881	0.00011	-0.00049	0.00206	0.00157	-3.13723
D26	-0.10725	0.00021	0.00085	0.00532	0.00618	-0.10108
D27	-2.46431	0.00017	-0.00155	0.00193	0.00038	-2.46393
D28	-0.43603	-0.00003	-0.00214	0.00116	-0.00098	-0.43701
D29	1.68106	0.00007	-0.00144	0.00118	-0.00026	1.68080
D30	0.80570	0.00008	-0.00310	-0.00181	-0.00491	0.80079
D31	2.83398	-0.00012	-0.00368	-0.00259	-0.00627	2.82771
D32	-1.33211	-0.00002	-0.00298	-0.00257	-0.00555	-1.33766
D33	-3.00463	-0.00007	0.00450	0.00231	0.00682	-2.99781
D34	1.21789	-0.00007	0.00496	0.00196	0.00693	1.22482
D35	-0.90322	-0.00007	0.00400	0.00291	0.00691	-0.89631

D36	1.16491	-0.00008	0.00467	0.00136	0.00603	1.17094
D37	-0.89575	-0.00007	0.00514	0.00101	0.00614	-0.88961
D38	-3.01687	-0.00008	0.00417	0.00195	0.00613	-3.01074
D39	-0.93199	0.00012	0.00553	0.00233	0.00786	-0.92413
D40	-2.99265	0.00012	0.00599	0.00198	0.00797	-2.98468
D41	1.16942	0.00012	0.00503	0.00292	0.00795	1.17737
D42	-3.13617	-0.00011	-0.00013	-0.00217	-0.00231	-3.13848
D43	-0.02212	-0.00011	0.00087	-0.00164	-0.00077	-0.02289
D44	-0.00883	-0.00004	0.00005	0.00029	0.00034	-0.00849
D45	3.10523	-0.00005	0.00105	0.00083	0.00188	3.10711
D46	-2.75150	-0.00008	0.00038	-0.00108	-0.00070	-2.75219
D47	-0.04306	-0.00012	-0.00006	-0.00095	-0.00101	-0.04407
D48	-0.02207	0.00001	-0.00018	-0.00096	-0.00114	-0.02321
D49	2.68636	-0.00004	-0.00062	-0.00082	-0.00144	2.68492
D50	0.27009	0.00018	0.00177	0.01209	0.01386	0.28395
D51	-2.10416	0.00023	0.00102	0.01119	0.01221	-2.09196
D52	2.57269	-0.00014	-0.00063	-0.00163	-0.00227	2.57042
D53	0.19390	-0.00015	-0.00127	-0.00213	-0.00340	0.19049
D54	2.55047	0.00000	-0.00030	0.00169	0.00140	2.55187
D55	-1.65853	0.00003	0.00048	0.00197	0.00246	-1.65607
D56	0.43497	0.00002	-0.00006	0.00217	0.00211	0.43709
D57	1.32263	0.00000	-0.00027	0.00223	0.00196	1.32459
D58	-2.88636	0.00003	0.00051	0.00251	0.00302	-2.88335
D59	-0.79286	0.00002	-0.00004	0.00271	0.00267	-0.79019
D60	-1.02090	-0.00003	-0.00086	0.00181	0.00095	-1.01995
D61	1.05328	0.00001	-0.00007	0.00208	0.00201	1.05529
D62	-3.13640	-0.00001	-0.00062	0.00229	0.00166	-3.13474
D63	1.52466	-0.00001	-0.00882	0.00136	-0.00748	1.51718
D64	2.83027	0.00007	-0.00804	0.00836	0.00033	2.83060
D65	2.28186	0.00002	-0.00299	0.00190	-0.00109	2.28077
D66	-0.84021	0.00011	-0.00110	0.00299	0.00190	-0.83831
D67	-1.90767	-0.00010	-0.00484	0.00235	-0.00249	-1.91015
D68	1.25345	0.00000	-0.00295	0.00345	0.00050	1.25395
D69	0.12350	0.00001	-0.00341	0.00254	-0.00087	0.12263
D70	-2.99857	0.00011	-0.00152	0.00364	0.00212	-2.99645
D71	2.93439	0.00012	0.00009	-0.00370	-0.00361	2.93079
D72	-0.18713	0.00021	0.00203	-0.00260	-0.00058	-0.18771
D73	-1.99381	0.00028	-0.00405	0.00723	0.00318	-1.99063

Item	Value	Threshold	Converged?
Maximum Force	0.000860	0.000450	NO
RMS Force	0.000205	0.000300	YES
Maximum Displacement	0.063365	0.001800	NO
RMS Displacement	0.016282	0.001200	NO

Predicted change in Energy=-1.918498D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.865957	1.654833	1.548922
2	6	0	-1.518542	0.462571	1.578560
3	7	0	-2.356354	0.446840	0.471713
4	6	0	-2.211546	1.600215	-0.199060
5	7	0	-1.307326	2.355141	0.436783
6	6	0	-0.763917	3.642515	-0.035414
7	1	0	-0.103357	2.045337	2.198858
8	1	0	-1.372596	-0.402246	2.236316
9	1	0	-1.595389	4.256640	-0.385792
10	1	0	-0.324826	4.127740	0.834058
11	35	0	-0.419326	-2.429932	2.926501
12	1	0	-2.734033	1.867832	-1.101400
13	6	0	-3.233227	-0.610978	0.067674
14	6	0	-3.198459	-1.828317	0.593701
15	1	0	-3.914961	-0.307868	-0.717235
16	1	0	-3.898853	-2.566221	0.223366
17	1	0	-2.486937	-2.134794	1.363408
18	6	0	2.556997	-0.677113	1.201674
19	6	0	3.985119	-0.363411	1.303350
20	8	0	2.997161	0.667018	1.580604
21	1	0	2.112632	-0.721803	0.211429
22	1	0	2.029729	-1.217448	1.983048
23	1	0	4.492398	-0.678418	2.212295
24	6	0	4.860577	-0.158308	0.098301
25	1	0	5.630943	0.591615	0.299981
26	1	0	5.364346	-1.096411	-0.153808
27	1	0	4.271807	0.162485	-0.763584
28	6	0	0.281860	3.463500	-1.143719
29	1	0	0.740298	4.439483	-1.333881
30	1	0	-0.176089	3.125008	-2.073971
31	6	0	1.378145	2.468458	-0.778843
32	8	0	1.720994	1.568742	-1.509302
33	8	0	1.873054	2.703266	0.434103
34	1	0	2.448703	1.935745	0.745353

Distance matrix (angstroms):

	1	2	3	4	5

1	C	0.000000				
2	C	1.359498	0.000000			
3	N	2.200206	1.388267	0.000000		
4	C	2.206589	2.221355	1.342080	0.000000	
5	N	1.386396	2.220380	2.177910	1.338590	0.000000
6	C	2.543897	3.645053	3.606295	2.508665	1.474990
7	H	1.075392	2.211937	3.257946	3.223756	2.156485
8	H	2.227278	1.096290	2.191472	3.262628	3.293291
9	H	3.323340	4.273119	3.978562	2.733334	2.091724
10	H	2.630423	3.925902	4.219884	3.318950	2.065246
11	Br	4.333879	3.375173	4.248985	5.405854	5.466641
12	H	3.249505	3.261037	2.153264	1.076489	2.153826
13	C	3.596104	2.524961	1.432178	2.450378	3.555728
14	C	4.299459	3.006698	2.429066	3.654764	4.593727
15	H	4.275990	3.406915	2.100580	2.609772	3.901683
16	H	5.364033	4.083627	3.394041	4.514934	5.566090
17	H	4.125926	2.780357	2.734412	4.058009	4.733881
18	C	4.156341	4.248640	5.092851	5.466926	4.971178
19	C	5.259900	5.572097	6.446891	6.671710	6.012606
20	O	3.987538	4.520329	5.471585	5.582892	4.763055
21	H	4.038474	4.056748	4.626587	4.925320	4.605917
22	H	4.101641	3.946682	4.928662	5.539786	5.127403
23	H	5.881844	6.151006	7.155504	7.479951	6.781720
24	C	6.179399	6.577979	7.251878	7.293541	6.668959
25	H	6.700746	7.264059	7.990454	7.922812	7.160189
26	H	7.020350	7.266751	7.898235	8.041640	7.534800
27	H	5.828499	6.253306	6.748284	6.664805	6.113538
28	C	3.440796	4.433714	4.320883	3.252888	2.500391
29	H	4.317972	5.422222	5.365689	4.250017	3.416503
30	H	3.970226	4.715054	4.290297	3.159648	2.859419
31	C	3.334137	4.239307	4.426884	3.738432	2.949973
32	O	4.006553	4.610109	4.669888	4.145189	3.684615
33	O	3.137549	4.222963	4.793825	4.278034	3.199377
34	H	3.422222	4.313178	5.037884	4.766803	3.791946

		6	7	8	9	10
6	C	0.000000				
7	H	2.824763	0.000000			
8	H	4.678818	2.757360	0.000000		
9	H	1.091449	3.714355	5.350730	0.000000	
10	H	1.088221	2.499626	4.856432	1.766063	0.000000
11	Br	6.765079	4.545034	2.344480	7.554115	6.884062
12	H	2.857828	4.224176	4.259943	2.741351	3.828506
13	C	4.919382	4.625369	2.865052	5.155759	5.612628
14	C	6.021028	5.211657	2.840006	6.368355	6.617413

15	H	5.098969	5.345043	3.898203	5.130789	5.913560
16	H	6.960114	6.290852	3.888023	7.226925	7.612866
17	H	6.188925	4.883946	2.237285	6.686179	6.646373
18	C	5.587311	3.934919	4.072805	6.641106	5.614861
19	C	6.355554	4.829041	5.438478	7.439096	6.242299
20	O	5.060712	3.448943	4.546214	6.151717	4.854846
21	H	5.232851	4.064177	4.043401	6.236264	5.463235
22	H	5.958010	3.904151	3.507779	6.979866	5.952743
23	H	7.165996	5.342283	5.871542	8.256271	6.942935
24	C	6.789629	5.823146	6.594168	7.836174	6.767566
25	H	7.093286	6.212989	7.333943	8.131579	6.946985
26	H	7.747712	6.730631	7.181988	8.783330	7.786804
27	H	6.164362	5.609211	6.416978	7.164414	6.277320
28	C	1.534286	3.651355	5.394984	2.174302	2.172759
29	H	2.140990	4.350164	6.375968	2.527398	2.435494
30	H	2.183820	4.407726	5.696642	2.478902	3.079647
31	C	2.553336	3.352698	4.989860	3.491989	2.873113
32	O	3.556355	4.160030	5.242590	4.414235	4.028050
33	O	2.838354	2.730097	4.840085	3.887840	2.649485
34	H	3.720697	2.938995	4.721387	4.797991	3.536265

		11	12	13	14	15
11	Br	0.000000				
12	H	6.328715	0.000000			
13	C	4.404489	2.785755	0.000000		
14	C	3.677971	4.092747	1.326585	0.000000	
15	H	5.477173	2.505164	1.082921	2.131594	0.000000
16	H	4.408244	4.772069	2.071297	1.082683	2.446456
17	H	2.608712	4.707160	2.134922	1.092080	3.115443
18	C	3.860816	6.306813	5.900595	5.900862	6.760532
19	C	5.128769	7.477183	7.327530	7.365687	8.154576
20	O	4.803636	6.440628	6.537581	6.751768	7.349006
21	H	4.086579	5.649769	5.348939	5.438583	6.112743
22	H	2.891037	6.459582	5.633398	5.444024	6.592283
23	H	5.263357	8.347770	8.018056	7.943009	8.910844
24	C	6.405963	7.951266	8.106510	8.245144	8.814620
25	H	7.254937	8.577029	8.948391	9.159731	9.641996
26	H	6.687111	8.675737	8.614114	8.626476	9.329780
27	H	6.507233	7.218319	7.590439	7.849229	8.200400
28	C	7.196589	3.412265	5.515857	6.567692	5.658481
29	H	8.166054	4.328788	6.577264	7.649489	6.677501
30	H	7.478051	3.011555	5.281130	6.386441	5.254002
31	C	6.399586	4.168308	5.609301	6.425842	5.977353
32	O	6.344030	4.483648	5.637583	6.337480	5.992748
33	O	6.149534	4.927572	6.098573	6.803011	6.625226

34	H	5.660577	5.502350	6.263335	6.788342	6.904286
		16	17	18	19	20
16	H	0.000000				
17	H	1.865296	0.000000			
18	C	6.797338	5.252833	0.000000		
19	C	8.256861	6.710359	1.465701	0.000000	
20	O	7.736338	6.162196	1.464248	1.454206	0.000000
21	H	6.288081	4.947689	1.086298	2.197031	2.141461
22	H	6.329593	4.650349	1.086516	2.239401	2.156177
23	H	8.827951	7.180025	2.183377	1.087540	2.108309
24	C	9.085224	7.713167	2.606352	1.503541	2.520060
25	H	10.039662	8.629262	3.445558	2.151177	2.929589
26	H	9.386664	8.063674	3.145529	2.136087	3.423658
27	H	8.670617	7.448638	2.740025	2.151969	2.715602
28	C	7.463566	6.729994	5.274637	5.860676	4.755535
29	H	8.545561	7.804584	5.992411	6.368017	5.274386
30	H	7.178218	6.694857	5.714521	6.394609	5.428366
31	C	7.362005	6.381068	3.899585	4.376223	3.381330
32	O	7.189071	6.298835	3.618309	4.095179	3.462547
33	O	7.818363	6.578750	3.533257	3.823730	2.593142
34	H	7.799463	6.427427	2.654616	2.821002	1.614967
		21	22	23	24	25
21	H	0.000000				
22	H	1.841513	0.000000			
23	H	3.109443	2.531372	0.000000		
24	C	2.807406	3.561986	2.207949	0.000000	
25	H	3.756518	4.367398	2.562463	1.093857	0.000000
26	H	3.293536	3.962383	2.556063	1.094248	1.768171
27	H	2.528766	3.804618	3.100264	1.091972	1.778362
28	C	4.764968	5.894319	6.793155	5.968649	6.240568
29	H	5.559690	6.683227	7.269562	6.337786	6.433817
30	H	5.025859	6.338925	7.391408	6.392726	6.765749
31	C	3.420216	4.651721	5.343062	4.449339	4.772075
32	O	2.891521	4.478246	5.155647	3.927349	4.417690
33	O	3.440651	4.218504	4.632355	4.150501	4.312631
34	H	2.731406	3.413217	3.628010	3.258968	3.483059
		26	27	28	29	30
26	H	0.000000				
27	H	1.774904	0.000000			
28	C	6.899593	5.192387	0.000000		
29	H	7.308934	5.575796	1.094929	0.000000	
30	H	7.225222	5.502494	1.090717	1.765033	0.000000
31	C	5.384121	3.700139	1.524823	2.144727	2.126983
32	O	4.713217	3.006710	2.407253	3.038698	2.517884

33	O	5.193486	3.693783	2.366301	2.724583	3.266082
34	H	4.301562	2.957203	3.255432	3.675672	4.031435

		31	32	33	34
31	C	0.000000			
32	O	1.208554	0.000000		
33	O	1.330905	2.255458	0.000000	
34	H	1.937280	2.397440	1.008631	0.000000

Stoichiometry C11H17BrN2O3
Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.058287	1.342782	1.253589
2	6	0	-1.167648	1.257803	0.672129
3	7	0	-1.224310	2.273155	-0.272929
4	6	0	-0.065184	2.949354	-0.253963
5	7	0	0.735463	2.401587	0.668391
6	6	0	2.143188	2.762017	0.921364
7	1	0	0.516540	0.720933	2.001771
8	1	0	-1.948755	0.497214	0.787149
9	1	0	2.217669	3.850567	0.949162
10	1	0	2.385140	2.378693	1.910681
11	35	0	-3.068998	-1.508436	0.319164
12	1	0	0.178313	3.789242	-0.881759
13	6	0	-2.313241	2.573197	-1.153462
14	6	0	-3.350842	1.766089	-1.331753
15	1	0	-2.187758	3.521934	-1.660286
16	1	0	-4.127023	2.074673	-2.020608
17	1	0	-3.454747	0.796503	-0.840076
18	6	0	0.618663	-2.474497	-0.292219
19	6	0	1.643154	-3.497072	-0.061918
20	8	0	1.656691	-2.271242	0.720306
21	1	0	0.728120	-1.826945	-1.157515
22	1	0	-0.388200	-2.569347	0.104958
23	1	0	1.355089	-4.350680	0.547274
24	6	0	2.797740	-3.717246	-0.999515
25	1	0	3.692721	-4.022786	-0.449808
26	1	0	2.550160	-4.515156	-1.706214

27	1	0	3.022164	-2.810054	-1.564352
28	6	0	3.093348	2.180893	-0.133872
29	1	0	4.119637	2.363776	0.201023
30	1	0	2.966677	2.672469	-1.099259
31	6	0	2.906409	0.682989	-0.349329
32	8	0	2.785188	0.184876	-1.443766
33	8	0	2.867737	0.020203	0.804157
34	1	0	2.550936	-0.927514	0.667024

Rotational constants (GHZ): 0.3307084 0.2541528 0.1601750

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 538 symmetry adapted cartesian basis functions of A symmetry.

There are 519 symmetry adapted basis functions of A symmetry.

519 basis functions, 823 primitive gaussians, 538 cartesian basis functions

78 alpha electrons 78 beta electrons

nuclear repulsion energy 1573.9950146262 Hartrees.

NAtoms= 34 NActive= 34 NUniq= 34 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 519 RedAO= T EigKep= 3.54D-06 NBF= 519

NBsUse= 519 1.00D-06 EigRej= -1.00D+00 NBFU= 519

Initial guess from the checkpoint file: "./coohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999914 0.000158 0.000774 0.013100 Ang= 1.50 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3338.90381449 A.U. after 12 cycles

NFock= 12 Conv=0.24D-08 -V/T= 2.0019

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000175281	-0.000350757	-0.000439282
2	6	0.000558279	0.000382798	0.000352461
3	7	-0.000623864	-0.000296379	0.000093035
4	6	-0.000255737	0.000029293	-0.000083285
5	7	0.000178808	0.000357853	-0.000016640
6	6	-0.000327495	-0.000286918	0.000448774
7	1	-0.000148495	0.000190665	0.000119215
8	1	-0.000352274	-0.000439750	-0.000144423
9	1	-0.000008913	-0.000033405	0.000077342
10	1	0.000041438	0.000045597	-0.000020971
11	35	0.000175977	0.000093075	0.000116058
12	1	0.000151575	-0.000026983	-0.000068656
13	6	0.000271181	0.000208798	0.000047442
14	6	-0.000100127	0.000262252	-0.000069975
15	1	-0.000000929	-0.000015673	-0.000066708
16	1	-0.000046853	-0.000115088	0.000042357
17	1	0.000021809	-0.000071460	-0.000041111
18	6	-0.000171975	-0.000378289	0.000135197
19	6	-0.000151588	0.000310927	0.000444357
20	8	0.000343716	-0.000871082	-0.000282502
21	1	0.000119340	0.000077927	0.000064862
22	1	-0.000060145	0.000106632	-0.000198124
23	1	0.000104095	0.000045786	-0.000030676
24	6	-0.000026664	-0.000067028	-0.000144861
25	1	0.000011762	-0.000011497	0.000020881
26	1	0.000000841	-0.000008410	0.000013640
27	1	-0.000045788	0.000006704	0.000034972
28	6	0.000460331	0.000151317	-0.000679655
29	1	-0.000061799	-0.000081669	0.000041606
30	1	0.000002235	-0.000057411	0.000074391
31	6	-0.000200327	0.000316563	0.000228787
32	8	0.000015561	-0.000205341	-0.000074527
33	8	0.000210025	-0.000466526	-0.000082733
34	1	-0.000259282	0.001197477	0.000088750

Cartesian Forces: Max 0.001197477 RMS 0.000263825

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000650368 RMS 0.000125038
Search for a local minimum.
Step number 27 out of a maximum of 175
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 21 22 23 24 25
26 27
DE= -5.44D-05 DEPred=-1.92D-05 R= 2.83D+00
TightC=F SS= 1.41D+00 RLast= 4.77D-02 DXNew= 1.3149D+00 1.4296D-01
Trust test= 2.83D+00 RLast= 4.77D-02 DXMaxT set to 7.82D-01
ITU= 1 1 -1 0 1 1 1 1 1 1 1 1 1 1 0 0 -1 1 1 1
ITU= 0 1 0 -1 0 1 0
Eigenvalues --- 0.00156 0.00291 0.00422 0.00567 0.00691
Eigenvalues --- 0.00782 0.00932 0.01185 0.01423 0.01611
Eigenvalues --- 0.02023 0.02094 0.02136 0.02265 0.02363
Eigenvalues --- 0.02422 0.02819 0.03027 0.03145 0.03214
Eigenvalues --- 0.03425 0.03566 0.03767 0.04213 0.04800
Eigenvalues --- 0.04896 0.05032 0.05345 0.05662 0.05745
Eigenvalues --- 0.05916 0.06324 0.06554 0.07804 0.09407
Eigenvalues --- 0.09538 0.11873 0.12617 0.12782 0.13196
Eigenvalues --- 0.13727 0.15099 0.15566 0.15783 0.15980
Eigenvalues --- 0.15996 0.16010 0.16030 0.16044 0.16177
Eigenvalues --- 0.17006 0.17624 0.20385 0.20890 0.22346
Eigenvalues --- 0.23111 0.23668 0.24008 0.25268 0.26009
Eigenvalues --- 0.28468 0.29173 0.30543 0.31573 0.32227
Eigenvalues --- 0.33694 0.34500 0.34571 0.34627 0.34805
Eigenvalues --- 0.34888 0.34956 0.34995 0.35105 0.35263
Eigenvalues --- 0.35338 0.35732 0.35783 0.36578 0.36947
Eigenvalues --- 0.37139 0.37485 0.37858 0.38393 0.40766
Eigenvalues --- 0.41261 0.45149 0.49150 0.50125 0.51592
Eigenvalues --- 0.53832 0.56032 0.56362 0.61098 0.90694
Eigenvalues --- 1.46585
En-DIIS/RFO-DIIS IScMMF= 0 using points: 27 26 25 24 23
RFO step: Lambda=-7.77004367D-06.
DidBck=F Rises=F RFO-DIIS coefs: 1.63709 -0.65092 0.09006 -0.32115
0.24492
Iteration 1 RMS(Cart)= 0.02554324 RMS(Int)= 0.00024727
Iteration 2 RMS(Cart)= 0.00049610 RMS(Int)= 0.00001680

Iteration 3 RMS(Cart)= 0.00000016 RMS(Int)= 0.00001680

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56908	-0.00004	0.00023	-0.00016	0.00006	2.56914
R2	2.61991	-0.00009	-0.00006	-0.00009	-0.00015	2.61976
R3	2.03220	0.00004	-0.00024	0.00012	-0.00012	2.03208
R4	2.62344	0.00040	0.00072	0.00018	0.00090	2.62434
R5	2.07169	0.00024	0.00098	-0.00027	0.00071	2.07240
R6	2.53616	0.00018	-0.00039	0.00000	-0.00040	2.53577
R7	2.70642	-0.00026	0.00028	-0.00024	0.00004	2.70646
R8	2.52957	0.00013	0.00024	0.00023	0.00047	2.53004
R9	2.03427	-0.00003	0.00004	-0.00005	-0.00001	2.03426
R10	2.78733	-0.00020	-0.00001	-0.00052	-0.00053	2.78679
R11	2.06254	-0.00004	0.00003	-0.00007	-0.00004	2.06250
R12	2.05644	0.00002	0.00005	0.00002	0.00007	2.05651
R13	2.89938	0.00046	0.00131	0.00070	0.00201	2.90139
R14	4.43043	0.00003	0.00327	-0.01390	-0.01063	4.41979
R15	2.50688	-0.00009	-0.00051	-0.00010	-0.00061	2.50627
R16	2.04642	0.00004	0.00005	-0.00004	0.00001	2.04643
R17	2.04597	0.00009	0.00043	0.00001	0.00044	2.04641
R18	2.06373	0.00001	0.00015	-0.00023	-0.00009	2.06364
R19	2.76977	0.00002	0.00037	0.00013	0.00044	2.77021
R20	2.76703	0.00012	0.00044	-0.00028	0.00019	2.76722
R21	2.05281	-0.00011	-0.00017	0.00007	-0.00010	2.05271
R22	2.05322	-0.00017	-0.00029	0.00028	-0.00001	2.05321
R23	2.74805	-0.00026	-0.00066	-0.00111	-0.00173	2.74632
R24	2.05515	0.00001	0.00002	-0.00006	-0.00004	2.05511
R25	2.84128	0.00004	0.00012	-0.00003	0.00009	2.84137
R26	3.05185	0.00065	0.00712	0.01125	0.01837	3.07021
R27	2.06709	0.00001	-0.00006	0.00002	-0.00004	2.06705
R28	2.06783	0.00000	-0.00001	0.00000	0.00000	2.06783
R29	2.06353	0.00001	0.00008	0.00021	0.00030	2.06383
R30	2.06912	-0.00011	-0.00019	0.00006	-0.00012	2.06899
R31	2.06116	-0.00005	-0.00020	0.00007	-0.00013	2.06102
R32	2.88150	-0.00009	-0.00050	-0.00035	-0.00085	2.88065
R33	2.28384	0.00020	-0.00029	-0.00033	-0.00062	2.28322
R34	2.51505	0.00003	0.00106	0.00085	0.00191	2.51696
R35	1.90604	-0.00037	-0.00110	-0.00159	-0.00269	1.90334
A1	1.88353	0.00019	0.00040	-0.00002	0.00038	1.88391
A2	2.27271	-0.00001	0.00065	0.00034	0.00099	2.27370
A3	2.12604	-0.00018	-0.00087	-0.00029	-0.00116	2.12488
A4	1.85693	-0.00010	-0.00056	0.00014	-0.00043	1.85650
A5	2.26659	-0.00011	-0.00028	0.00024	-0.00004	2.26655
A6	2.15288	0.00021	0.00072	-0.00028	0.00045	2.15332

A7	1.90036	-0.00008	0.00025	-0.00013	0.00012	1.90049
A8	2.21780	0.00032	0.00045	-0.00008	0.00037	2.21817
A9	2.16496	-0.00024	-0.00072	0.00019	-0.00053	2.16443
A10	1.89668	0.00001	0.00008	-0.00001	0.00007	1.89675
A11	2.18980	0.00004	0.00038	0.00023	0.00061	2.19041
A12	2.19669	-0.00006	-0.00046	-0.00022	-0.00069	2.19601
A13	1.88727	-0.00002	-0.00017	0.00003	-0.00014	1.88712
A14	2.19001	-0.00010	0.00085	-0.00035	0.00048	2.19049
A15	2.20066	0.00012	-0.00023	0.00070	0.00046	2.20112
A16	1.88937	-0.00008	-0.00057	-0.00035	-0.00092	1.88845
A17	1.85672	0.00002	0.00025	0.00012	0.00037	1.85709
A18	1.96117	0.00009	0.00203	-0.00002	0.00201	1.96318
A19	1.88913	0.00000	-0.00094	0.00004	-0.00089	1.88824
A20	1.93158	0.00006	-0.00024	0.00052	0.00028	1.93186
A21	1.93281	-0.00008	-0.00061	-0.00034	-0.00095	1.93186
A22	2.72143	-0.00006	0.00459	0.00242	0.00700	2.72843
A23	2.15300	0.00013	-0.00082	0.00012	-0.00070	2.15231
A24	1.96404	-0.00005	0.00000	-0.00001	-0.00001	1.96403
A25	2.16609	-0.00008	0.00083	-0.00012	0.00072	2.16681
A26	2.06330	0.00008	0.00060	0.00063	0.00123	2.06454
A27	2.15805	0.00002	0.00029	0.00040	0.00069	2.15874
A28	2.06155	-0.00010	-0.00090	-0.00104	-0.00193	2.05962
A29	2.06079	-0.00002	-0.00131	-0.00147	-0.00276	2.05803
A30	2.12868	0.00009	0.00117	0.00046	0.00161	2.13029
A31	1.97865	-0.00004	-0.00115	-0.00101	-0.00217	1.97647
A32	2.00015	0.00009	0.00131	-0.00028	0.00104	2.00119
A33	2.02261	-0.00003	0.00016	0.00144	0.00160	2.02420
A34	2.03809	0.00014	0.00061	0.00058	0.00116	2.03925
A35	2.14234	-0.00020	-0.00148	-0.00115	-0.00260	2.13974
A36	1.94206	0.00006	0.00059	0.00035	0.00094	1.94300
A37	2.03949	-0.00011	-0.00032	-0.00047	-0.00081	2.03869
A38	2.02392	0.00003	0.00048	0.00047	0.00095	2.02487
A39	2.07742	-0.00001	0.00318	0.00439	0.00743	2.08485
A40	2.33061	0.00012	0.00804	0.01022	0.01822	2.34882
A41	1.93459	0.00000	0.00031	0.00034	0.00064	1.93523
A42	1.91322	0.00001	0.00067	0.00035	0.00101	1.91423
A43	1.93770	-0.00008	-0.00056	-0.00062	-0.00118	1.93652
A44	1.88178	0.00000	0.00020	0.00010	0.00030	1.88208
A45	1.90059	0.00004	-0.00024	-0.00014	-0.00037	1.90021
A46	1.89466	0.00004	-0.00037	-0.00001	-0.00039	1.89427
A47	1.88266	0.00006	-0.00145	-0.00047	-0.00191	1.88075
A48	1.94563	0.00009	-0.00008	0.00020	0.00013	1.94576
A49	1.97505	-0.00036	-0.00055	-0.00084	-0.00139	1.97366
A50	1.87999	-0.00001	0.00084	0.00030	0.00113	1.88112

A51	1.89886	0.00015	0.00088	0.00077	0.00164	1.90050
A52	1.87909	0.00009	0.00046	0.00012	0.00058	1.87967
A53	2.14734	-0.00007	0.00064	0.00028	0.00091	2.14826
A54	1.95013	0.00018	-0.00010	-0.00010	-0.00021	1.94993
A55	2.18547	-0.00011	-0.00059	-0.00022	-0.00081	2.18466
A56	1.93822	-0.00017	-0.00193	-0.00127	-0.00320	1.93502
A57	2.82800	0.00001	-0.00040	-0.00272	-0.00311	2.82489
D1	0.00268	-0.00002	0.00157	-0.00252	-0.00095	0.00173
D2	3.02021	0.00003	0.00050	-0.00160	-0.00110	3.01911
D3	-3.09287	-0.00014	-0.00348	-0.00331	-0.00679	-3.09966
D4	-0.07534	-0.00009	-0.00454	-0.00240	-0.00694	-0.08228
D5	-0.00121	-0.00001	-0.00192	0.00178	-0.00014	-0.00136
D6	-3.03818	-0.00004	-0.00636	-0.00204	-0.00840	-3.04657
D7	3.09901	0.00010	0.00265	0.00251	0.00516	3.10416
D8	0.06204	0.00008	-0.00179	-0.00131	-0.00310	0.05894
D9	-0.00323	0.00005	-0.00068	0.00240	0.00172	-0.00151
D10	3.12602	0.00001	-0.00128	0.00070	-0.00057	3.12545
D11	-3.03087	0.00003	0.00038	0.00152	0.00190	-3.02897
D12	0.09838	-0.00001	-0.00022	-0.00019	-0.00040	0.09798
D13	-1.52122	0.00019	-0.00076	0.00058	-0.00018	-1.52140
D14	1.47777	0.00022	-0.00208	0.00167	-0.00042	1.47736
D15	0.00253	-0.00006	-0.00051	-0.00133	-0.00185	0.00068
D16	3.13896	-0.00008	-0.00108	-0.00242	-0.00350	3.13546
D17	-3.12719	-0.00003	0.00005	0.00031	0.00036	-3.12683
D18	0.00925	-0.00005	-0.00052	-0.00077	-0.00130	0.00795
D19	-0.20102	0.00005	0.00166	0.00662	0.00828	-0.19274
D20	2.95097	0.00003	0.00010	0.00699	0.00709	2.95807
D21	2.92649	0.00000	0.00098	0.00467	0.00566	2.93214
D22	-0.20471	-0.00001	-0.00057	0.00504	0.00447	-0.20023
D23	-0.00083	0.00005	0.00149	-0.00026	0.00123	0.00041
D24	3.03533	0.00005	0.00605	0.00350	0.00955	3.04488
D25	-3.13723	0.00006	0.00206	0.00083	0.00289	-3.13434
D26	-0.10108	0.00007	0.00662	0.00459	0.01121	-0.08987
D27	-2.46393	0.00005	0.00047	-0.00145	-0.00098	-2.46491
D28	-0.43701	0.00001	-0.00077	-0.00151	-0.00228	-0.43929
D29	1.68080	-0.00003	-0.00016	-0.00185	-0.00201	1.67879
D30	0.80079	0.00003	-0.00478	-0.00588	-0.01066	0.79013
D31	2.82771	-0.00001	-0.00602	-0.00594	-0.01196	2.81575
D32	-1.33766	-0.00004	-0.00540	-0.00629	-0.01169	-1.34936
D33	-2.99781	0.00002	0.00272	-0.00371	-0.00099	-2.99880
D34	1.22482	-0.00006	0.00263	-0.00389	-0.00126	1.22356
D35	-0.89631	0.00002	0.00248	-0.00359	-0.00110	-0.89742
D36	1.17094	0.00002	0.00222	-0.00362	-0.00140	1.16954
D37	-0.88961	-0.00005	0.00213	-0.00380	-0.00167	-0.89128

D38	-3.01074	0.00003	0.00198	-0.00350	-0.00152	-3.01226
D39	-0.92413	0.00004	0.00395	-0.00379	0.00016	-0.92398
D40	-2.98468	-0.00003	0.00387	-0.00398	-0.00011	-2.98480
D41	1.17737	0.00005	0.00372	-0.00367	0.00004	1.17741
D42	-3.13848	-0.00003	-0.00189	0.00017	-0.00171	-3.14019
D43	-0.02289	-0.00007	-0.00180	-0.00032	-0.00213	-0.02501
D44	-0.00849	-0.00002	-0.00016	-0.00024	-0.00040	-0.00889
D45	3.10711	-0.00005	-0.00007	-0.00074	-0.00081	3.10630
D46	-2.75219	-0.00005	-0.00044	-0.00053	-0.00096	-2.75315
D47	-0.04407	-0.00010	-0.00132	-0.00065	-0.00196	-0.04602
D48	-0.02321	0.00004	-0.00035	0.00096	0.00061	-0.02260
D49	2.68492	0.00000	-0.00123	0.00085	-0.00039	2.68453
D50	0.28395	0.00019	0.00971	0.01224	0.02196	0.30591
D51	-2.09196	0.00018	0.00930	0.01143	0.02075	-2.07120
D52	2.57042	-0.00013	-0.00220	-0.00337	-0.00560	2.56482
D53	0.19049	-0.00013	-0.00327	-0.00399	-0.00728	0.18321
D54	2.55187	0.00001	0.00091	0.00119	0.00210	2.55397
D55	-1.65607	0.00002	0.00177	0.00173	0.00351	-1.65256
D56	0.43709	0.00002	0.00138	0.00155	0.00294	0.44003
D57	1.32459	0.00000	0.00123	0.00167	0.00288	1.32747
D58	-2.88335	0.00001	0.00209	0.00221	0.00429	-2.87906
D59	-0.79019	0.00001	0.00170	0.00203	0.00372	-0.78647
D60	-1.01995	-0.00001	0.00007	0.00110	0.00117	-1.01878
D61	1.05529	0.00000	0.00093	0.00165	0.00258	1.05788
D62	-3.13474	0.00000	0.00055	0.00147	0.00201	-3.13272
D63	1.51718	-0.00001	-0.01355	0.00521	-0.00842	1.50876
D64	2.83060	0.00007	-0.00809	0.01268	0.00467	2.83527
D65	2.28077	-0.00005	-0.00054	0.00212	0.00158	2.28235
D66	-0.83831	0.00007	0.00202	0.00405	0.00608	-0.83223
D67	-1.91015	-0.00009	-0.00210	0.00152	-0.00059	-1.91074
D68	1.25395	0.00002	0.00046	0.00345	0.00391	1.25786
D69	0.12263	0.00001	-0.00041	0.00233	0.00193	0.12455
D70	-2.99645	0.00013	0.00215	0.00427	0.00642	-2.99003
D71	2.93079	-0.00009	-0.00130	-0.00642	-0.00772	2.92306
D72	-0.18771	0.00003	0.00131	-0.00444	-0.00314	-0.19085
D73	-1.99063	0.00030	0.00444	0.01761	0.02205	-1.96857

Item	Value	Threshold	Converged?
Maximum Force	0.000650	0.000450	NO
RMS Force	0.000125	0.000300	YES
Maximum Displacement	0.110547	0.001800	NO
RMS Displacement	0.025521	0.001200	NO

Predicted change in Energy=-2.041346D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.854215	1.647814	1.541399
2	6	0	-1.509612	0.457218	1.576936
3	7	0	-2.359696	0.445464	0.478837
4	6	0	-2.217383	1.598235	-0.193086
5	7	0	-1.304685	2.350361	0.434429
6	6	0	-0.769573	3.641286	-0.036663
7	1	0	-0.087383	2.038694	2.186002
8	1	0	-1.358562	-0.409033	2.232274
9	1	0	-1.606191	4.251954	-0.380713
10	1	0	-0.329250	4.126851	0.832043
11	35	0	-0.414846	-2.435123	2.921181
12	1	0	-2.745978	1.867606	-1.091331
13	6	0	-3.243646	-0.609240	0.082064
14	6	0	-3.211786	-1.824571	0.612086
15	1	0	-3.928255	-0.304796	-0.699826
16	1	0	-3.917947	-2.561222	0.249619
17	1	0	-2.497059	-2.132763	1.378062
18	6	0	2.555677	-0.684840	1.162298
19	6	0	3.980133	-0.370940	1.308417
20	8	0	2.984749	0.657980	1.558592
21	1	0	2.144051	-0.724352	0.157843
22	1	0	2.003664	-1.227758	1.924549
23	1	0	4.460876	-0.688726	2.230696
24	6	0	4.888903	-0.162780	0.128763
25	1	0	5.654578	0.585301	0.353701
26	1	0	5.397729	-1.100522	-0.114363
27	1	0	4.323563	0.162648	-0.747157
28	6	0	0.273399	3.473074	-1.150763
29	1	0	0.723036	4.453613	-1.338098
30	1	0	-0.185977	3.134287	-2.080121
31	6	0	1.376916	2.484497	-0.792042
32	8	0	1.724915	1.589729	-1.525597
33	8	0	1.869319	2.715209	0.423819
34	1	0	2.443607	1.946558	0.730137

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.359532	0.000000			

3	N	2.200263	1.388741	0.000000		
4	C	2.206608	2.221674	1.341870	0.000000	
5	N	1.386318	2.220655	2.177993	1.338837	0.000000
6	C	2.543890	3.645497	3.606593	2.508920	1.474707
7	H	1.075329	2.212411	3.258251	3.223501	2.155682
8	H	2.227621	1.096665	2.192481	3.263291	3.293843
9	H	3.322879	4.271035	3.974414	2.729649	2.090794
10	H	2.631425	3.926108	4.219014	3.318107	2.065305
11	Br	4.332115	3.372112	4.247972	5.405162	5.465950
12	H	3.249360	3.261509	2.153400	1.076484	2.153676
13	C	3.596294	2.525638	1.432199	2.449871	3.555695
14	C	4.298746	3.005809	2.428347	3.654140	4.593327
15	H	4.276154	3.407953	2.100598	2.608716	3.901220
16	H	5.363873	4.083237	3.394237	4.515417	5.566592
17	H	4.125334	2.778957	2.733995	4.057964	4.733984
18	C	4.148778	4.242970	5.089755	5.461831	4.964337
19	C	5.244098	5.558349	6.445785	6.673932	6.008214
20	O	3.964557	4.498880	5.456568	5.569078	4.746277
21	H	4.065833	4.093798	4.664251	4.953752	4.628622
22	H	4.072246	3.911916	4.891693	5.503440	5.095936
23	H	5.846772	6.114516	7.132713	7.463514	6.760497
24	C	6.185240	6.589582	7.282492	7.328305	6.691027
25	H	6.701040	7.268997	8.016470	7.955676	7.180062
26	H	7.027212	7.280000	7.932188	8.079568	7.558580
27	H	5.852571	6.286024	6.800661	6.719514	6.153000
28	C	3.442502	4.440141	4.330728	3.261312	2.502732
29	H	4.318765	5.427090	5.373058	4.255619	3.417188
30	H	3.971341	4.721523	4.301523	3.169696	2.861645
31	C	3.335106	4.248995	4.442417	3.750093	2.951815
32	O	4.007711	4.622819	4.691604	4.161415	3.687647
33	O	3.131446	4.224379	4.799931	4.281277	3.194922
34	H	3.409256	4.308496	5.038666	4.764294	3.781560

		6	7	8	9	10
6	C	0.000000				
7	H	2.823814	0.000000			
8	H	4.679751	2.758514	0.000000		
9	H	1.091428	3.713937	5.349189	0.000000	
10	H	1.088259	2.500421	4.857404	1.765505	0.000000
11	Br	6.767379	4.545630	2.338853	7.552404	6.887040
12	H	2.857348	4.223542	4.260793	2.736641	3.826765
13	C	4.919563	4.626024	2.866536	5.150401	5.611304
14	C	6.021700	5.211901	2.839577	6.362998	6.616405
15	H	5.097904	5.345301	3.900179	5.124235	5.910918
16	H	6.961704	6.291425	3.887582	7.222251	7.612377

17	H	6.190743	4.884706	2.235419	6.682181	6.646826
18	C	5.586606	3.930824	4.067209	6.638823	5.619986
19	C	6.361360	4.808448	5.418176	7.445221	6.247226
20	O	5.053701	3.426078	4.522911	6.144452	4.852168
21	H	5.252221	4.089884	4.083012	6.254436	5.486887
22	H	5.936732	3.887228	3.474129	6.955037	5.942044
23	H	7.158737	5.303534	5.826156	8.248580	6.934790
24	C	6.820310	5.817400	6.596682	7.869923	6.791513
25	H	7.124685	6.199983	7.328156	8.167158	6.969761
26	H	7.779871	6.725534	7.185565	8.819004	7.811491
27	H	6.208522	5.619556	6.441302	7.212398	6.313275
28	C	1.535351	3.649878	5.401758	2.175428	2.173046
29	H	2.140441	4.348321	6.381687	2.526371	2.433843
30	H	2.184801	4.405662	5.703230	2.480761	3.080002
31	C	2.552680	3.348382	5.000185	3.491708	2.871582
32	O	3.556442	4.154751	5.255899	4.415254	4.026791
33	O	2.834328	2.718758	4.842584	3.884331	2.644444
34	H	3.712763	2.921292	4.718232	4.790585	3.528852

		11	12	13	14	15
11	Br	0.000000				
12	H	6.328341	0.000000			
13	C	4.404151	2.785551	0.000000		
14	C	3.677984	4.092771	1.326261	0.000000	
15	H	5.476681	2.504074	1.082926	2.131703	0.000000
16	H	4.407365	4.773487	2.071954	1.082913	2.448063
17	H	2.609262	4.707740	2.134977	1.092033	3.115671
18	C	3.870551	6.300902	5.899557	5.904689	6.756724
19	C	5.116414	7.484012	7.331010	7.370320	8.159658
20	O	4.793869	6.428570	6.525250	6.742105	7.336008
21	H	4.136512	5.673716	5.389459	5.486511	6.146911
22	H	2.881006	6.421519	5.595675	5.411068	6.551860
23	H	5.224876	8.337231	7.998912	7.923369	8.894542
24	C	6.410217	7.993903	8.144928	8.283496	8.857144
25	H	7.249332	8.619846	8.982154	9.191662	9.681574
26	H	6.691914	8.722626	8.657558	8.670394	9.378162
27	H	6.531281	7.280366	7.651540	7.910630	8.265182
28	C	7.208411	3.420189	5.527635	6.581731	5.668292
29	H	8.178686	4.333864	6.586646	7.661699	6.684635
30	H	7.488907	3.022547	5.295128	6.402638	5.266607
31	C	6.418808	4.179519	5.628931	6.449483	5.994456
32	O	6.368033	4.500521	5.666272	6.371668	6.019091
33	O	6.162803	4.931032	6.108287	6.816353	6.632863
34	H	5.671909	5.500524	6.268727	6.798442	6.907533

		16	17	18	19	20

16	H	0.000000				
17	H	1.864372	0.000000			
18	C	6.801588	5.260530	0.000000		
19	C	8.264264	6.712889	1.465932	0.000000	
20	O	7.728123	6.153946	1.464348	1.453290	0.000000
21	H	6.334851	5.001245	1.086245	2.195432	2.140026
22	H	6.296745	4.623222	1.086511	2.240577	2.156956
23	H	8.811105	7.157170	2.184324	1.087520	2.108148
24	C	9.128402	7.745580	2.604742	1.503588	2.518701
25	H	10.076938	8.653691	3.445326	2.151661	2.930022
26	H	9.436522	8.100650	3.143233	2.136860	3.422510
27	H	8.737020	7.503755	2.736727	2.151289	2.711872
28	C	7.479383	6.745057	5.277054	5.879106	4.755710
29	H	8.559642	7.818368	6.001188	6.394453	5.283274
30	H	7.196813	6.711330	5.711014	6.412899	5.424558
31	C	7.387822	6.405944	3.905588	4.397975	3.383308
32	O	7.226596	6.333502	3.617818	4.118478	3.459416
33	O	7.833487	6.593836	3.546375	3.842182	2.600786
34	H	7.811552	6.439786	2.669003	2.840090	1.624686

		21	22	23	24	25
21	H	0.000000				
22	H	1.842384	0.000000			
23	H	3.108966	2.534200	0.000000		
24	C	2.801860	3.561408	2.208608	0.000000	
25	H	3.751980	4.368514	2.563431	1.093838	0.000000
26	H	3.286643	3.961443	2.558626	1.094246	1.768348
27	H	2.521124	3.801733	3.100209	1.092130	1.778236
28	C	4.778093	5.877855	6.803661	6.013277	6.289653
29	H	5.573907	6.675541	7.290499	6.388835	6.492005
30	H	5.032554	6.313426	7.402149	6.442377	6.821502
31	C	3.433291	4.642577	5.358833	4.493329	4.818512
32	O	2.892164	4.463120	5.175574	3.977312	4.470222
33	O	3.460751	4.221046	4.644108	4.181837	4.343916
34	H	2.747910	3.420008	3.642220	3.284878	3.507856

		26	27	28	29	30
26	H	0.000000				
27	H	1.774785	0.000000			
28	C	6.946270	5.246489	0.000000		
29	H	7.361977	5.632529	1.094863	0.000000	
30	H	7.278433	5.562677	1.090646	1.765651	0.000000
31	C	5.429415	3.751762	1.524374	2.145496	2.126972
32	O	4.766403	3.065207	2.407154	3.039860	2.518862
33	O	5.224856	3.729619	2.366565	2.727703	3.266433
34	H	4.327206	2.983113	3.252359	3.677402	4.027774

		31	32	33	34
31	C	0.000000			
32	O	1.208228	0.000000		
33	O	1.331918	2.255611	0.000000	
34	H	1.935003	2.394197	1.007205	0.000000

Stoichiometry C11H17BrN2O3
Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.064827	1.333823	1.243793
2	6	0	-1.164157	1.251410	0.668352
3	7	0	-1.226903	2.274313	-0.268843
4	6	0	-0.067906	2.950381	-0.252282
5	7	0	0.738119	2.397107	0.662430
6	6	0	2.143612	2.763405	0.917720
7	1	0	0.526788	0.710890	1.988696
8	1	0	-1.943712	0.488459	0.781817
9	1	0	2.212147	3.852278	0.947268
10	1	0	2.386044	2.380811	1.907244
11	35	0	-3.071813	-1.506974	0.317198
12	1	0	0.173166	3.793187	-0.877086
13	6	0	-2.320206	2.579855	-1.142071
14	6	0	-3.361311	1.776524	-1.314489
15	1	0	-2.194880	3.529477	-1.647283
16	1	0	-4.142622	2.088171	-1.996494
17	1	0	-3.464875	0.805749	-0.825196
18	6	0	0.622757	-2.467150	-0.322630
19	6	0	1.625047	-3.502156	-0.052196
20	8	0	1.646523	-2.261243	0.703929
21	1	0	0.762325	-1.840669	-1.198970
22	1	0	-0.392946	-2.534727	0.057220
23	1	0	1.312191	-4.338321	0.568811
24	6	0	2.790741	-3.759483	-0.966371
25	1	0	3.671525	-4.070195	-0.397020
26	1	0	2.541244	-4.564890	-1.663826
27	1	0	3.039790	-2.865876	-1.542731
28	6	0	3.100922	2.188072	-0.135776

```
      29          1          0        4.124327    2.378076    0.203731
      30          1          0        2.973840    2.678876   -1.101421
      31          6          0        2.922406    0.689503   -0.350581
      32          8          0        2.808047    0.188973   -1.444294
      33          8          0        2.876868    0.027910    0.804506
      34          1          0        2.558681   -0.917368    0.664261
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.3303186           0.2537696           0.1596456
 Standard basis: 6-311++G(d,p) (5D, 7F)
 There are     538 symmetry adapted cartesian basis functions of A      symmetry.
 There are     519 symmetry adapted basis functions of A      symmetry.
   519 basis functions,      823 primitive gaussians,      538 cartesian basis functions
    78 alpha electrons              78 beta electrons
         nuclear repulsion energy           1573.1222749987 Hartrees.
 NAtoms=       34 NActive=       34 NUniq=       34 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      519 RedAO= T EigKep=    3.50D-06    NBF=      519
 NBsUse=      519 1.00D-06 EigRej= -1.00D+00 NBFU=      519
 Initial guess from the checkpoint file:    "./coohpo.chk"
 B after Tr=          0.000000        0.000000        0.000000
            Rot=        1.000000        0.000240        0.000068        0.000587 Ang=      0.07 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn=                5 AccDes=
0.00D+00
 Harris functional with IExCor=    402 and IRadAn=             5 diagonalized for initial guess.
 HarFok:    IExCor=    402 AccDes= 0.00D+00 IRadAn=                5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=    3500011 ScaDFX=    1.000000    1.000000    1.000000    1.000000
 FoFCou: FMM=F IPFlag=                  0 FMFlag=           100000 FMFlg1=                  0
            NFxFlg=                   0 DoJE=T BraDBF=F KetDBF=T FulRan=T
            wScrn=      0.000000 ICntrl=             500 IOpCl=      0 I1Cent=        200000004 NGrid=
0
            NMat0=         1 NMatS0=             1 NMatT0=         0 NMatD0=         1 NMtDS0=         0
NMtDT0=         0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                      energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3338.90384433          A.U. after      12 cycles
                  NFock= 12    Conv=0.35D-08         -V/T= 2.0019
 Calling FoFJK, ICntrl=             2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
```

NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000009638	-0.000213684	-0.000268060
2	6	0.000386945	0.000526030	0.000157415
3	7	-0.000214683	-0.000513485	-0.000017388
4	6	-0.000071069	0.000376412	-0.000038053
5	7	-0.000057173	0.000184866	-0.000113797
6	6	-0.000113682	-0.000176849	0.000190427
7	1	-0.000012951	0.000026032	0.000108907
8	1	-0.000482595	-0.000335166	-0.000148904
9	1	0.000034232	-0.000025320	-0.000041159
10	1	0.000048177	-0.000018744	-0.000027795
11	35	0.000259728	-0.000021567	0.000140206
12	1	0.000034128	-0.000026675	-0.000009479
13	6	0.000342401	0.000492878	0.000123758
14	6	-0.000249740	-0.000369501	0.000009337
15	1	-0.000024644	-0.000036325	-0.000037281
16	1	0.000030375	0.000059974	-0.000030575
17	1	0.000060502	0.000045654	-0.000017012
18	6	-0.000031570	-0.000006145	-0.000089352
19	6	-0.000208500	0.000202363	0.000285487
20	8	0.000025640	-0.000688638	-0.000153693
21	1	0.000000691	0.000006802	-0.000040892
22	1	0.000007571	0.000040354	0.000096127
23	1	0.000082135	0.000006671	-0.000032126
24	6	0.000003106	0.000000537	-0.000170516
25	1	0.000014764	-0.000012978	0.000038021
26	1	-0.000002791	-0.000014706	0.000058347
27	1	0.000005435	-0.000002809	0.000058497
28	6	0.000012326	0.000313870	-0.000152532
29	1	0.000031850	-0.000112858	-0.000078225
30	1	0.000051575	-0.000033265	0.000028632
31	6	-0.000368634	0.000052017	0.000662856
32	8	0.000127989	-0.000152498	-0.000237164
33	8	0.000207753	-0.000606637	-0.000377373
34	1	0.000061071	0.001033389	0.000123356

Cartesian Forces: Max 0.001033389 RMS 0.000230439

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000427431 RMS 0.000114624
Search for a local minimum.
Step number 28 out of a maximum of 175
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 21 22 23 24 25
26 27 28
DE= -2.98D-05 DEPred=-2.04D-05 R= 1.46D+00
TightC=F SS= 1.41D+00 RLast= 6.22D-02 DXNew= 1.3149D+00 1.8657D-01
Trust test= 1.46D+00 RLast= 6.22D-02 DXMaxT set to 7.82D-01
ITU= 1 1 1 -1 0 1 1 1 1 1 1 1 1 1 0 0 -1 1 1
ITU= 1 0 1 0 -1 0 1 0
Eigenvalues --- 0.00152 0.00333 0.00395 0.00571 0.00665
Eigenvalues --- 0.00725 0.00863 0.01161 0.01376 0.01646
Eigenvalues --- 0.01976 0.02087 0.02181 0.02264 0.02346
Eigenvalues --- 0.02410 0.02665 0.02821 0.03126 0.03197
Eigenvalues --- 0.03444 0.03549 0.03843 0.04246 0.04824
Eigenvalues --- 0.04898 0.05053 0.05392 0.05717 0.05878
Eigenvalues --- 0.05914 0.06070 0.06492 0.07653 0.09468
Eigenvalues --- 0.09577 0.11844 0.12618 0.12764 0.13250
Eigenvalues --- 0.13684 0.15160 0.15586 0.15872 0.15983
Eigenvalues --- 0.15992 0.16011 0.16034 0.16068 0.16254
Eigenvalues --- 0.17024 0.17680 0.20442 0.21791 0.22166
Eigenvalues --- 0.23102 0.23781 0.24303 0.25262 0.26198
Eigenvalues --- 0.28521 0.29397 0.30419 0.31450 0.32262
Eigenvalues --- 0.33663 0.34499 0.34577 0.34632 0.34824
Eigenvalues --- 0.34890 0.34959 0.34985 0.35108 0.35302
Eigenvalues --- 0.35406 0.35723 0.35862 0.36586 0.36952
Eigenvalues --- 0.37176 0.37551 0.37979 0.38481 0.40519
Eigenvalues --- 0.41737 0.45136 0.48972 0.50372 0.51667
Eigenvalues --- 0.54002 0.55984 0.56943 0.62137 0.90883
Eigenvalues --- 1.50855
En-DIIS/RFO-DIIS IScMMF= 0 using points: 28 27 26 25 24
RFO step: Lambda=-4.20278436D-06.
DidBck=F Rises=F RFO-DIIS coefs: 1.19749 -0.03499 -0.47317 0.39820 -0.08752
Iteration 1 RMS(Cart)= 0.01406884 RMS(Int)= 0.00006787
Iteration 2 RMS(Cart)= 0.00012986 RMS(Int)= 0.00000644
Iteration 3 RMS(Cart)= 0.00000001 RMS(Int)= 0.00000644
Variable Old X -DE/DX Delta X Delta X Delta X New X

			(Linear)	(Quad)	(Total)	
R1	2.56914	-0.00014	-0.00007	0.00001	-0.00006	2.56909
R2	2.61976	-0.00001	-0.00009	0.00008	0.00000	2.61976
R3	2.03208	0.00007	0.00000	0.00010	0.00010	2.03218
R4	2.62434	0.00013	0.00029	0.00011	0.00040	2.62474
R5	2.07240	0.00025	-0.00005	0.00070	0.00066	2.07305
R6	2.53577	0.00031	0.00011	0.00023	0.00034	2.53611
R7	2.70646	-0.00025	-0.00013	-0.00033	-0.00046	2.70601
R8	2.53004	-0.00009	0.00011	-0.00008	0.00002	2.53006
R9	2.03426	-0.00002	0.00000	-0.00001	-0.00001	2.03425
R10	2.78679	-0.00019	-0.00018	-0.00049	-0.00067	2.78612
R11	2.06250	-0.00003	-0.00002	-0.00007	-0.00008	2.06242
R12	2.05651	-0.00001	-0.00003	0.00012	0.00009	2.05660
R13	2.90139	0.00003	0.00063	0.00038	0.00100	2.90240
R14	4.41979	0.00017	0.00535	0.00067	0.00601	4.42580
R15	2.50627	0.00023	-0.00015	0.00027	0.00012	2.50639
R16	2.04643	0.00003	0.00005	0.00008	0.00013	2.04656
R17	2.04641	-0.00005	0.00013	-0.00006	0.00007	2.04648
R18	2.06364	0.00002	0.00003	0.00002	0.00005	2.06369
R19	2.77021	0.00001	0.00018	0.00019	0.00034	2.77056
R20	2.76722	-0.00007	-0.00008	0.00013	0.00005	2.76727
R21	2.05271	0.00004	-0.00008	0.00021	0.00012	2.05283
R22	2.05321	0.00004	-0.00014	0.00024	0.00010	2.05330
R23	2.74632	-0.00020	-0.00057	-0.00083	-0.00139	2.74493
R24	2.05511	0.00000	0.00002	-0.00001	0.00000	2.05512
R25	2.84137	0.00004	0.00000	0.00020	0.00020	2.84157
R26	3.07021	0.00032	0.00393	0.00444	0.00837	3.07858
R27	2.06705	0.00001	-0.00001	0.00000	-0.00001	2.06704
R28	2.06783	0.00000	0.00000	-0.00002	-0.00003	2.06780
R29	2.06383	-0.00004	0.00007	-0.00007	0.00001	2.06384
R30	2.06899	-0.00008	-0.00014	-0.00032	-0.00046	2.06854
R31	2.06102	-0.00004	-0.00013	-0.00010	-0.00023	2.06079
R32	2.88065	0.00006	-0.00012	-0.00021	-0.00033	2.88032
R33	2.28322	0.00029	0.00004	0.00017	0.00021	2.28343
R34	2.51696	-0.00018	0.00027	0.00045	0.00071	2.51768
R35	1.90334	-0.00043	-0.00085	-0.00103	-0.00187	1.90147
A1	1.88391	0.00013	0.00024	0.00016	0.00040	1.88432
A2	2.27370	-0.00011	0.00012	0.00007	0.00018	2.27388
A3	2.12488	-0.00002	-0.00027	-0.00014	-0.00042	2.12446
A4	1.85650	-0.00003	-0.00017	-0.00012	-0.00029	1.85622
A5	2.26655	-0.00015	-0.00022	0.00066	0.00043	2.26698
A6	2.15332	0.00017	0.00037	-0.00059	-0.00021	2.15311
A7	1.90049	-0.00008	0.00000	-0.00001	0.00000	1.90048
A8	2.21817	0.00023	0.00026	0.00028	0.00054	2.21871

A9	2.16443	-0.00015	-0.00028	-0.00028	-0.00055	2.16388
A10	1.89675	-0.00002	0.00000	0.00004	0.00003	1.89679
A11	2.19041	0.00000	0.00012	0.00007	0.00019	2.19060
A12	2.19601	0.00002	-0.00012	-0.00013	-0.00026	2.19575
A13	1.88712	0.00000	-0.00008	-0.00008	-0.00015	1.88697
A14	2.19049	-0.00009	-0.00005	0.00036	0.00031	2.19080
A15	2.20112	0.00009	0.00024	-0.00036	-0.00012	2.20100
A16	1.88845	0.00015	-0.00008	0.00010	0.00001	1.88846
A17	1.85709	0.00013	-0.00002	0.00077	0.00075	1.85784
A18	1.96318	-0.00039	0.00037	-0.00017	0.00020	1.96338
A19	1.88824	-0.00002	-0.00009	0.00007	-0.00002	1.88821
A20	1.93186	0.00009	0.00015	-0.00038	-0.00023	1.93163
A21	1.93186	0.00006	-0.00034	-0.00033	-0.00067	1.93119
A22	2.72843	-0.00018	-0.00546	0.00284	-0.00261	2.72582
A23	2.15231	0.00029	-0.00023	0.00074	0.00051	2.15281
A24	1.96403	-0.00010	0.00003	-0.00031	-0.00028	1.96375
A25	2.16681	-0.00019	0.00020	-0.00043	-0.00023	2.16658
A26	2.06454	-0.00002	0.00037	0.00006	0.00042	2.06496
A27	2.15874	-0.00006	-0.00024	0.00021	-0.00003	2.15870
A28	2.05962	0.00007	-0.00014	-0.00027	-0.00041	2.05921
A29	2.05803	0.00007	-0.00037	-0.00067	-0.00103	2.05700
A30	2.13029	-0.00009	0.00049	0.00015	0.00063	2.13091
A31	1.97647	0.00003	-0.00053	-0.00028	-0.00082	1.97566
A32	2.00119	-0.00004	0.00014	-0.00010	0.00004	2.00123
A33	2.02420	0.00004	0.00015	0.00068	0.00083	2.02503
A34	2.03925	0.00005	0.00048	0.00053	0.00099	2.04024
A35	2.13974	-0.00001	-0.00070	-0.00066	-0.00136	2.13838
A36	1.94300	0.00003	0.00021	0.00066	0.00087	1.94387
A37	2.03869	0.00001	-0.00011	-0.00028	-0.00040	2.03829
A38	2.02487	-0.00005	0.00012	-0.00011	0.00002	2.02488
A39	2.08485	0.00001	0.00139	0.00298	0.00432	2.08917
A40	2.34882	0.00010	0.00472	0.00325	0.00796	2.35679
A41	1.93523	-0.00002	0.00005	0.00008	0.00012	1.93535
A42	1.91423	-0.00006	0.00014	0.00008	0.00022	1.91446
A43	1.93652	-0.00001	-0.00024	-0.00032	-0.00055	1.93597
A44	1.88208	0.00002	0.00006	0.00011	0.00016	1.88225
A45	1.90021	0.00003	-0.00003	0.00004	0.00001	1.90022
A46	1.89427	0.00005	0.00003	0.00002	0.00005	1.89433
A47	1.88075	0.00022	0.00012	0.00049	0.00061	1.88136
A48	1.94576	0.00006	0.00000	-0.00012	-0.00012	1.94563
A49	1.97366	-0.00032	-0.00055	-0.00083	-0.00138	1.97228
A50	1.88112	-0.00006	0.00019	0.00057	0.00076	1.88188
A51	1.90050	0.00006	0.00033	0.00015	0.00048	1.90098
A52	1.87967	0.00005	-0.00004	-0.00019	-0.00023	1.87944

A53	2.14826	-0.00009	0.00028	0.00028	0.00055	2.14881
A54	1.94993	0.00011	0.00016	-0.00017	-0.00001	1.94992
A55	2.18466	-0.00001	-0.00046	-0.00006	-0.00052	2.18414
A56	1.93502	0.00022	-0.00115	0.00002	-0.00113	1.93390
A57	2.82489	-0.00037	-0.00004	-0.00333	-0.00338	2.82151
D1	0.00173	-0.00002	0.00079	0.00117	0.00196	0.00369
D2	3.01911	-0.00003	0.00066	0.00067	0.00133	3.02044
D3	-3.09966	0.00000	-0.00144	-0.00160	-0.00304	-3.10270
D4	-0.08228	-0.00001	-0.00157	-0.00210	-0.00367	-0.08595
D5	-0.00136	0.00005	-0.00117	-0.00017	-0.00134	-0.00270
D6	-3.04657	0.00011	-0.00242	0.00066	-0.00176	-3.04833
D7	3.10416	0.00004	0.00084	0.00232	0.00316	3.10732
D8	0.05894	0.00009	-0.00041	0.00315	0.00274	0.06168
D9	-0.00151	-0.00003	-0.00013	-0.00177	-0.00190	-0.00341
D10	3.12545	-0.00002	-0.00117	-0.00222	-0.00339	3.12206
D11	-3.02897	0.00001	0.00003	-0.00141	-0.00138	-3.03036
D12	0.09798	0.00002	-0.00100	-0.00187	-0.00287	0.09512
D13	-1.52140	0.00023	0.00094	0.00282	0.00376	-1.51764
D14	1.47736	0.00020	0.00076	0.00228	0.00304	1.48040
D15	0.00068	0.00006	-0.00060	0.00169	0.00110	0.00178
D16	3.13546	-0.00003	-0.00128	-0.00134	-0.00262	3.13284
D17	-3.12683	0.00005	0.00039	0.00212	0.00251	-3.12432
D18	0.00795	-0.00005	-0.00029	-0.00091	-0.00120	0.00675
D19	-0.19274	-0.00002	-0.00095	0.00104	0.00009	-0.19265
D20	2.95807	-0.00001	-0.00131	0.00156	0.00025	2.95832
D21	2.93214	-0.00001	-0.00213	0.00053	-0.00160	2.93055
D22	-0.20023	0.00000	-0.00248	0.00105	-0.00144	-0.20167
D23	0.00041	-0.00007	0.00108	-0.00094	0.00014	0.00055
D24	3.04488	-0.00014	0.00232	-0.00173	0.00059	3.04547
D25	-3.13434	0.00002	0.00177	0.00210	0.00386	-3.13048
D26	-0.08987	-0.00004	0.00300	0.00131	0.00431	-0.08556
D27	-2.46491	-0.00009	-0.00016	-0.00491	-0.00506	-2.46998
D28	-0.43929	0.00002	-0.00032	-0.00439	-0.00470	-0.44400
D29	1.67879	-0.00006	-0.00053	-0.00439	-0.00492	1.67387
D30	0.79013	-0.00002	-0.00160	-0.00396	-0.00556	0.78457
D31	2.81575	0.00010	-0.00176	-0.00343	-0.00520	2.81055
D32	-1.34936	0.00002	-0.00198	-0.00343	-0.00541	-1.35477
D33	-2.99880	0.00005	-0.00229	0.00169	-0.00060	-2.99940
D34	1.22356	-0.00004	-0.00259	0.00076	-0.00183	1.22173
D35	-0.89742	0.00007	-0.00214	0.00170	-0.00044	-0.89786
D36	1.16954	0.00006	-0.00254	0.00196	-0.00059	1.16895
D37	-0.89128	-0.00003	-0.00285	0.00103	-0.00182	-0.89310
D38	-3.01226	0.00008	-0.00240	0.00196	-0.00043	-3.01269
D39	-0.92398	-0.00001	-0.00231	0.00233	0.00003	-0.92395

D40	-2.98480	-0.00010	-0.00261	0.00140	-0.00121	-2.98600
D41	1.17741	0.00002	-0.00216	0.00234	0.00018	1.17759
D42	-3.14019	0.00003	-0.00080	0.00077	-0.00003	-3.14022
D43	-0.02501	-0.00003	-0.00134	0.00044	-0.00090	-0.02591
D44	-0.00889	0.00001	-0.00040	0.00020	-0.00021	-0.00909
D45	3.10630	-0.00004	-0.00095	-0.00013	-0.00108	3.10522
D46	-2.75315	-0.00001	-0.00054	0.00043	-0.00010	-2.75326
D47	-0.04602	-0.00005	-0.00076	-0.00021	-0.00097	-0.04700
D48	-0.02260	0.00005	0.00023	0.00103	0.00126	-0.02134
D49	2.68453	0.00002	0.00001	0.00038	0.00039	2.68492
D50	0.30591	0.00009	0.00549	0.00382	0.00931	0.31523
D51	-2.07120	0.00003	0.00570	0.00318	0.00889	-2.06232
D52	2.56482	-0.00008	-0.00096	-0.00372	-0.00470	2.56012
D53	0.18321	-0.00005	-0.00127	-0.00400	-0.00528	0.17794
D54	2.55397	0.00003	0.00052	0.00094	0.00146	2.55543
D55	-1.65256	0.00000	0.00071	0.00117	0.00188	-1.65067
D56	0.44003	0.00001	0.00069	0.00105	0.00174	0.44177
D57	1.32747	0.00001	0.00074	0.00106	0.00179	1.32927
D58	-2.87906	-0.00002	0.00093	0.00129	0.00221	-2.87684
D59	-0.78647	0.00000	0.00090	0.00117	0.00207	-0.78440
D60	-1.01878	0.00001	0.00039	0.00044	0.00083	-1.01795
D61	1.05788	-0.00001	0.00057	0.00067	0.00125	1.05913
D62	-3.13272	0.00000	0.00055	0.00055	0.00111	-3.13162
D63	1.50876	-0.00008	-0.00008	-0.00591	-0.00601	1.50275
D64	2.83527	0.00005	0.00298	-0.00188	0.00113	2.83640
D65	2.28235	-0.00006	0.00170	-0.00715	-0.00545	2.27690
D66	-0.83223	-0.00014	0.00250	-0.00903	-0.00653	-0.83877
D67	-1.91074	0.00006	0.00173	-0.00696	-0.00523	-1.91598
D68	1.25786	-0.00003	0.00252	-0.00884	-0.00632	1.25154
D69	0.12455	0.00004	0.00210	-0.00631	-0.00421	0.12035
D70	-2.99003	-0.00004	0.00290	-0.00819	-0.00529	-2.99533
D71	2.92306	-0.00004	-0.00190	0.00338	0.00148	2.92455
D72	-0.19085	-0.00013	-0.00109	0.00144	0.00035	-0.19050
D73	-1.96857	0.00019	0.00764	0.01562	0.02326	-1.94531

Item	Value	Threshold	Converged?
Maximum Force	0.000427	0.000450	YES
RMS Force	0.000115	0.000300	YES
Maximum Displacement	0.058576	0.001800	NO
RMS Displacement	0.014030	0.001200	NO

Predicted change in Energy=-8.397139D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.850025	1.644284	1.537782
2	6	0	-1.509318	0.455997	1.577175
3	7	0	-2.366627	0.448008	0.484404
4	6	0	-2.226143	1.601816	-0.186488
5	7	0	-1.306794	2.350331	0.435635
6	6	0	-0.772454	3.640711	-0.036708
7	1	0	-0.079311	2.033425	2.178887
8	1	0	-1.356964	-0.411740	2.230825
9	1	0	-1.609685	4.251896	-0.378198
10	1	0	-0.328749	4.126380	0.830278
11	35	0	-0.408874	-2.443121	2.908868
12	1	0	-2.758181	1.873148	-1.082098
13	6	0	-3.254252	-0.604170	0.090011
14	6	0	-3.221222	-1.821373	0.615804
15	1	0	-3.943097	-0.296240	-0.686871
16	1	0	-3.930656	-2.555969	0.255458
17	1	0	-2.501851	-2.133514	1.375849
18	6	0	2.561270	-0.687680	1.144358
19	6	0	3.982992	-0.371570	1.312502
20	8	0	2.983052	0.655573	1.547057
21	1	0	2.166128	-0.726943	0.133224
22	1	0	1.997623	-1.230876	1.897921
23	1	0	4.450973	-0.688685	2.241554
24	6	0	4.908180	-0.162724	0.145663
25	1	0	5.670410	0.585541	0.381391
26	1	0	5.420488	-1.100198	-0.091040
27	1	0	4.354560	0.163015	-0.737602
28	6	0	0.267392	3.472336	-1.154431
29	1	0	0.716779	4.452359	-1.343646
30	1	0	-0.194783	3.132373	-2.081828
31	6	0	1.370831	2.483346	-0.797357
32	8	0	1.713433	1.584227	-1.528306
33	8	0	1.871550	2.719602	0.414451
34	1	0	2.446397	1.952148	0.719462

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.359502	0.000000			
3	N	2.200174	1.388953	0.000000		
4	C	2.206494	2.221992	1.342053	0.000000	

5	N	1.386315	2.220953	2.178178	1.338849	0.000000
6	C	2.543769	3.645544	3.606425	2.508534	1.474350
7	H	1.075382	2.212523	3.258318	3.223380	2.155475
8	H	2.228122	1.097013	2.192846	3.263937	3.294580
9	H	3.323809	4.271113	3.973237	2.727581	2.090458
10	H	2.633076	3.927252	4.219360	3.317731	2.065590
11	Br	4.333748	3.374800	4.250818	5.407885	5.468119
12	H	3.249186	3.261856	2.153663	1.076476	2.153542
13	C	3.596094	2.525946	1.431957	2.449455	3.555436
14	C	4.299232	3.006870	2.428515	3.654049	4.593540
15	H	4.275723	3.408085	2.100249	2.607859	3.900571
16	H	5.364398	4.084330	3.394477	4.515291	5.566767
17	H	4.126319	2.780508	2.734450	4.058276	4.734663
18	C	4.150875	4.250296	5.099951	5.471039	4.969277
19	C	5.241418	5.560610	6.455627	6.685401	6.013275
20	O	3.958549	4.496902	5.458149	5.571021	4.744496
21	H	4.085667	4.122286	4.695712	4.981705	4.649974
22	H	4.062677	3.904748	4.885014	5.496281	5.087484
23	H	5.834262	6.105470	7.131572	7.464962	6.756392
24	C	6.193561	6.604265	7.308253	7.356799	6.710099
25	H	6.706284	7.279778	8.038874	7.981908	7.197138
26	H	7.035949	7.295677	7.960355	8.110547	7.578909
27	H	5.870198	6.311029	6.837315	6.758663	6.181566
28	C	3.440698	4.440345	4.332482	3.263966	2.503051
29	H	4.317730	5.427487	5.374383	4.257394	3.417486
30	H	3.968038	4.720094	4.302124	3.171962	2.861080
31	C	3.330030	4.247799	4.444559	3.753463	2.950870
32	O	3.996976	4.615521	4.689231	4.161856	3.683171
33	O	3.134510	4.231560	4.809073	4.289716	3.199794
34	H	3.410399	4.315301	5.048059	4.772433	3.784911

		6	7	8	9	10
6	C	0.000000				
7	H	2.823593	0.000000			
8	H	4.680355	2.759335	0.000000		
9	H	1.091384	3.715150	5.349801	0.000000	
10	H	1.088307	2.502284	4.859350	1.765493	0.000000
11	Br	6.769167	4.547631	2.342035	7.554469	6.890957
12	H	2.856612	4.223275	4.261406	2.733671	3.825751
13	C	4.918780	4.626074	2.867022	5.148319	5.611119
14	C	6.021346	5.212898	2.840918	6.361579	6.617262
15	H	5.096594	5.344974	3.900561	5.121096	5.909722
16	H	6.961211	6.292454	3.888918	7.220488	7.613011
17	H	6.190946	4.886405	2.237466	6.681774	6.648781
18	C	5.589597	3.930309	4.075427	6.641871	5.623702

19	C	6.366556	4.799680	5.418493	7.450701	6.249416
20	O	5.052048	3.416980	4.521331	6.142751	4.850598
21	H	5.266929	4.104433	4.112355	6.269542	5.501367
22	H	5.928615	3.879209	3.469159	6.946523	5.937344
23	H	7.156698	5.285573	5.814546	8.246455	6.929811
24	C	6.838785	5.816540	6.607718	7.889605	6.803714
25	H	7.142784	6.195696	7.334778	8.186509	6.980612
26	H	7.799468	6.724579	7.197145	8.840289	7.824300
27	H	6.234733	5.627038	6.462461	7.240189	6.332447
28	C	1.535882	3.647147	5.402271	2.175700	2.173068
29	H	2.141185	4.346636	6.382532	2.526799	2.434202
30	H	2.185092	4.401672	5.701787	2.481458	3.079993
31	C	2.551813	3.341163	4.999227	3.490981	2.870074
32	O	3.554381	4.142341	5.248074	4.413879	4.024421
33	O	2.835973	2.718443	4.850548	3.885257	2.644476
34	H	3.712686	2.918172	4.726282	4.790146	3.527180

		11	12	13	14	15
11	Br	0.000000				
12	H	6.330658	0.000000			
13	C	4.407253	2.785144	0.000000		
14	C	3.681578	4.092281	1.326323	0.000000	
15	H	5.479888	2.503292	1.082993	2.131689	0.000000
16	H	4.410926	4.772927	2.072297	1.082948	2.448370
17	H	2.612768	4.707499	2.135037	1.092060	3.115699
18	C	3.875154	6.309636	5.910915	5.916235	6.768561
19	C	5.111575	7.497752	7.343452	7.381600	8.174721
20	O	4.791826	6.430918	6.527932	6.745036	7.339477
21	H	4.156934	5.699675	5.421943	5.518533	6.179053
22	H	2.877981	6.413513	5.589588	5.406372	6.545750
23	H	5.209747	8.341555	8.000423	7.923927	8.898881
24	C	6.411440	8.026535	8.174550	8.310194	8.891346
25	H	7.246974	8.651062	9.008324	9.214625	9.712787
26	H	6.692111	8.758631	8.690796	8.700510	9.416905
27	H	6.540565	7.323545	7.692043	7.947451	8.310511
28	C	7.208354	3.422970	5.528879	6.582364	5.670008
29	H	8.179158	4.335445	6.587332	7.662050	6.685431
30	H	7.485921	3.025908	5.295185	6.401262	5.267936
31	C	6.416660	4.183558	5.631302	6.450936	5.998011
32	O	6.357061	4.503100	5.664443	6.367585	6.020008
33	O	6.170588	4.938679	6.117725	6.826223	6.642163
34	H	5.680181	5.508129	6.279201	6.809707	6.917995

		16	17	18	19	20
16	H	0.000000				
17	H	1.864196	0.000000			

18	C	6.813644	5.270600	0.000000		
19	C	8.277365	6.720242	1.466115	0.000000	
20	O	7.731855	6.155687	1.464375	1.452556	0.000000
21	H	6.366400	5.031162	1.086311	2.194990	2.139542
22	H	6.292698	4.618721	1.086562	2.241164	2.157050
23	H	8.813797	7.153931	2.185135	1.087522	2.108114
24	C	9.157766	7.765689	2.604027	1.503696	2.517863
25	H	10.102743	8.669952	3.445281	2.151838	2.930115
26	H	9.470123	8.122990	3.141896	2.137107	3.421577
27	H	8.776322	7.533332	2.735205	2.150993	2.709855
28	C	7.480097	6.745115	5.277503	5.887874	4.754683
29	H	8.559933	7.818502	6.001027	6.402622	5.282779
30	H	7.195616	6.708775	5.709370	6.422842	5.422359
31	C	7.389782	6.405926	3.904203	4.407429	3.381758
32	O	7.223487	6.326479	3.608811	4.128708	3.454300
33	O	7.843629	6.603307	3.552189	3.849678	2.603546
34	H	7.823377	6.450476	2.676271	2.848242	1.629116

		21	22	23	24	25
21	H	0.000000				
22	H	1.842959	0.000000			
23	H	3.109185	2.535938	0.000000		
24	C	2.799525	3.561278	2.208717	0.000000	
25	H	3.750226	4.369050	2.563374	1.093830	0.000000
26	H	3.283363	3.960941	2.559355	1.094233	1.768437
27	H	2.517855	3.800535	3.100009	1.092135	1.778240
28	C	4.785102	5.867773	6.808021	6.036623	6.315453
29	H	5.577359	6.666895	7.295766	6.409749	6.516633
30	H	5.037328	6.299444	7.407777	6.469900	6.852320
31	C	3.435757	4.631720	5.365074	4.517057	4.845357
32	O	2.882207	4.443489	5.183830	4.007545	4.505772
33	O	3.470524	4.221712	4.648456	4.195375	4.357367
34	H	2.756765	3.423713	3.648162	3.295801	3.517978

		26	27	28	29	30
26	H	0.000000				
27	H	1.774811	0.000000			
28	C	6.970888	5.275443	0.000000		
29	H	7.384091	5.656785	1.094622	0.000000	
30	H	7.308157	5.596477	1.090525	1.765848	0.000000
31	C	5.453475	3.780230	1.524199	2.145515	2.126558
32	O	4.797304	3.101710	2.407442	3.041974	2.518816
33	O	5.238449	3.745491	2.366712	2.725225	3.266729
34	H	4.338081	2.994181	3.251232	3.674106	4.026908

		31	32	33	34
31	C	0.000000			

32	O	1.208337	0.000000	
33	O	1.332296	2.255744	0.000000
34	H	1.933844	2.392710	1.006213	0.000000

Stoichiometry C11H17BrN2O3
Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.061034	1.332047	1.240297
2	6	0	-1.170677	1.245267	0.671437
3	7	0	-1.244201	2.272382	-0.260669
4	6	0	-0.089596	2.956315	-0.245530
5	7	0	0.724446	2.403306	0.662233
6	6	0	2.128030	2.778228	0.913420
7	1	0	0.529998	0.709858	1.981512
8	1	0	-1.945539	0.477079	0.785078
9	1	0	2.189753	3.867446	0.943632
10	1	0	2.376819	2.396365	1.901699
11	35	0	-3.060336	-1.527846	0.313241
12	1	0	0.144240	3.802342	-0.868714
13	6	0	-2.341883	2.574203	-1.129288
14	6	0	-3.377833	1.764504	-1.303435
15	1	0	-2.224557	3.527280	-1.630040
16	1	0	-4.163244	2.073913	-1.981796
17	1	0	-3.473011	0.790094	-0.819636
18	6	0	0.643935	-2.464622	-0.333013
19	6	0	1.643101	-3.497453	-0.042462
20	8	0	1.661523	-2.247596	0.697428
21	1	0	0.791528	-1.849780	-1.216335
22	1	0	-0.374413	-2.525096	0.041055
23	1	0	1.325766	-4.325849	0.586634
24	6	0	2.813805	-3.766843	-0.946885
25	1	0	3.690803	-4.072497	-0.369030
26	1	0	2.567183	-4.579338	-1.637084
27	1	0	3.067385	-2.879762	-1.531300
28	6	0	3.086254	2.209919	-0.143824
29	1	0	4.109413	2.406439	0.191917
30	1	0	2.951780	2.699556	-1.108924

```
      31        6        0        2.915737      0.710455     -0.357637
      32        8        0        2.795066      0.208910     -1.450326
      33        8        0        2.885964      0.047859      0.797825
      34        1        0        2.574300     -0.898751      0.659038
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.3293246           0.2540810           0.1593612
 Standard basis: 6-311++G(d,p) (5D, 7F)
 There are     538 symmetry adapted cartesian basis functions of A      symmetry.
 There are     519 symmetry adapted basis functions of A      symmetry.
   519 basis functions,      823 primitive gaussians,      538 cartesian basis functions
    78 alpha electrons              78 beta electrons
         nuclear repulsion energy           1572.5258892189 Hartrees.
 NAtoms=       34 NActive=       34 NUniq=       34 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      519 RedAO= T EigKep=    3.53D-06    NBF=      519
 NBsUse=      519 1.00D-06 EigRej= -1.00D+00 NBFU=      519
 Initial guess from the checkpoint file:    "./coohpo.chk"
 B after Tr=          0.000000        0.000000        0.000000
             Rot=        0.999995        0.000054      -0.000398      -0.003002 Ang=      0.35 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn=                5 AccDes=
0.00D+00
 Harris functional with IExCor=    402 and IRadAn=             5 diagonalized for initial guess.
 HarFok:    IExCor=    402 AccDes= 0.00D+00 IRadAn=                5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=    3500011 ScaDFX=    1.000000    1.000000    1.000000    1.000000
 FoFCou: FMM=F IPFlag=                  0 FMFlag=           100000 FMFlg1=                  0
             NFxFlg=                   0 DoJE=T BraDBF=F KetDBF=T FulRan=T
             wScrn=      0.000000  ICntrl=             500  IOpCl=      0  I1Cent=        200000004  NGrid=
0
             NMat0=        1 NMatS0=            1 NMatT0=        0 NMatD0=        1 NMtDS0=        0
NMtDT0=        0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                    energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3338.90385331          A.U. after      11 cycles
                  NFock= 11    Conv=0.28D-08         -V/T= 2.0019
 Calling FoFJK, ICntrl=             2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
```

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000088946	0.000044731	0.000073286
2	6	0.000416426	0.000223413	0.000014526
3	7	-0.000103500	-0.000283220	-0.000004399
4	6	0.000095777	0.000190579	-0.000043772
5	7	-0.000141112	-0.000057230	-0.000104443
6	6	0.000101383	0.000038770	-0.000020864
7	1	0.000027334	-0.000047435	0.000061332
8	1	-0.000434318	-0.000164910	-0.000308200
9	1	0.000008287	-0.000026778	-0.000035074
10	1	0.000005524	-0.000045103	-0.000013602
11	35	0.000182303	0.000093214	0.000072860
12	1	-0.000035160	-0.000021299	0.000032368
13	6	0.000169664	0.000379913	0.000105010
14	6	-0.000135390	-0.000373861	0.000023889
15	1	-0.000030214	-0.000060725	0.000011484
16	1	0.000034345	0.000109408	-0.000047347
17	1	0.000038745	0.000089443	0.000012003
18	6	0.000029997	0.000118442	-0.000177798
19	6	-0.000194177	0.000061407	0.000156229
20	8	-0.000108083	-0.000493765	-0.000069855
21	1	-0.000050930	-0.000005429	-0.000006306
22	1	0.000064293	-0.000001973	0.000173188
23	1	0.000043948	-0.000016711	-0.000020689
24	6	0.000019430	0.000008563	-0.000087903
25	1	0.000019820	-0.000006307	0.000028355
26	1	-0.000003272	-0.000011965	0.000046072
27	1	0.000030338	-0.000013166	0.000027408
28	6	-0.000192380	0.000035188	0.000114557
29	1	0.000060864	0.000000173	-0.000061916
30	1	0.000007707	-0.000020913	-0.000034002
31	6	0.000030140	-0.000088683	0.000472842
32	8	-0.000045480	0.000092489	-0.000062791
33	8	0.000002848	-0.000415356	-0.000525902
34	1	0.000173791	0.000669098	0.000199457

Cartesian Forces: Max 0.000669098 RMS 0.000167680

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000568873 RMS 0.000113385
Search for a local minimum.
Step number 29 out of a maximum of 175
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 21 22 23 24 25
26 27 28 29
DE= -8.98D-06 DEPred=-8.40D-06 R= 1.07D+00
TightC=F SS= 1.41D+00 RLast= 3.96D-02 DXNew= 1.3149D+00 1.1865D-01
Trust test= 1.07D+00 RLast= 3.96D-02 DXMaxT set to 7.82D-01
ITU= 1 1 1 1 -1 0 1 1 1 1 1 1 1 1 1 0 0 -1 1
ITU= 1 1 0 1 0 -1 0 1 0
Eigenvalues --- 0.00152 0.00301 0.00355 0.00523 0.00619
Eigenvalues --- 0.00719 0.00803 0.01164 0.01328 0.01636
Eigenvalues --- 0.01989 0.02189 0.02245 0.02264 0.02395
Eigenvalues --- 0.02460 0.02673 0.02806 0.03131 0.03198
Eigenvalues --- 0.03430 0.03541 0.03891 0.04267 0.04818
Eigenvalues --- 0.04901 0.05005 0.05371 0.05726 0.05853
Eigenvalues --- 0.05940 0.06007 0.06545 0.07463 0.09364
Eigenvalues --- 0.09571 0.11815 0.12618 0.12798 0.13367
Eigenvalues --- 0.13862 0.15279 0.15590 0.15906 0.15990
Eigenvalues --- 0.16010 0.16032 0.16040 0.16131 0.16296
Eigenvalues --- 0.17012 0.17609 0.20469 0.21593 0.22514
Eigenvalues --- 0.23306 0.23924 0.24473 0.25515 0.25876
Eigenvalues --- 0.28802 0.29267 0.30820 0.31544 0.32636
Eigenvalues --- 0.33420 0.34499 0.34581 0.34637 0.34826
Eigenvalues --- 0.34893 0.34958 0.34993 0.35133 0.35304
Eigenvalues --- 0.35483 0.35720 0.36032 0.36578 0.37001
Eigenvalues --- 0.37151 0.37478 0.37760 0.39250 0.40481
Eigenvalues --- 0.41597 0.45258 0.49205 0.50722 0.51689
Eigenvalues --- 0.54210 0.55992 0.56832 0.61906 0.90977
Eigenvalues --- 1.52088
En-DIIS/RFO-DIIS IScMMF= 0 using points: 29 28 27 26 25
RFO step: Lambda=-3.30324637D-06.
DidBck=F Rises=F RFO-DIIS coefs: 1.67664 -0.46715 -0.62815 0.62351 -0.20485
Iteration 1 RMS(Cart)= 0.01595576 RMS(Int)= 0.00009278
Iteration 2 RMS(Cart)= 0.00015375 RMS(Int)= 0.00000386
Iteration 3 RMS(Cart)= 0.00000003 RMS(Int)= 0.00000386

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56909	-0.00018	-0.00003	-0.00015	-0.00018	2.56891

R2	2.61976	-0.00002	0.00001	0.00008	0.00009	2.61985
R3	2.03218	0.00004	0.00011	-0.00003	0.00008	2.03226
R4	2.62474	-0.00005	0.00019	-0.00001	0.00018	2.62492
R5	2.07305	-0.00011	0.00037	0.00023	0.00060	2.07366
R6	2.53611	0.00013	0.00018	0.00005	0.00023	2.53634
R7	2.70601	-0.00018	-0.00044	-0.00032	-0.00076	2.70525
R8	2.53006	-0.00007	-0.00002	-0.00003	-0.00006	2.53000
R9	2.03425	-0.00002	-0.00003	-0.00001	-0.00004	2.03420
R10	2.78612	-0.00011	-0.00057	0.00019	-0.00038	2.78574
R11	2.06242	-0.00001	-0.00007	-0.00003	-0.00010	2.06231
R12	2.05660	-0.00003	0.00011	-0.00009	0.00002	2.05662
R13	2.90240	-0.00017	0.00037	0.00014	0.00051	2.90291
R14	4.42580	0.00002	-0.00159	-0.00260	-0.00420	4.42161
R15	2.50639	0.00016	0.00015	0.00003	0.00018	2.50657
R16	2.04656	-0.00001	0.00004	0.00003	0.00007	2.04663
R17	2.04648	-0.00008	-0.00004	-0.00002	-0.00006	2.04641
R18	2.06369	0.00001	-0.00014	0.00024	0.00009	2.06379
R19	2.77056	-0.00003	0.00015	-0.00001	0.00012	2.77068
R20	2.76727	-0.00012	0.00007	-0.00008	0.00000	2.76727
R21	2.05283	0.00003	0.00017	-0.00001	0.00016	2.05299
R22	2.05330	0.00008	0.00023	0.00004	0.00027	2.05358
R23	2.74493	-0.00006	-0.00091	-0.00042	-0.00132	2.74362
R24	2.05512	0.00000	-0.00004	0.00004	0.00000	2.05512
R25	2.84157	0.00005	0.00012	0.00020	0.00033	2.84190
R26	3.07858	0.00024	0.00641	0.00451	0.01092	3.08950
R27	2.06704	0.00002	0.00001	0.00002	0.00003	2.06707
R28	2.06780	0.00000	-0.00001	-0.00002	-0.00004	2.06776
R29	2.06384	-0.00004	0.00000	-0.00002	-0.00002	2.06381
R30	2.06854	0.00004	-0.00020	0.00006	-0.00014	2.06840
R31	2.06079	0.00003	0.00002	-0.00009	-0.00008	2.06072
R32	2.88032	0.00009	-0.00022	0.00049	0.00027	2.88059
R33	2.28343	-0.00005	-0.00002	-0.00013	-0.00015	2.28328
R34	2.51768	-0.00028	0.00055	-0.00043	0.00011	2.51779
R35	1.90147	-0.00016	-0.00105	-0.00088	-0.00194	1.89953
A1	1.88432	-0.00003	0.00006	-0.00003	0.00003	1.88435
A2	2.27388	-0.00006	0.00021	-0.00035	-0.00014	2.27374
A3	2.12446	0.00009	-0.00021	0.00037	0.00017	2.12462
A4	1.85622	0.00009	-0.00003	0.00006	0.00003	1.85624
A5	2.26698	-0.00014	0.00043	-0.00032	0.00011	2.26709
A6	2.15311	0.00005	-0.00037	0.00033	-0.00004	2.15308
A7	1.90048	-0.00006	-0.00005	-0.00001	-0.00006	1.90042
A8	2.21871	0.00002	0.00034	-0.00009	0.00025	2.21896
A9	2.16388	0.00004	-0.00031	0.00010	-0.00021	2.16367
A10	1.89679	-0.00006	-0.00002	-0.00005	-0.00006	1.89672

A11	2.19060	-0.00001	0.00014	-0.00011	0.00003	2.19062
A12	2.19575	0.00007	-0.00014	0.00016	0.00002	2.19577
A13	1.88697	0.00006	0.00004	0.00003	0.00006	1.88704
A14	2.19080	-0.00023	0.00010	-0.00022	-0.00012	2.19068
A15	2.20100	0.00016	-0.00009	-0.00001	-0.00010	2.20090
A16	1.88846	0.00023	-0.00008	-0.00019	-0.00027	1.88819
A17	1.85784	0.00012	0.00068	0.00010	0.00078	1.85862
A18	1.96338	-0.00057	-0.00027	-0.00019	-0.00046	1.96292
A19	1.88821	-0.00005	0.00006	0.00018	0.00024	1.88845
A20	1.93163	0.00014	-0.00002	0.00005	0.00003	1.93166
A21	1.93119	0.00014	-0.00034	0.00007	-0.00026	1.93092
A22	2.72582	-0.00022	0.00002	0.00702	0.00703	2.73285
A23	2.15281	0.00010	0.00073	-0.00033	0.00040	2.15321
A24	1.96375	0.00002	-0.00024	0.00054	0.00029	1.96405
A25	2.16658	-0.00012	-0.00049	-0.00020	-0.00069	2.16589
A26	2.06496	-0.00005	0.00023	-0.00031	-0.00009	2.06488
A27	2.15870	-0.00007	0.00033	-0.00057	-0.00024	2.15846
A28	2.05921	0.00013	-0.00058	0.00091	0.00034	2.05955
A29	2.05700	0.00013	-0.00094	0.00108	0.00015	2.05715
A30	2.13091	-0.00019	0.00044	-0.00161	-0.00118	2.12974
A31	1.97566	0.00004	-0.00046	-0.00044	-0.00091	1.97475
A32	2.00123	-0.00008	-0.00022	0.00034	0.00011	2.00135
A33	2.02503	0.00006	0.00080	0.00049	0.00129	2.02632
A34	2.04024	-0.00002	0.00060	-0.00008	0.00052	2.04076
A35	2.13838	0.00010	-0.00089	0.00025	-0.00064	2.13774
A36	1.94387	0.00002	0.00059	0.00052	0.00111	1.94498
A37	2.03829	0.00006	-0.00028	0.00015	-0.00013	2.03816
A38	2.02488	-0.00008	0.00003	-0.00044	-0.00041	2.02447
A39	2.08917	0.00007	0.00321	0.00196	0.00514	2.09431
A40	2.35679	0.00013	0.00519	0.00307	0.00824	2.36503
A41	1.93535	-0.00002	0.00015	0.00000	0.00014	1.93550
A42	1.91446	-0.00005	0.00019	-0.00027	-0.00007	1.91438
A43	1.93597	0.00004	-0.00046	0.00045	-0.00001	1.93595
A44	1.88225	0.00001	0.00012	-0.00006	0.00006	1.88231
A45	1.90022	0.00000	0.00004	-0.00003	0.00001	1.90023
A46	1.89433	0.00002	-0.00002	-0.00011	-0.00013	1.89420
A47	1.88136	0.00017	0.00013	0.00043	0.00056	1.88192
A48	1.94563	0.00006	-0.00001	-0.00023	-0.00024	1.94539
A49	1.97228	-0.00030	-0.00086	0.00009	-0.00077	1.97151
A50	1.88188	-0.00005	0.00049	0.00008	0.00057	1.88245
A51	1.90098	0.00010	0.00031	-0.00009	0.00022	1.90120
A52	1.87944	0.00004	0.00001	-0.00027	-0.00026	1.87918
A53	2.14881	-0.00016	0.00001	0.00007	0.00008	2.14889
A54	1.94992	0.00008	0.00013	-0.00002	0.00011	1.95002

A55	2.18414	0.00008	-0.00012	-0.00008	-0.00020	2.18394
A56	1.93390	0.00026	-0.00028	0.00061	0.00033	1.93422
A57	2.82151	-0.00049	-0.00295	-0.00195	-0.00491	2.81661
D1	0.00369	-0.00010	-0.00009	-0.00034	-0.00043	0.00326
D2	3.02044	-0.00009	0.00019	0.00027	0.00046	3.02090
D3	-3.10270	0.00003	-0.00229	-0.00012	-0.00241	-3.10511
D4	-0.08595	0.00004	-0.00202	0.00049	-0.00152	-0.08747
D5	-0.00270	0.00012	0.00055	-0.00018	0.00037	-0.00233
D6	-3.04833	0.00019	-0.00001	0.00207	0.00206	-3.04628
D7	3.10732	0.00000	0.00253	-0.00039	0.00214	3.10946
D8	0.06168	0.00007	0.00197	0.00185	0.00383	0.06551
D9	-0.00341	0.00005	-0.00041	0.00074	0.00034	-0.00307
D10	3.12206	0.00004	-0.00148	0.00096	-0.00052	3.12155
D11	-3.03036	0.00006	-0.00073	0.00024	-0.00049	-3.03085
D12	0.09512	0.00005	-0.00180	0.00046	-0.00135	0.09377
D13	-1.51764	0.00019	0.00211	0.00007	0.00217	-1.51547
D14	1.48040	0.00019	0.00246	0.00074	0.00320	1.48360
D15	0.00178	0.00003	0.00076	-0.00087	-0.00011	0.00166
D16	3.13284	-0.00004	-0.00172	-0.00035	-0.00207	3.13078
D17	-3.12432	0.00004	0.00178	-0.00108	0.00070	-3.12361
D18	0.00675	-0.00003	-0.00070	-0.00055	-0.00125	0.00550
D19	-0.19265	-0.00002	0.00231	-0.00084	0.00147	-0.19118
D20	2.95832	0.00000	0.00308	-0.00151	0.00156	2.95988
D21	2.93055	-0.00003	0.00109	-0.00060	0.00050	2.93104
D22	-0.20167	-0.00001	0.00186	-0.00127	0.00059	-0.20108
D23	0.00055	-0.00009	-0.00080	0.00065	-0.00016	0.00039
D24	3.04547	-0.00018	-0.00023	-0.00163	-0.00186	3.04361
D25	-3.13048	-0.00002	0.00168	0.00012	0.00180	-3.12868
D26	-0.08556	-0.00011	0.00226	-0.00215	0.00010	-0.08545
D27	-2.46998	-0.00010	-0.00393	-0.00274	-0.00667	-2.47665
D28	-0.44400	0.00002	-0.00356	-0.00258	-0.00613	-0.45013
D29	1.67387	-0.00007	-0.00368	-0.00253	-0.00621	1.66766
D30	0.78457	-0.00001	-0.00460	-0.00009	-0.00469	0.77988
D31	2.81055	0.00011	-0.00422	0.00007	-0.00415	2.80640
D32	-1.35477	0.00002	-0.00435	0.00011	-0.00424	-1.35900
D33	-2.99940	0.00009	-0.00101	-0.00053	-0.00154	-3.00094
D34	1.22173	0.00002	-0.00168	-0.00076	-0.00244	1.21929
D35	-0.89786	0.00014	-0.00107	-0.00030	-0.00136	-0.89923
D36	1.16895	0.00008	-0.00071	-0.00018	-0.00089	1.16806
D37	-0.89310	0.00001	-0.00138	-0.00041	-0.00179	-0.89489
D38	-3.01269	0.00013	-0.00077	0.00005	-0.00071	-3.01341
D39	-0.92395	-0.00004	-0.00055	-0.00048	-0.00103	-0.92498
D40	-2.98600	-0.00011	-0.00122	-0.00071	-0.00193	-2.98793
D41	1.17759	0.00001	-0.00061	-0.00025	-0.00086	1.17673

D42	-3.14022	0.00003	0.00076	-0.00081	-0.00005	-3.14028
D43	-0.02591	0.00001	0.00001	0.00026	0.00027	-0.02563
D44	-0.00909	0.00002	-0.00009	-0.00006	-0.00015	-0.00925
D45	3.10522	0.00000	-0.00084	0.00101	0.00017	3.10540
D46	-2.75326	0.00000	0.00022	-0.00045	-0.00022	-2.75348
D47	-0.04700	-0.00003	-0.00040	-0.00126	-0.00166	-0.04866
D48	-0.02134	0.00003	0.00121	-0.00041	0.00080	-0.02054
D49	2.68492	0.00000	0.00059	-0.00123	-0.00064	2.68428
D50	0.31523	0.00000	0.00632	0.00166	0.00799	0.32321
D51	-2.06232	-0.00004	0.00583	0.00103	0.00687	-2.05545
D52	2.56012	-0.00004	-0.00360	-0.00157	-0.00517	2.55496
D53	0.17794	0.00000	-0.00401	-0.00164	-0.00565	0.17228
D54	2.55543	0.00003	0.00083	0.00107	0.00190	2.55733
D55	-1.65067	0.00000	0.00119	0.00083	0.00202	-1.64866
D56	0.44177	0.00001	0.00100	0.00080	0.00180	0.44357
D57	1.32927	0.00001	0.00101	0.00085	0.00186	1.33112
D58	-2.87684	-0.00002	0.00137	0.00061	0.00198	-2.87487
D59	-0.78440	-0.00001	0.00118	0.00058	0.00176	-0.78264
D60	-1.01795	0.00001	0.00034	0.00035	0.00069	-1.01726
D61	1.05913	-0.00002	0.00070	0.00011	0.00081	1.05993
D62	-3.13162	-0.00001	0.00051	0.00008	0.00059	-3.13103
D63	1.50275	-0.00014	-0.00384	-0.00498	-0.00884	1.49391
D64	2.83640	0.00001	0.00117	-0.00203	-0.00084	2.83556
D65	2.27690	-0.00010	-0.00374	-0.00591	-0.00965	2.26726
D66	-0.83877	-0.00007	-0.00434	-0.00484	-0.00918	-0.84795
D67	-1.91598	-0.00001	-0.00392	-0.00537	-0.00929	-1.92526
D68	1.25154	0.00002	-0.00452	-0.00430	-0.00882	1.24272
D69	0.12035	0.00000	-0.00316	-0.00547	-0.00864	0.11171
D70	-2.99533	0.00003	-0.00377	-0.00441	-0.00817	-3.00350
D71	2.92455	-0.00026	0.00055	-0.00345	-0.00290	2.92165
D72	-0.19050	-0.00021	-0.00007	-0.00236	-0.00242	-0.19292
D73	-1.94531	0.00007	0.01652	0.01463	0.03115	-1.91416

Item	Value	Threshold	Converged?
Maximum Force	0.000569	0.000450	NO
RMS Force	0.000113	0.000300	YES
Maximum Displacement	0.061180	0.001800	NO
RMS Displacement	0.015928	0.001200	NO

Predicted change in Energy=-7.181017D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.841594	1.640218	1.532769
2	6	0	-1.501083	0.452186	1.573348
3	7	0	-2.369213	0.449498	0.489008
4	6	0	-2.234372	1.606169	-0.178347
5	7	0	-1.308417	2.351255	0.438007
6	6	0	-0.776213	3.642007	-0.035104
7	1	0	-0.065714	2.026777	2.169259
8	1	0	-1.343290	-0.418574	2.222206
9	1	0	-1.615102	4.253458	-0.371840
10	1	0	-0.327726	4.126951	0.829837
11	35	0	-0.399100	-2.450231	2.897197
12	1	0	-2.773659	1.881045	-1.068496
13	6	0	-3.260701	-0.600209	0.098219
14	6	0	-3.224323	-1.819787	0.618504
15	1	0	-3.956168	-0.288998	-0.671474
16	1	0	-3.937581	-2.552064	0.261100
17	1	0	-2.498762	-2.135569	1.371197
18	6	0	2.560695	-0.687525	1.126475
19	6	0	3.979828	-0.373074	1.318478
20	8	0	2.978226	0.655708	1.533643
21	1	0	2.182512	-0.727009	0.108793
22	1	0	1.984403	-1.228839	1.871993
23	1	0	4.432048	-0.689743	2.255456
24	6	0	4.924758	-0.168370	0.166600
25	1	0	5.685291	0.577954	0.413766
26	1	0	5.437986	-1.107682	-0.060547
27	1	0	4.386652	0.157777	-0.726037
28	6	0	0.258045	3.474254	-1.158464
29	1	0	0.706209	4.454231	-1.350388
30	1	0	-0.208874	3.133236	-2.083044
31	6	0	1.363365	2.485398	-0.806247
32	8	0	1.696152	1.580327	-1.534248
33	8	0	1.877482	2.728860	0.398569
34	1	0	2.451315	1.962079	0.703801

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.359408	0.000000			
3	N	2.200198	1.389047	0.000000		
4	C	2.206560	2.222122	1.342175	0.000000	
5	N	1.386362	2.220941	2.178203	1.338819	0.000000
6	C	2.543552	3.645203	3.606169	2.508262	1.474149

7	H	1.075424	2.212404	3.258399	3.223545	2.155650
8	H	2.228373	1.097333	2.193181	3.264394	3.294925
9	H	3.324887	4.271584	3.972387	2.725633	2.090044
10	H	2.634770	3.928546	4.219893	3.317541	2.066007
11	Br	4.334655	3.375050	4.253134	5.411245	5.470716
12	H	3.249223	3.261967	2.153769	1.076454	2.153504
13	C	3.595765	2.525826	1.431555	2.449071	3.554998
14	C	4.299408	3.007182	2.428504	3.654059	4.593567
15	H	4.275644	3.408228	2.100123	2.607569	3.900316
16	H	5.364467	4.084610	3.394274	4.514968	5.566537
17	H	4.126606	2.780774	2.734522	4.058521	4.734908
18	C	4.142346	4.242249	5.099332	5.473231	4.967716
19	C	5.229281	5.548549	6.455616	6.691350	6.013546
20	O	3.944653	4.484106	5.452421	5.568254	4.738207
21	H	4.095935	4.135733	4.716665	5.003501	4.665905
22	H	4.041388	3.881191	4.866563	5.480805	5.071099
23	H	5.810533	6.080404	7.118663	7.458938	6.745645
24	C	6.195823	6.607228	7.327191	7.383842	6.728644
25	H	6.706773	7.280413	8.055880	8.008051	7.215063
26	H	7.037239	7.297498	7.979923	8.139037	7.597812
27	H	5.885099	6.327659	6.870455	6.799687	6.212902
28	C	3.437387	4.437366	4.331951	3.265350	2.502729
29	H	4.315896	5.425563	5.373964	4.258186	3.417540
30	H	3.962769	4.714555	4.299415	3.172135	2.859403
31	C	3.323729	4.242816	4.444628	3.756463	2.950353
32	O	3.981247	4.599148	4.679693	4.157902	3.675806
33	O	3.140848	4.240054	4.820591	4.301234	3.208441
34	H	3.410870	4.319414	5.056830	4.781267	3.789154

		6	7	8	9	10
6	C	0.000000				
7	H	2.823648	0.000000			
8	H	4.680314	2.759483	0.000000		
9	H	1.091329	3.716974	5.350780	0.000000	
10	H	1.088318	2.504681	4.861261	1.765608	0.000000
11	Br	6.771703	4.548037	2.339815	7.556766	6.894808
12	H	2.856339	4.223418	4.261798	2.730554	3.824964
13	C	4.918013	4.625819	2.867190	5.146556	5.611030
14	C	6.020932	5.213224	2.841398	6.360399	6.618053
15	H	5.096065	5.344924	3.900936	5.119011	5.909326
16	H	6.960495	6.292711	3.889481	7.218702	7.613393
17	H	6.190738	4.886896	2.237723	6.681220	6.650235
18	C	5.588297	3.918272	4.063749	6.640447	5.622290
19	C	6.369693	4.780117	5.399479	7.454208	6.248520
20	O	5.047252	3.398442	4.505962	6.137860	4.845016

21	H	5.278547	4.108938	4.122247	6.281554	5.511997
22	H	5.914656	3.858806	3.442777	6.931580	5.925918
23	H	7.150993	5.255166	5.781795	8.240506	6.920142
24	C	6.860083	5.808109	6.601253	7.912791	6.817496
25	H	7.165259	6.185054	7.325603	8.211105	6.994631
26	H	7.821538	6.714728	7.188291	8.864805	7.838213
27	H	6.266771	5.630227	6.469663	7.274689	6.356133
28	C	1.536154	3.643315	5.398825	2.175917	2.173127
29	H	2.141788	4.344687	6.380290	2.527123	2.435060
30	H	2.185127	4.396228	5.695386	2.482054	3.080012
31	C	2.551510	3.332602	4.993052	3.490847	2.869016
32	O	3.551133	4.125463	5.229221	4.411487	4.021227
33	O	2.839720	2.721080	4.858536	3.887939	2.646430
34	H	3.712826	2.913278	4.729914	4.789903	3.525000

		11	12	13	14	15
11	Br	0.000000				
12	H	6.334446	0.000000			
13	C	4.409718	2.784791	0.000000		
14	C	3.683990	4.092093	1.326419	0.000000	
15	H	5.482615	2.503007	1.083030	2.131421	0.000000
16	H	4.413640	4.772316	2.072302	1.082915	2.447756
17	H	2.614626	4.707533	2.135030	1.092110	3.115503
18	C	3.873367	6.314331	5.912156	5.916628	6.772071
19	C	5.097249	7.509213	7.346148	7.381242	8.182116
20	O	4.786697	6.430921	6.523954	6.740709	7.337631
21	H	4.172459	5.722900	5.444700	5.539660	6.203552
22	H	2.867739	6.399766	5.572482	5.389924	6.530153
23	H	5.181809	8.341452	7.989998	7.910539	8.893238
24	C	6.403633	8.061711	8.197128	8.327000	8.921198
25	H	7.235823	8.686137	9.028755	9.228884	9.741000
26	H	6.679989	8.796565	8.714923	8.718016	9.449529
27	H	6.544689	7.372718	7.728903	7.977812	8.354952
28	C	7.209698	3.426023	5.528298	6.581137	5.670875
29	H	8.181398	4.337075	6.586517	7.660869	6.685574
30	H	7.484255	3.029094	5.292464	6.397165	5.267488
31	C	6.417337	4.189150	5.632142	6.450691	6.001073
32	O	6.346115	4.504060	5.655977	6.356586	6.015603
33	O	6.184574	4.950170	6.129751	6.838639	6.654618
34	H	5.692480	5.517966	6.289609	6.820751	6.929255

		16	17	18	19	20
16	H	0.000000				
17	H	1.864399	0.000000			
18	C	6.815641	5.268285	0.000000		
19	C	8.279578	6.714261	1.466180	0.000000	

20	O	7.729007	6.149391	1.464375	1.451859	0.000000
21	H	6.388236	5.048964	1.086397	2.195212	2.138986
22	H	6.278199	4.601274	1.086706	2.240633	2.157240
23	H	8.803203	7.135016	2.185535	1.087525	2.108282
24	C	9.177798	7.773647	2.603782	1.503868	2.517320
25	H	10.120276	8.675172	3.445648	2.152106	2.930592
26	H	9.491625	8.130093	3.140757	2.137190	3.420731
27	H	8.809684	7.554254	2.735042	2.151128	2.708828
28	C	7.478967	6.743092	5.276699	5.898207	4.753001
29	H	8.558612	7.816926	6.000968	6.414226	5.282846
30	H	7.191725	6.703408	5.706990	6.435043	5.419978
31	C	7.390216	6.403954	3.903391	4.419412	3.380921
32	O	7.213797	6.312432	3.601393	4.143549	3.451171
33	O	7.856336	6.615149	3.559258	3.858508	2.607295
34	H	7.835270	6.460604	2.685334	2.857817	1.634893

		21	22	23	24	25
21	H	0.000000				
22	H	1.843896	0.000000			
23	H	3.109656	2.535475	0.000000		
24	C	2.799167	3.560709	2.208600	0.000000	
25	H	3.750386	4.368924	2.563102	1.093846	0.000000
26	H	3.282027	3.959372	2.559385	1.094214	1.768473
27	H	2.517542	3.800429	3.099944	1.092122	1.778247
28	C	4.791672	5.855174	6.812930	6.066524	6.349446
29	H	5.581570	6.656936	7.303728	6.439398	6.552024
30	H	5.042257	6.283349	7.414573	6.505050	6.892365
31	C	3.439166	4.621063	5.373301	4.546696	4.879121
32	O	2.874009	4.424588	5.196172	4.046569	4.551125
33	O	3.481385	4.224428	4.654104	4.211133	4.373332
34	H	2.767215	3.429962	3.655557	3.308371	3.529663

		26	27	28	29	30
26	H	0.000000				
27	H	1.774702	0.000000			
28	C	7.002238	5.313323	0.000000		
29	H	7.415407	5.691659	1.094550	0.000000	
30	H	7.345944	5.640361	1.090484	1.766122	0.000000
31	C	5.483505	3.816348	1.524344	2.145750	2.126461
32	O	4.837200	3.148911	2.407555	3.045178	2.518298
33	O	5.254239	3.764457	2.366968	2.721697	3.267231
34	H	4.350616	3.007568	3.250406	3.670954	4.026750

		31	32	33	34
31	C	0.000000			
32	O	1.208257	0.000000		
33	O	1.332356	2.255613	0.000000	

34 H 1.933325 2.392669 1.005189 0.000000

Stoichiometry C11H17BrN2O3

Framework group C1[X(C11H17BrN2O3)]

Deg. of freedom 96

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.070539	1.326470	1.235648
2	6	0	-1.162847	1.242872	0.670174
3	7	0	-1.240796	2.277737	-0.253098
4	6	0	-0.086741	2.962798	-0.236289
5	7	0	0.730939	2.403095	0.664027
6	6	0	2.135469	2.775911	0.911855
7	1	0	0.541897	0.699718	1.971543
8	1	0	-1.936937	0.472960	0.780447
9	1	0	2.198070	3.864946	0.944745
10	1	0	2.387883	2.390978	1.898034
11	35	0	-3.060352	-1.524991	0.310485
12	1	0	0.144718	3.813149	-0.854417
13	6	0	-2.341024	2.585217	-1.115829
14	6	0	-3.377333	1.776498	-1.293099
15	1	0	-2.226025	3.541984	-1.610124
16	1	0	-4.164753	2.090898	-1.966765
17	1	0	-3.470723	0.798520	-0.816085
18	6	0	0.641139	-2.460779	-0.342386
19	6	0	1.625059	-3.502677	-0.032492
20	8	0	1.656849	-2.243691	0.689892
21	1	0	0.801798	-1.859304	-1.232709
22	1	0	-0.379700	-2.503801	0.027704
23	1	0	1.293833	-4.318768	0.605469
24	6	0	2.796107	-3.799728	-0.928051
25	1	0	3.666099	-4.110659	-0.342444
26	1	0	2.541041	-4.616980	-1.609480
27	1	0	3.064879	-2.923603	-1.522103
28	6	0	3.089410	2.209637	-0.150735
29	1	0	4.114121	2.405066	0.180647
30	1	0	2.950177	2.700829	-1.114322
31	6	0	2.916816	0.710526	-0.366379
32	8	0	2.781465	0.211885	-1.458589

```
      33        8        0        2.902675        0.044620        0.787546
      34        1        0        2.587460       -0.900064        0.651103
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.3286909           0.2544853           0.1592032
 Standard basis: 6-311++G(d,p) (5D, 7F)
 There are     538 symmetry adapted cartesian basis functions of A      symmetry.
 There are     519 symmetry adapted basis functions of A      symmetry.
    519 basis functions,      823 primitive gaussians,      538 cartesian basis functions
     78 alpha electrons              78 beta electrons
          nuclear repulsion energy           1572.3460511184 Hartrees.
 NAtoms=       34 NActive=       34 NUniq=       34 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      519 RedAO= T EigKep=    3.52D-06    NBF=      519
 NBsUse=      519 1.00D-06 EigRej= -1.00D+00 NBFU=      519
 Initial guess from the checkpoint file:    "./coohpo.chk"
 B after Tr=          0.000000        0.000000        0.000000
             Rot=        0.999999      -0.000034      -0.000582        0.001112 Ang=    -0.14 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn=                5 AccDes=
0.00D+00
 Harris functional with IExCor=    402 and IRadAn=             5 diagonalized for initial guess.
 HarFok:    IExCor=    402 AccDes= 0.00D+00 IRadAn=                5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=    3500011 ScaDFX=    1.000000    1.000000    1.000000    1.000000
 FoFCou: FMM=F IPFlag=                  0 FMFlag=           100000 FMFlg1=                  0
             NFxFlg=                   0 DoJE=T BraDBF=F KetDBF=T FulRan=T
             wScrn=      0.000000 ICntrl=             500 IOpCl=      0 I1Cent=        200000004 NGrid=
0
             NMat0=        1 NMatS0=           1 NMatT0=        0 NMatD0=        1 NMtDS0=        0
NMtDT0=        0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                    energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3338.90386576          A.U. after      11 cycles
                  NFock= 11    Conv=0.43D-08         -V/T= 2.0019
 Calling FoFJK, ICntrl=             2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 ---------------------------------------------------------------------
 Center         Atomic                             Forces (Hartrees/Bohr)
```

Number	Number	X	Y	Z
1	6	-0.000079513	0.000102527	0.000102166
2	6	0.000314183	0.000079369	0.000029573
3	7	0.000107698	-0.000059919	-0.000036238
4	6	0.000176374	0.000063250	-0.000004426
5	7	-0.000147661	-0.000074573	-0.000032725
6	6	0.000184458	0.000087934	-0.000168558
7	1	0.000067568	-0.000066387	0.000016145
8	1	-0.000490854	-0.000072649	-0.000313234
9	1	0.000009225	0.000017469	-0.000042227
10	1	-0.000024301	-0.000062378	0.000016966
11	35	0.000162820	0.000072090	0.000071866
12	1	-0.000069901	-0.000000237	0.000044179
13	6	-0.000001154	0.000120008	0.000062999
14	6	-0.000036660	-0.000261280	0.000036020
15	1	-0.000014022	-0.000026368	0.000035239
16	1	0.000035054	0.000086794	-0.000041269
17	1	-0.000010985	0.000077473	0.000012634
18	6	0.000080315	0.000176580	-0.000185907
19	6	-0.000091072	-0.000031984	-0.000113917
20	8	-0.000210171	-0.000240949	0.000071550
21	1	-0.000046352	-0.000062076	0.000037515
22	1	0.000055332	-0.000005857	0.000167045
23	1	0.000002222	-0.000012778	0.000004305
24	6	0.000022553	0.000007750	0.000017135
25	1	0.000006485	-0.000002858	0.000018298
26	1	0.000008541	-0.000013556	0.000025748
27	1	0.000025323	-0.000011725	0.000013799
28	6	-0.000127187	-0.000049812	0.000204116
29	1	0.000034545	0.000042302	-0.000030431
30	1	-0.000008777	-0.000012274	-0.000043502
31	6	0.000001241	-0.000204392	0.000290121
32	8	-0.000066361	0.000136821	-0.000070647
33	8	-0.000119740	-0.000090437	-0.000307223
34	1	0.000250773	0.000292121	0.000112887

Cartesian Forces: Max 0.000490854 RMS 0.000122779

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000367830 RMS 0.000080398

Search for a local minimum.
Step number 30 out of a maximum of 175
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 21 22 23 24 25
26 27 28 29 30
DE= -1.24D-05 DEPred=-7.18D-06 R= 1.73D+00
TightC=F SS= 1.41D+00 RLast= 4.83D-02 DXNew= 1.3149D+00 1.4483D-01
Trust test= 1.73D+00 RLast= 4.83D-02 DXMaxT set to 7.82D-01
ITU= 1 1 1 1 1 -1 0 1 1 1 1 1 1 1 1 1 0 0 -1
ITU= 1 1 1 0 1 0 -1 0 1 0
Eigenvalues --- 0.00156 0.00274 0.00346 0.00513 0.00675
Eigenvalues --- 0.00727 0.00847 0.01199 0.01275 0.01603
Eigenvalues --- 0.01991 0.02209 0.02249 0.02275 0.02363
Eigenvalues --- 0.02443 0.02616 0.02792 0.03124 0.03168
Eigenvalues --- 0.03426 0.03586 0.03960 0.04279 0.04816
Eigenvalues --- 0.04898 0.04971 0.05320 0.05687 0.05769
Eigenvalues --- 0.05887 0.05989 0.06457 0.07301 0.09278
Eigenvalues --- 0.09573 0.11797 0.12608 0.12831 0.13221
Eigenvalues --- 0.13916 0.15471 0.15650 0.15763 0.15986
Eigenvalues --- 0.16010 0.16034 0.16041 0.16099 0.16178
Eigenvalues --- 0.16987 0.17539 0.20364 0.20827 0.22451
Eigenvalues --- 0.23309 0.23774 0.24037 0.25481 0.25892
Eigenvalues --- 0.28776 0.29268 0.30705 0.31644 0.32582
Eigenvalues --- 0.33290 0.34500 0.34581 0.34627 0.34809
Eigenvalues --- 0.34891 0.34957 0.35015 0.35160 0.35290
Eigenvalues --- 0.35442 0.35719 0.35861 0.36570 0.36974
Eigenvalues --- 0.37179 0.37573 0.37865 0.39277 0.41015
Eigenvalues --- 0.41378 0.45227 0.49487 0.50714 0.51637
Eigenvalues --- 0.53897 0.56123 0.56475 0.61248 0.91408
Eigenvalues --- 1.43733
En-DIIS/RFO-DIIS IScMMF= 0 using points: 30 29 28 27 26
RFO step: Lambda=-1.91289586D-06.
DidBck=F Rises=F RFO-DIIS coefs: 1.40987 -0.30355 -0.32657 0.06270 0.15755
Iteration 1 RMS(Cart)= 0.00639300 RMS(Int)= 0.00001729
Iteration 2 RMS(Cart)= 0.00004519 RMS(Int)= 0.00001211
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001211

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56891	-0.00009	-0.00011	0.00004	-0.00007	2.56884
R2	2.61985	0.00000	0.00006	0.00003	0.00009	2.61994
R3	2.03226	0.00004	0.00011	0.00004	0.00016	2.03242

R4	2.62492	-0.00015	-0.00018	-0.00026	-0.00044	2.62448
R5	2.07366	-0.00019	-0.00006	-0.00045	-0.00052	2.07314
R6	2.53634	0.00003	0.00031	-0.00010	0.00021	2.53655
R7	2.70525	-0.00001	-0.00051	0.00008	-0.00043	2.70481
R8	2.53000	-0.00007	-0.00018	-0.00002	-0.00020	2.52980
R9	2.03420	0.00000	-0.00003	0.00000	-0.00003	2.03417
R10	2.78574	-0.00002	-0.00014	0.00006	-0.00007	2.78566
R11	2.06231	0.00002	-0.00005	0.00005	0.00000	2.06231
R12	2.05662	-0.00002	0.00000	-0.00002	-0.00002	2.05660
R13	2.90291	-0.00025	-0.00036	-0.00038	-0.00074	2.90217
R14	4.42161	0.00003	0.00230	0.00088	0.00319	4.42479
R15	2.50657	0.00010	0.00032	-0.00007	0.00024	2.50681
R16	2.04663	-0.00003	0.00004	-0.00006	-0.00002	2.04661
R17	2.04641	-0.00007	-0.00018	-0.00002	-0.00020	2.04621
R18	2.06379	-0.00002	0.00002	-0.00008	-0.00006	2.06373
R19	2.77068	-0.00005	-0.00005	-0.00018	-0.00018	2.77049
R20	2.76727	-0.00011	-0.00008	0.00000	-0.00009	2.76718
R21	2.05299	-0.00001	0.00011	-0.00018	-0.00006	2.05293
R22	2.05358	0.00008	0.00013	0.00001	0.00014	2.05372
R23	2.74362	0.00006	-0.00021	-0.00007	-0.00031	2.74331
R24	2.05512	0.00001	0.00001	0.00003	0.00003	2.05516
R25	2.84190	0.00000	0.00013	-0.00004	0.00009	2.84199
R26	3.08950	0.00011	0.00003	0.00361	0.00363	3.09313
R27	2.06707	0.00001	0.00004	0.00001	0.00004	2.06711
R28	2.06776	0.00001	-0.00001	0.00004	0.00003	2.06779
R29	2.06381	-0.00002	-0.00011	0.00000	-0.00011	2.06370
R30	2.06840	0.00006	-0.00005	0.00015	0.00010	2.06850
R31	2.06072	0.00004	0.00002	0.00011	0.00013	2.06084
R32	2.88059	-0.00002	0.00037	-0.00024	0.00012	2.88071
R33	2.28328	-0.00008	0.00015	-0.00023	-0.00008	2.28320
R34	2.51779	-0.00016	-0.00053	0.00003	-0.00050	2.51729
R35	1.89953	0.00002	-0.00014	-0.00018	-0.00032	1.89921
A1	1.88435	-0.00005	-0.00012	-0.00018	-0.00029	1.88406
A2	2.27374	-0.00004	-0.00032	0.00000	-0.00032	2.27343
A3	2.12462	0.00009	0.00040	0.00018	0.00059	2.12521
A4	1.85624	0.00008	0.00018	0.00013	0.00030	1.85655
A5	2.26709	-0.00006	0.00019	0.00038	0.00057	2.26766
A6	2.15308	-0.00002	-0.00028	-0.00044	-0.00072	2.15235
A7	1.90042	-0.00002	-0.00010	0.00002	-0.00008	1.90035
A8	2.21896	-0.00009	0.00006	-0.00051	-0.00045	2.21851
A9	2.16367	0.00011	0.00003	0.00049	0.00053	2.16420
A10	1.89672	-0.00003	-0.00007	-0.00003	-0.00010	1.89663
A11	2.19062	-0.00002	-0.00015	-0.00004	-0.00020	2.19042
A12	2.19577	0.00005	0.00021	0.00008	0.00030	2.19606

A13	1.88704	0.00003	0.00011	0.00005	0.00016	1.88720
A14	2.19068	-0.00015	-0.00025	-0.00007	-0.00032	2.19036
A15	2.20090	0.00012	-0.00017	0.00000	-0.00016	2.20074
A16	1.88819	0.00020	0.00015	0.00011	0.00027	1.88845
A17	1.85862	0.00002	0.00034	-0.00048	-0.00014	1.85848
A18	1.96292	-0.00037	-0.00098	0.00011	-0.00087	1.96205
A19	1.88845	-0.00003	0.00044	-0.00003	0.00041	1.88886
A20	1.93166	0.00005	0.00000	0.00001	0.00001	1.93167
A21	1.93092	0.00015	0.00010	0.00026	0.00036	1.93129
A22	2.73285	-0.00016	-0.00229	-0.00151	-0.00381	2.72905
A23	2.15321	0.00003	0.00055	-0.00040	0.00015	2.15336
A24	1.96405	0.00002	0.00012	0.00029	0.00041	1.96446
A25	2.16589	-0.00005	-0.00067	0.00011	-0.00056	2.16532
A26	2.06488	-0.00005	-0.00035	-0.00004	-0.00039	2.06449
A27	2.15846	-0.00004	-0.00033	-0.00016	-0.00049	2.15797
A28	2.05955	0.00009	0.00068	0.00022	0.00090	2.06044
A29	2.05715	0.00009	0.00080	0.00036	0.00114	2.05829
A30	2.12974	-0.00014	-0.00081	-0.00070	-0.00150	2.12824
A31	1.97475	0.00007	0.00026	0.00044	0.00072	1.97546
A32	2.00135	-0.00011	-0.00043	-0.00021	-0.00064	2.00070
A33	2.02632	0.00004	0.00010	0.00017	0.00027	2.02659
A34	2.04076	-0.00008	0.00003	-0.00020	-0.00015	2.04062
A35	2.13774	0.00016	0.00037	0.00045	0.00080	2.13855
A36	1.94498	-0.00004	0.00026	-0.00004	0.00021	1.94519
A37	2.03816	0.00010	0.00020	0.00020	0.00041	2.03857
A38	2.02447	-0.00007	-0.00051	-0.00028	-0.00080	2.02368
A39	2.09431	0.00010	0.00022	0.00152	0.00183	2.09615
A40	2.36503	0.00005	-0.00166	0.00151	-0.00011	2.36492
A41	1.93550	-0.00002	-0.00013	-0.00004	-0.00017	1.93533
A42	1.91438	-0.00003	-0.00036	0.00008	-0.00028	1.91410
A43	1.93595	0.00003	0.00028	0.00008	0.00036	1.93631
A44	1.88231	0.00001	-0.00006	-0.00002	-0.00008	1.88223
A45	1.90023	0.00000	0.00017	-0.00002	0.00014	1.90037
A46	1.89420	0.00000	0.00011	-0.00008	0.00002	1.89422
A47	1.88192	0.00006	0.00095	-0.00049	0.00046	1.88238
A48	1.94539	0.00002	-0.00012	-0.00011	-0.00023	1.94516
A49	1.97151	-0.00012	-0.00008	0.00034	0.00026	1.97177
A50	1.88245	-0.00002	-0.00005	0.00012	0.00008	1.88253
A51	1.90120	0.00007	-0.00040	0.00005	-0.00034	1.90085
A52	1.87918	-0.00001	-0.00031	0.00008	-0.00023	1.87895
A53	2.14889	-0.00017	-0.00035	-0.00034	-0.00069	2.14819
A54	1.95002	0.00003	0.00021	-0.00030	-0.00008	1.94994
A55	2.18394	0.00014	0.00017	0.00066	0.00083	2.18478
A56	1.93422	0.00009	0.00121	0.00048	0.00168	1.93591

A57	2.81661	-0.00030	-0.00100	0.00049	-0.00051	2.81609
D1	0.00326	-0.00004	-0.00005	0.00030	0.00026	0.00351
D2	3.02090	-0.00003	0.00071	0.00088	0.00159	3.02249
D3	-3.10511	0.00005	0.00055	0.00025	0.00080	-3.10431
D4	-0.08747	0.00006	0.00131	0.00083	0.00214	-0.08534
D5	-0.00233	0.00006	0.00038	-0.00058	-0.00020	-0.00253
D6	-3.04628	0.00011	0.00355	-0.00037	0.00318	-3.04309
D7	3.10946	-0.00002	-0.00018	-0.00054	-0.00071	3.10875
D8	0.06551	0.00002	0.00300	-0.00033	0.00268	0.06819
D9	-0.00307	0.00001	-0.00030	0.00008	-0.00022	-0.00329
D10	3.12155	0.00003	-0.00043	0.00036	-0.00008	3.12147
D11	-3.03085	0.00001	-0.00104	-0.00052	-0.00155	-3.03240
D12	0.09377	0.00003	-0.00117	-0.00024	-0.00141	0.09236
D13	-1.51547	0.00016	0.00196	0.00254	0.00450	-1.51097
D14	1.48360	0.00017	0.00287	0.00325	0.00612	1.48972
D15	0.00166	0.00003	0.00055	-0.00045	0.00009	0.00176
D16	3.13078	0.00001	-0.00029	0.00055	0.00027	3.13104
D17	-3.12361	0.00001	0.00067	-0.00070	-0.00003	-3.12364
D18	0.00550	-0.00001	-0.00016	0.00030	0.00014	0.00564
D19	-0.19118	-0.00002	-0.00231	-0.00247	-0.00477	-0.19595
D20	2.95988	-0.00001	-0.00162	-0.00275	-0.00437	2.95551
D21	2.93104	0.00000	-0.00246	-0.00216	-0.00462	2.92643
D22	-0.20108	0.00001	-0.00177	-0.00245	-0.00421	-0.20529
D23	0.00039	-0.00005	-0.00057	0.00064	0.00007	0.00046
D24	3.04361	-0.00012	-0.00378	0.00042	-0.00336	3.04025
D25	-3.12868	-0.00003	0.00027	-0.00037	-0.00010	-3.12878
D26	-0.08545	-0.00010	-0.00294	-0.00059	-0.00353	-0.08898
D27	-2.47665	-0.00005	-0.00312	-0.00024	-0.00336	-2.48001
D28	-0.45013	0.00002	-0.00236	-0.00046	-0.00282	-0.45295
D29	1.66766	-0.00001	-0.00259	-0.00040	-0.00299	1.66467
D30	0.77988	0.00001	0.00061	0.00001	0.00061	0.78049
D31	2.80640	0.00008	0.00137	-0.00022	0.00115	2.80755
D32	-1.35900	0.00005	0.00114	-0.00015	0.00099	-1.35802
D33	-3.00094	0.00007	-0.00155	-0.00016	-0.00171	-3.00265
D34	1.21929	0.00005	-0.00201	0.00005	-0.00196	1.21734
D35	-0.89923	0.00013	-0.00145	-0.00022	-0.00167	-0.90089
D36	1.16806	0.00004	-0.00107	-0.00039	-0.00146	1.16660
D37	-0.89489	0.00002	-0.00153	-0.00017	-0.00170	-0.89659
D38	-3.01341	0.00010	-0.00097	-0.00044	-0.00141	-3.01482
D39	-0.92498	-0.00005	-0.00169	-0.00053	-0.00222	-0.92720
D40	-2.98793	-0.00007	-0.00215	-0.00031	-0.00246	-2.99039
D41	1.17673	0.00001	-0.00159	-0.00058	-0.00217	1.17456
D42	-3.14028	0.00003	0.00072	-0.00017	0.00055	-3.13973
D43	-0.02563	0.00004	0.00061	0.00084	0.00144	-0.02419

D44	-0.00925	0.00002	-0.00005	0.00015	0.00010	-0.00914
D45	3.10540	0.00002	-0.00016	0.00116	0.00100	3.10639
D46	-2.75348	0.00004	0.00022	0.00043	0.00065	-2.75284
D47	-0.04866	0.00003	-0.00020	0.00028	0.00008	-0.04858
D48	-0.02054	0.00001	0.00051	-0.00001	0.00050	-0.02004
D49	2.68428	0.00000	0.00009	-0.00016	-0.00006	2.68422
D50	0.32321	-0.00006	-0.00276	0.00115	-0.00161	0.32160
D51	-2.05545	-0.00008	-0.00273	0.00063	-0.00213	-2.05758
D52	2.55496	-0.00003	-0.00103	-0.00147	-0.00247	2.55248
D53	0.17228	0.00001	-0.00074	-0.00120	-0.00192	0.17036
D54	2.55733	0.00003	0.00025	0.00012	0.00036	2.55769
D55	-1.64866	0.00001	-0.00013	0.00012	-0.00002	-1.64868
D56	0.44357	0.00002	-0.00006	0.00012	0.00005	0.44362
D57	1.33112	-0.00002	0.00001	-0.00019	-0.00017	1.33095
D58	-2.87487	-0.00003	-0.00038	-0.00018	-0.00055	-2.87542
D59	-0.78264	-0.00003	-0.00030	-0.00019	-0.00048	-0.78312
D60	-1.01726	0.00001	-0.00004	-0.00002	-0.00006	-1.01732
D61	1.05993	-0.00001	-0.00042	-0.00002	-0.00044	1.05949
D62	-3.13103	0.00000	-0.00035	-0.00002	-0.00036	-3.13139
D63	1.49391	-0.00011	-0.00123	-0.00944	-0.01062	1.48329
D64	2.83556	-0.00001	-0.00131	-0.00761	-0.00898	2.82658
D65	2.26726	-0.00004	-0.00471	0.00023	-0.00448	2.26278
D66	-0.84795	-0.00006	-0.00610	-0.00072	-0.00681	-0.85476
D67	-1.92526	0.00001	-0.00384	-0.00013	-0.00397	-1.92923
D68	1.24272	-0.00001	-0.00523	-0.00108	-0.00630	1.23642
D69	0.11171	0.00002	-0.00427	0.00009	-0.00419	0.10752
D70	-3.00350	0.00000	-0.00566	-0.00086	-0.00652	-3.01002
D71	2.92165	-0.00011	0.00124	0.00212	0.00336	2.92501
D72	-0.19292	-0.00013	-0.00017	0.00117	0.00100	-0.19192
D73	-1.91416	0.00001	0.00988	0.00564	0.01553	-1.89863

Item	Value	Threshold	Converged?
Maximum Force	0.000368	0.000450	YES
RMS Force	0.000080	0.000300	YES
Maximum Displacement	0.020512	0.001800	NO
RMS Displacement	0.006391	0.001200	NO

Predicted change in Energy=-3.312781D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.843904	1.639526	1.532202

2	6	0	-1.504545	0.452138	1.571651
3	7	0	-2.374193	0.451843	0.488824
4	6	0	-2.239492	1.609651	-0.176808
5	7	0	-1.312038	2.352802	0.439396
6	6	0	-0.776769	3.641983	-0.034418
7	1	0	-0.066225	2.023658	2.168105
8	1	0	-1.347971	-0.419561	2.219080
9	1	0	-1.614045	4.255595	-0.371240
10	1	0	-0.326371	4.125808	0.830143
11	35	0	-0.397784	-2.452916	2.886342
12	1	0	-2.780176	1.886349	-1.065522
13	6	0	-3.266778	-0.596723	0.098316
14	6	0	-3.226924	-1.818625	0.613187
15	1	0	-3.966391	-0.283327	-0.666703
16	1	0	-3.941305	-2.549617	0.255719
17	1	0	-2.497898	-2.136295	1.361679
18	6	0	2.567189	-0.686277	1.132487
19	6	0	3.986457	-0.370310	1.320214
20	8	0	2.984837	0.658378	1.534633
21	1	0	2.185604	-0.729615	0.116268
22	1	0	1.994259	-1.225754	1.882024
23	1	0	4.441037	-0.684230	2.256996
24	6	0	4.929544	-0.168469	0.166259
25	1	0	5.690113	0.578871	0.410320
26	1	0	5.442921	-1.108271	-0.058581
27	1	0	4.390246	0.154667	-0.726685
28	6	0	0.255933	3.469910	-1.158021
29	1	0	0.706158	4.448449	-1.352740
30	1	0	-0.212663	3.127622	-2.081363
31	6	0	1.359800	2.479603	-0.805048
32	8	0	1.686477	1.570091	-1.530206
33	8	0	1.881174	2.729547	0.395022
34	1	0	2.456793	1.965211	0.702455

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.359371	0.000000			
3	N	2.200230	1.388813	0.000000		
4	C	2.206643	2.221957	1.342286	0.000000	
5	N	1.386412	2.220717	2.178133	1.338713	0.000000
6	C	2.543352	3.644753	3.605904	2.508029	1.474110
7	H	1.075508	2.212283	3.258421	3.223835	2.156113
8	H	2.228390	1.097060	2.192319	3.263862	3.294627

9	H	3.325661	4.272364	3.973168	2.725803	2.090205
10	H	2.634829	3.928584	4.219963	3.317383	2.065859
11	Br	4.333681	3.375303	4.253458	5.411029	5.469765
12	H	3.249344	3.261729	2.153746	1.076435	2.153552
13	C	3.595435	2.525132	1.431326	2.449306	3.554862
14	C	4.299091	3.006927	2.428506	3.654066	4.593234
15	H	4.275800	3.407612	2.100193	2.608743	3.901053
16	H	5.363974	4.084117	3.393957	4.514728	5.566013
17	H	4.125723	2.780436	2.734161	4.057811	4.733800
18	C	4.147853	4.250632	5.111445	5.485410	4.976422
19	C	5.236102	5.557944	6.467226	6.702519	6.022062
20	O	3.952457	4.494269	5.464025	5.579208	4.746973
21	H	4.098246	4.139068	4.725081	5.013934	4.673244
22	H	4.048132	3.892722	4.882490	5.495722	5.081225
23	H	5.818571	6.091877	7.131931	7.470928	6.754636
24	C	6.202205	6.614966	7.337125	7.394220	6.737118
25	H	6.713940	7.288886	8.065689	8.017847	7.223420
26	H	7.043092	7.304780	7.990048	8.149880	7.606344
27	H	5.890984	6.333987	6.879201	6.809755	6.221542
28	C	3.434712	4.433659	4.328786	3.263508	2.501640
29	H	4.314584	5.423077	5.371478	4.256576	3.417104
30	H	3.958629	4.708681	4.293934	3.168532	2.857130
31	C	3.320358	4.238370	4.441691	3.755849	2.950159
32	O	3.973159	4.588459	4.670760	4.152888	3.671928
33	O	3.147599	4.246662	4.827513	4.308253	3.215667
34	H	3.418940	4.328636	5.066986	4.791098	3.797830

		6	7	8	9	10
6	C	0.000000				
7	H	2.823997	0.000000			
8	H	4.679815	2.759491	0.000000		
9	H	1.091329	3.718274	5.351414	0.000000	
10	H	1.088306	2.505364	4.861398	1.765863	0.000000
11	Br	6.769214	4.545933	2.341501	7.556139	6.892942
12	H	2.856408	4.223829	4.261108	2.730424	3.824903
13	C	4.917763	4.625361	2.865458	5.147523	5.611048
14	C	6.020041	5.212575	2.840201	6.361338	6.617897
15	H	5.097208	5.345055	3.899029	5.120804	5.910225
16	H	6.959482	6.291925	3.888098	7.219427	7.613082
17	H	6.188689	4.885547	2.237106	6.681351	6.649209
18	C	5.592634	3.918051	4.071891	6.645751	5.623189
19	C	6.373526	4.782701	5.409853	7.458259	6.249458
20	O	5.051089	3.402095	4.517039	6.141826	4.845974
21	H	5.282919	4.106250	4.123604	6.287075	5.513145
22	H	5.919984	3.858253	3.454570	6.938461	5.927140

23	H	7.154872	5.258894	5.795179	8.244604	6.921022
24	C	6.864533	5.811241	6.609411	7.917057	6.819545
25	H	7.169450	6.189721	7.335060	8.214613	6.996791
26	H	7.826240	6.716978	7.195712	8.869587	7.840289
27	H	6.272053	5.633211	6.475678	7.279797	6.359256
28	C	1.535762	3.641229	5.394933	2.175578	2.173034
29	H	2.141829	4.344253	6.377685	2.526633	2.436225
30	H	2.184666	4.392967	5.689046	2.482078	3.079963
31	C	2.551455	3.328825	4.988239	3.490858	2.868277
32	O	3.549324	4.117668	5.217637	4.410054	4.019265
33	O	2.842819	2.726622	4.865332	3.890056	2.648042
34	H	3.716244	2.918418	4.739570	4.792744	3.525689

		11	12	13	14	15
11	Br	0.000000				
12	H	6.334212	0.000000			
13	C	4.410178	2.785130	0.000000		
14	C	3.684236	4.092002	1.326546	0.000000	
15	H	5.483266	2.504727	1.083019	2.131213	0.000000
16	H	4.414303	4.771970	2.072091	1.082808	2.446950
17	H	2.614445	4.706660	2.134841	1.092078	3.115172
18	C	3.871444	6.328030	5.925597	5.926519	6.788749
19	C	5.100154	7.521407	7.358921	7.391236	8.197755
20	O	4.790552	6.442367	6.536129	6.750599	7.352024
21	H	4.161366	5.735753	5.454031	5.543314	6.217657
22	H	2.869921	6.416264	5.590689	5.405756	6.550842
23	H	5.190232	8.354215	8.004871	7.923799	8.910307
24	C	6.402965	8.073372	8.207784	8.333710	8.935585
25	H	7.237741	8.696747	9.039097	9.235946	9.754560
26	H	6.677909	8.809143	8.726119	8.724797	9.464961
27	H	6.540541	7.384340	7.737908	7.981880	8.368322
28	C	7.201672	3.425518	5.524978	6.575414	5.670643
29	H	8.174187	4.336055	6.583581	7.655731	6.685287
30	H	7.473604	3.027344	5.286716	6.388406	5.265577
31	C	6.406653	4.190370	5.628950	6.443927	6.001769
32	O	6.327291	4.501881	5.646406	6.341848	6.011298
33	O	6.185325	4.957051	6.136247	6.842963	6.663234
34	H	5.695420	5.527912	6.299822	6.828618	6.941744

		16	17	18	19	20
16	H	0.000000				
17	H	1.864781	0.000000			
18	C	6.826511	5.273536	0.000000		
19	C	8.290473	6.720660	1.466083	0.000000	
20	O	7.739399	6.156337	1.464326	1.451695	0.000000
21	H	6.393033	5.046284	1.086364	2.195828	2.139407

22	H	6.295109	4.612951	1.086779	2.239702	2.156822
23	H	8.817507	7.145551	2.185367	1.087542	2.108298
24	C	9.185305	7.776134	2.604313	1.503917	2.517541
25	H	10.127959	8.678752	3.445981	2.152045	2.930686
26	H	9.499472	8.132071	3.141107	2.137042	3.420754
27	H	8.814364	7.553561	2.736283	2.151381	2.709697
28	C	7.473297	6.735132	5.278468	5.899640	4.754158
29	H	8.553303	7.809795	6.000434	6.412915	5.281471
30	H	7.183020	6.692208	5.709837	6.437303	5.421863
31	C	7.383766	6.393986	3.903156	4.420189	3.381082
32	O	7.199545	6.293591	3.599553	4.144871	3.451115
33	O	7.860677	6.617183	3.561225	3.859703	2.608932
34	H	7.843399	6.465747	2.688402	2.859398	1.636815

		21	22	23	24	25
21	H	0.000000				
22	H	1.844088	0.000000			
23	H	3.109945	2.533885	0.000000		
24	C	2.801177	3.560561	2.208128	0.000000	
25	H	3.752358	4.368286	2.562387	1.093869	0.000000
26	H	3.283910	3.958916	2.558413	1.094228	1.768451
27	H	2.520510	3.801536	3.099787	1.092066	1.778310
28	C	4.794106	5.857723	6.814273	6.069115	6.352017
29	H	5.582033	6.657288	7.302322	6.438966	6.551475
30	H	5.045745	6.287355	7.416771	6.508327	6.895462
31	C	3.439456	4.620884	5.374009	4.549593	4.882777
32	O	2.872046	4.422080	5.197351	4.051921	4.558208
33	O	3.483703	4.227100	4.655504	4.212290	4.374204
34	H	2.771146	3.433305	3.656960	3.309772	3.530105

		26	27	28	29	30
26	H	0.000000				
27	H	1.774683	0.000000			
28	C	7.005237	5.316900	0.000000		
29	H	7.415450	5.692189	1.094604	0.000000	
30	H	7.349835	5.644501	1.090552	1.766269	0.000000
31	C	5.486522	3.820349	1.524408	2.145593	2.126394
32	O	4.842538	3.155857	2.407133	3.045893	2.517223
33	O	5.255534	3.766121	2.366747	2.718448	3.267277
34	H	4.352290	3.009776	3.251042	3.668109	4.028255

		31	32	33	34
31	C	0.000000			
32	O	1.208215	0.000000		
33	O	1.332093	2.255825	0.000000	
34	H	1.934052	2.394636	1.005018	0.000000

Stoichiometry C11H17BrN2O3

Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.058922	1.328888	1.236178
2	6	0	-1.174407	1.235579	0.672189
3	7	0	-1.262995	2.271149	-0.248978
4	6	0	-0.115062	2.966641	-0.232416
5	7	0	0.708708	2.412618	0.665700
6	6	0	2.111309	2.795055	0.909528
7	1	0	0.536724	0.704283	1.969862
8	1	0	-1.942220	0.459798	0.782488
9	1	0	2.166743	3.884470	0.942725
10	1	0	2.369323	2.410964	1.894573
11	35	0	-3.043012	-1.551587	0.307920
12	1	0	0.107609	3.820271	-0.849218
13	6	0	-2.367347	2.569691	-1.109195
14	6	0	-3.394037	1.749396	-1.290168
15	1	0	-2.264576	3.530126	-1.599024
16	1	0	-4.185117	2.057956	-1.962072
17	1	0	-3.475433	0.768481	-0.817079
18	6	0	0.664643	-2.462119	-0.334191
19	6	0	1.661180	-3.493008	-0.028281
20	8	0	1.683169	-2.233181	0.692670
21	1	0	0.813145	-1.859455	-1.225779
22	1	0	-0.353474	-2.517047	0.041988
23	1	0	1.341713	-4.312076	0.611888
24	6	0	2.831082	-3.779446	-0.928864
25	1	0	3.706761	-4.080804	-0.346698
26	1	0	2.581003	-4.600421	-1.607683
27	1	0	3.088360	-2.901787	-1.525631
28	6	0	3.064664	2.235821	-0.156745
29	1	0	4.089512	2.439066	0.169652
30	1	0	2.917061	2.725508	-1.119929
31	6	0	2.902911	0.735287	-0.371349
32	8	0	2.762305	0.236552	-1.462806
33	8	0	2.907387	0.068951	0.782101
34	1	0	2.602264	-0.879450	0.649825

```
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.3279281           0.2549611           0.1591747
 Standard basis: 6-311++G(d,p) (5D, 7F)
 There are      538 symmetry adapted cartesian basis functions of A      symmetry.
 There are      519 symmetry adapted basis functions of A      symmetry.
    519 basis functions,      823 primitive gaussians,      538 cartesian basis functions
     78 alpha electrons              78 beta electrons
          nuclear repulsion energy           1572.2077314013 Hartrees.
 NAtoms=       34 NActive=       34 NUniq=       34 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      519 RedAO= T EigKep=    3.55D-06    NBF=      519
 NBsUse=      519 1.00D-06 EigRej= -1.00D+00 NBFU=      519
 Initial guess from the checkpoint file:    "./coohpo.chk"
 B after Tr=          0.000000        0.000000        0.000000
             Rot=        0.999990      -0.000019      -0.000403      -0.004502 Ang=    -0.52 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn=                5 AccDes=
0.00D+00
 Harris functional with IExCor=    402 and IRadAn=             5 diagonalized for initial guess.
 HarFok:    IExCor=    402 AccDes= 0.00D+00 IRadAn=                5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=    3500011 ScaDFX=    1.000000    1.000000    1.000000    1.000000
 FoFCou: FMM=F IPFlag=                  0 FMFlag=           100000 FMFlg1=                  0
             NFxFlg=                    0 DoJE=T BraDBF=F KetDBF=T FulRan=T
             wScrn=      0.000000  ICntrl=             500  IOpCl=      0  I1Cent=        200000004  NGrid=
0
             NMat0=         1 NMatS0=            1 NMatT0=         0 NMatD0=         1 NMtDS0=         0
NMtDT0=         0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                       energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3338.90386462          A.U. after      10 cycles
                   NFock= 10    Conv=0.69D-08         -V/T= 2.0019
 Calling FoFJK, ICntrl=             2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 ---------------------------------------------------------------------
 Center         Atomic                             Forces (Hartrees/Bohr)
 Number          Number                       X                       Y                       Z
 ---------------------------------------------------------------------
```

1	6	-0.000049279	0.000082855	0.000094159
2	6	0.000272943	0.000031527	0.000108051
3	7	0.000086384	0.000127264	-0.000024036
4	6	0.000086352	-0.000091753	0.000019121
5	7	-0.000047986	-0.000064181	0.000003252
6	6	0.000103585	0.000061720	-0.000087342
7	1	0.000021776	-0.000022826	-0.000037773
8	1	-0.000338173	-0.000126626	-0.000250247
9	1	-0.000002075	0.000013854	-0.000003325
10	1	-0.000021735	0.000006571	0.000011970
11	35	0.000129851	0.000093413	0.000082716
12	1	-0.000042848	0.000016493	0.000022870
13	6	-0.000112538	-0.000085342	-0.000030117
14	6	-0.000000289	0.000005597	0.000023317
15	1	0.000005688	0.000013120	0.000012755
16	1	0.000002347	0.000010845	-0.000014094
17	1	-0.000009077	-0.000012216	0.000018629
18	6	0.000029969	0.000079736	-0.000027780
19	6	0.000065235	-0.000035084	-0.000128251
20	8	-0.000204362	-0.000096586	0.000048067
21	1	-0.000027321	-0.000038335	0.000052868
22	1	-0.000000445	0.000021170	-0.000011776
23	1	-0.000013494	-0.000009707	0.000024868
24	6	0.000018183	-0.000018129	0.000065697
25	1	-0.000003993	-0.000001749	0.000001073
26	1	0.000004053	-0.000002444	0.000010338
27	1	-0.000005578	-0.000004989	-0.000011364
28	6	-0.000028200	-0.000032043	0.000045005
29	1	0.000005961	0.000020067	0.000002040
30	1	0.000001182	0.000002144	-0.000001612
31	6	0.000026823	-0.000055335	-0.000032454
32	8	-0.000013119	0.000010133	0.000029289
33	8	-0.000054011	-0.000004736	0.000019151
34	1	0.000114190	0.000105572	-0.000035068

Cartesian Forces: Max 0.000338173 RMS 0.000074269

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000316249 RMS 0.000067608

Search for a local minimum.

Step number 31 out of a maximum of 175

All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 21 22 23 24 25
26 27 28 29 30
31
DE= 1.15D-06 DEPred=-3.31D-06 R=-3.46D-01
Trust test=-3.46D-01 RLast= 3.11D-02 DXMaxT set to 3.91D-01
ITU= -1 1 1 1 1 1 -1 0 1 1 1 1 1 1 1 1 1 0 0
ITU= -1 1 1 1 0 1 0 -1 0 1 0
Eigenvalues --- 0.00114 0.00224 0.00373 0.00513 0.00661
Eigenvalues --- 0.00723 0.00853 0.01199 0.01272 0.01568
Eigenvalues --- 0.01986 0.02118 0.02251 0.02269 0.02395
Eigenvalues --- 0.02424 0.02751 0.02881 0.03098 0.03239
Eigenvalues --- 0.03451 0.03677 0.03966 0.04271 0.04819
Eigenvalues --- 0.04912 0.05144 0.05446 0.05704 0.05738
Eigenvalues --- 0.05921 0.06032 0.06567 0.07292 0.09286
Eigenvalues --- 0.09578 0.11773 0.12571 0.12850 0.13105
Eigenvalues --- 0.13755 0.15085 0.15620 0.15805 0.15967
Eigenvalues --- 0.16005 0.16013 0.16040 0.16053 0.16226
Eigenvalues --- 0.17044 0.17559 0.20138 0.21311 0.22275
Eigenvalues --- 0.23299 0.23618 0.23966 0.25392 0.26416
Eigenvalues --- 0.28461 0.29436 0.30720 0.31581 0.32359
Eigenvalues --- 0.33270 0.34500 0.34579 0.34625 0.34817
Eigenvalues --- 0.34889 0.34961 0.35009 0.35135 0.35287
Eigenvalues --- 0.35487 0.35720 0.35834 0.36578 0.37007
Eigenvalues --- 0.37214 0.37682 0.38157 0.39000 0.40777
Eigenvalues --- 0.43961 0.45430 0.49313 0.50391 0.51951
Eigenvalues --- 0.53889 0.56077 0.56890 0.61341 0.91651
Eigenvalues --- 1.38470
En-DIIS/RFO-DIIS IScMMF= 0 using points: 31 30 29 28 27
RFO step: Lambda=-1.22121076D-06.
DidBck=T Rises=F RFO-DIIS coefs: 0.72458 0.88288 -0.65312 -0.11823 0.16388
Iteration 1 RMS(Cart)= 0.00864713 RMS(Int)= 0.00002821
Iteration 2 RMS(Cart)= 0.00004487 RMS(Int)= 0.00000385
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000385

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56884	-0.00005	-0.00010	0.00006	-0.00004	2.56880
R2	2.61994	-0.00003	0.00005	0.00005	0.00010	2.62004
R3	2.03242	-0.00001	0.00002	0.00000	0.00002	2.03244
R4	2.62448	0.00001	0.00006	-0.00020	-0.00013	2.62434
R5	2.07314	-0.00010	0.00036	-0.00034	0.00003	2.07317

R6	2.53655	-0.00001	0.00013	-0.00009	0.00004	2.53660
R7	2.70481	0.00012	-0.00033	0.00023	-0.00010	2.70471
R8	2.52980	-0.00001	-0.00006	0.00000	-0.00006	2.52974
R9	2.03417	0.00000	-0.00001	0.00002	0.00000	2.03417
R10	2.78566	0.00005	-0.00009	0.00021	0.00011	2.78578
R11	2.06231	0.00001	-0.00005	0.00005	0.00000	2.06231
R12	2.05660	0.00001	0.00000	-0.00001	-0.00001	2.05659
R13	2.90217	-0.00008	0.00014	-0.00024	-0.00010	2.90207
R14	4.42479	0.00000	-0.00196	0.00027	-0.00169	4.42311
R15	2.50681	0.00001	0.00014	-0.00002	0.00011	2.50692
R16	2.04661	-0.00001	0.00004	-0.00005	-0.00001	2.04660
R17	2.04621	0.00000	-0.00006	0.00000	-0.00006	2.04615
R18	2.06373	0.00001	0.00009	-0.00006	0.00003	2.06375
R19	2.77049	0.00002	0.00004	-0.00007	-0.00002	2.77048
R20	2.76718	-0.00006	-0.00001	-0.00016	-0.00017	2.76700
R21	2.05293	-0.00004	0.00013	-0.00017	-0.00004	2.05289
R22	2.05372	-0.00002	0.00012	0.00003	0.00015	2.05387
R23	2.74331	0.00007	-0.00037	0.00014	-0.00024	2.74307
R24	2.05516	0.00002	0.00000	0.00004	0.00004	2.05520
R25	2.84199	-0.00003	0.00015	-0.00012	0.00003	2.84202
R26	3.09313	0.00002	0.00224	0.00175	0.00399	3.09712
R27	2.06711	0.00000	0.00001	-0.00001	0.00001	2.06712
R28	2.06779	0.00000	-0.00003	0.00003	0.00000	2.06780
R29	2.06370	0.00001	-0.00003	0.00003	-0.00001	2.06370
R30	2.06850	0.00002	-0.00007	0.00005	-0.00002	2.06848
R31	2.06084	0.00000	-0.00005	0.00001	-0.00004	2.06080
R32	2.88071	-0.00004	0.00029	-0.00028	0.00001	2.88072
R33	2.28320	-0.00003	0.00002	-0.00008	-0.00006	2.28314
R34	2.51729	-0.00005	-0.00014	0.00012	-0.00002	2.51727
R35	1.89921	-0.00004	-0.00056	-0.00016	-0.00072	1.89849
A1	1.88406	0.00001	0.00002	-0.00006	-0.00004	1.88402
A2	2.27343	-0.00001	-0.00017	-0.00002	-0.00018	2.27325
A3	2.12521	0.00000	0.00015	0.00006	0.00021	2.12542
A4	1.85655	0.00000	0.00002	0.00007	0.00008	1.85663
A5	2.26766	-0.00011	-0.00011	0.00014	0.00003	2.26769
A6	2.15235	0.00011	0.00011	-0.00014	-0.00002	2.15233
A7	1.90035	-0.00001	-0.00003	-0.00002	-0.00005	1.90030
A8	2.21851	0.00000	0.00019	-0.00029	-0.00010	2.21841
A9	2.16420	0.00001	-0.00016	0.00032	0.00016	2.16436
A10	1.89663	-0.00001	-0.00003	0.00008	0.00006	1.89668
A11	2.19042	-0.00001	-0.00004	-0.00009	-0.00013	2.19029
A12	2.19606	0.00001	0.00005	0.00003	0.00008	2.19614
A13	1.88720	0.00000	0.00003	-0.00008	-0.00005	1.88714
A14	2.19036	-0.00021	-0.00008	-0.00008	-0.00016	2.19020

A15	2.20074	0.00020	-0.00009	0.00012	0.00003	2.20076
A16	1.88845	0.00014	-0.00009	0.00023	0.00014	1.88859
A17	1.85848	-0.00004	0.00042	-0.00043	-0.00001	1.85847
A18	1.96205	-0.00017	-0.00038	0.00013	-0.00025	1.96180
A19	1.88886	-0.00003	0.00018	-0.00014	0.00004	1.88890
A20	1.93167	0.00002	-0.00002	-0.00009	-0.00011	1.93156
A21	1.93129	0.00008	-0.00007	0.00028	0.00021	1.93149
A22	2.72905	-0.00005	0.00429	0.00038	0.00468	2.73372
A23	2.15336	0.00003	0.00030	-0.00010	0.00019	2.15355
A24	1.96446	-0.00003	0.00008	-0.00005	0.00003	1.96449
A25	2.16532	0.00000	-0.00037	0.00015	-0.00022	2.16510
A26	2.06449	-0.00003	-0.00017	-0.00012	-0.00029	2.06420
A27	2.15797	0.00003	-0.00012	0.00015	0.00002	2.15800
A28	2.06044	0.00000	0.00029	-0.00002	0.00027	2.06071
A29	2.05829	0.00003	0.00027	0.00022	0.00049	2.05877
A30	2.12824	-0.00001	-0.00060	-0.00028	-0.00088	2.12736
A31	1.97546	0.00004	-0.00036	0.00047	0.00012	1.97558
A32	2.00070	-0.00004	0.00008	-0.00065	-0.00057	2.00013
A33	2.02659	-0.00003	0.00041	0.00010	0.00051	2.02710
A34	2.04062	-0.00003	0.00012	-0.00025	-0.00012	2.04050
A35	2.13855	0.00006	-0.00012	0.00051	0.00038	2.13893
A36	1.94519	-0.00003	0.00042	-0.00026	0.00016	1.94536
A37	2.03857	0.00006	-0.00004	0.00025	0.00021	2.03877
A38	2.02368	-0.00002	-0.00019	-0.00017	-0.00036	2.02332
A39	2.09615	0.00001	0.00120	0.00117	0.00241	2.09856
A40	2.36492	0.00000	0.00169	0.00058	0.00227	2.36719
A41	1.93533	0.00000	0.00002	-0.00001	0.00001	1.93534
A42	1.91410	0.00000	-0.00014	0.00011	-0.00004	1.91407
A43	1.93631	0.00000	0.00011	-0.00003	0.00009	1.93640
A44	1.88223	0.00000	0.00000	-0.00001	-0.00001	1.88221
A45	1.90037	0.00000	0.00003	-0.00001	0.00001	1.90039
A46	1.89422	0.00000	-0.00003	-0.00005	-0.00007	1.89415
A47	1.88238	0.00001	0.00050	-0.00016	0.00033	1.88271
A48	1.94516	0.00008	-0.00010	-0.00008	-0.00018	1.94497
A49	1.97177	-0.00017	-0.00025	-0.00004	-0.00029	1.97148
A50	1.88253	-0.00002	0.00010	0.00010	0.00021	1.88273
A51	1.90085	0.00014	-0.00006	0.00018	0.00012	1.90097
A52	1.87895	-0.00002	-0.00018	0.00002	-0.00016	1.87879
A53	2.14819	-0.00003	0.00006	0.00001	0.00007	2.14826
A54	1.94994	0.00008	0.00012	-0.00031	-0.00019	1.94975
A55	2.18478	-0.00004	-0.00019	0.00032	0.00012	2.18490
A56	1.93591	-0.00032	0.00031	-0.00025	0.00006	1.93597
A57	2.81609	-0.00029	-0.00218	-0.00062	-0.00279	2.81330
D1	0.00351	-0.00004	-0.00026	0.00030	0.00004	0.00355

D2	3.02249	-0.00001	-0.00004	0.00093	0.00089	3.02338
D3	-3.10431	0.00002	-0.00043	0.00080	0.00037	-3.10394
D4	-0.08534	0.00005	-0.00021	0.00143	0.00123	-0.08411
D5	-0.00253	0.00004	0.00037	-0.00054	-0.00018	-0.00271
D6	-3.04309	0.00005	0.00183	-0.00016	0.00167	-3.04143
D7	3.10875	-0.00001	0.00051	-0.00099	-0.00048	3.10827
D8	0.06819	0.00000	0.00197	-0.00061	0.00136	0.06955
D9	-0.00329	0.00002	0.00007	0.00004	0.00011	-0.00318
D10	3.12147	0.00004	-0.00004	0.00087	0.00082	3.12229
D11	-3.03240	0.00002	-0.00012	-0.00056	-0.00068	-3.03308
D12	0.09236	0.00003	-0.00023	0.00027	0.00004	0.09240
D13	-1.51097	0.00015	-0.00006	0.00083	0.00077	-1.51020
D14	1.48972	0.00017	0.00019	0.00157	0.00176	1.49148
D15	0.00176	0.00000	0.00016	-0.00038	-0.00022	0.00154
D16	3.13104	0.00000	-0.00064	0.00104	0.00040	3.13145
D17	-3.12364	-0.00001	0.00026	-0.00117	-0.00091	-3.12455
D18	0.00564	-0.00001	-0.00053	0.00025	-0.00028	0.00536
D19	-0.19595	0.00000	0.00085	0.00002	0.00086	-0.19509
D20	2.95551	0.00000	0.00098	-0.00014	0.00084	2.95635
D21	2.92643	0.00002	0.00072	0.00096	0.00167	2.92810
D22	-0.20529	0.00002	0.00085	0.00080	0.00165	-0.20364
D23	0.00046	-0.00003	-0.00032	0.00057	0.00025	0.00070
D24	3.04025	-0.00006	-0.00180	0.00017	-0.00163	3.03863
D25	-3.12878	-0.00003	0.00047	-0.00086	-0.00038	-3.12916
D26	-0.08898	-0.00006	-0.00100	-0.00125	-0.00225	-0.09123
D27	-2.48001	0.00001	-0.00274	-0.00127	-0.00401	-2.48402
D28	-0.45295	0.00002	-0.00236	-0.00154	-0.00390	-0.45685
D29	1.66467	0.00000	-0.00240	-0.00140	-0.00380	1.66087
D30	0.78049	0.00004	-0.00102	-0.00081	-0.00183	0.77866
D31	2.80755	0.00005	-0.00064	-0.00108	-0.00173	2.80582
D32	-1.35802	0.00002	-0.00068	-0.00094	-0.00163	-1.35964
D33	-3.00265	0.00011	-0.00027	0.00121	0.00094	-3.00172
D34	1.21734	0.00009	-0.00065	0.00124	0.00059	1.21792
D35	-0.90089	0.00018	-0.00017	0.00130	0.00113	-0.89976
D36	1.16660	0.00003	0.00012	0.00089	0.00101	1.16761
D37	-0.89659	0.00001	-0.00026	0.00092	0.00066	-0.89593
D38	-3.01482	0.00010	0.00022	0.00098	0.00121	-3.01361
D39	-0.92720	0.00000	-0.00004	0.00094	0.00090	-0.92630
D40	-2.99039	-0.00002	-0.00042	0.00097	0.00055	-2.98984
D41	1.17456	0.00007	0.00006	0.00103	0.00110	1.17566
D42	-3.13973	0.00001	0.00010	0.00036	0.00046	-3.13927
D43	-0.02419	0.00001	0.00016	0.00054	0.00069	-0.02350
D44	-0.00914	0.00001	-0.00005	0.00054	0.00049	-0.00865
D45	3.10639	0.00001	0.00001	0.00071	0.00073	3.10712

D46	-2.75284	0.00001	-0.00015	0.00029	0.00013	-2.75270
D47	-0.04858	0.00001	-0.00067	0.00046	-0.00021	-0.04879
D48	-0.02004	-0.00001	0.00019	0.00040	0.00059	-0.01945
D49	2.68422	0.00000	-0.00033	0.00058	0.00025	2.68447
D50	0.32160	-0.00003	0.00127	0.00030	0.00157	0.32317
D51	-2.05758	0.00002	0.00095	0.00034	0.00128	-2.05630
D52	2.55248	0.00002	-0.00133	-0.00132	-0.00264	2.54985
D53	0.17036	0.00002	-0.00147	-0.00102	-0.00249	0.16787
D54	2.55769	0.00000	0.00064	-0.00048	0.00016	2.55785
D55	-1.64868	-0.00001	0.00057	-0.00044	0.00013	-1.64855
D56	0.44362	-0.00001	0.00052	-0.00045	0.00007	0.44369
D57	1.33095	0.00000	0.00062	-0.00066	-0.00004	1.33091
D58	-2.87542	0.00000	0.00055	-0.00062	-0.00007	-2.87549
D59	-0.78312	0.00000	0.00050	-0.00063	-0.00013	-0.78325
D60	-1.01732	0.00000	0.00020	-0.00033	-0.00012	-1.01744
D61	1.05949	0.00000	0.00013	-0.00028	-0.00015	1.05934
D62	-3.13139	0.00000	0.00008	-0.00029	-0.00021	-3.13160
D63	1.48329	0.00000	-0.00079	-0.00013	-0.00091	1.48238
D64	2.82658	0.00001	0.00114	0.00110	0.00223	2.82881
D65	2.26278	-0.00004	-0.00464	-0.00091	-0.00555	2.25723
D66	-0.85476	0.00010	-0.00440	-0.00128	-0.00568	-0.86044
D67	-1.92923	-0.00005	-0.00421	-0.00102	-0.00523	-1.93446
D68	1.23642	0.00009	-0.00397	-0.00139	-0.00536	1.23105
D69	0.10752	-0.00001	-0.00422	-0.00079	-0.00501	0.10251
D70	-3.01002	0.00013	-0.00398	-0.00116	-0.00514	-3.01516
D71	2.92501	-0.00021	-0.00149	0.00025	-0.00124	2.92378
D72	-0.19192	-0.00007	-0.00125	-0.00013	-0.00137	-0.19330
D73	-1.89863	0.00013	0.00997	0.00580	0.01577	-1.88286

Item	Value	Threshold	Converged?
Maximum Force	0.000316	0.000450	YES
RMS Force	0.000068	0.000300	YES
Maximum Displacement	0.037652	0.001800	NO
RMS Displacement	0.008645	0.001200	NO

Predicted change in Energy=-2.641986D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.839277	1.638370	1.529673
2	6	0	-1.499417	0.450741	1.569558
3	7	0	-2.373929	0.452422	0.490748

4	6	0	-2.242459	1.611636	-0.173129
5	7	0	-1.312603	2.353865	0.440492
6	6	0	-0.778399	3.643290	-0.034049
7	1	0	-0.058626	2.021067	2.162814
8	1	0	-1.340185	-0.422054	2.214882
9	1	0	-1.616298	4.256941	-0.369243
10	1	0	-0.326405	4.126948	0.829767
11	35	0	-0.393048	-2.455151	2.884131
12	1	0	-2.787528	1.890064	-1.058620
13	6	0	-3.268550	-0.595280	0.102785
14	6	0	-3.227481	-1.817818	0.616205
15	1	0	-3.971047	-0.280823	-0.659145
16	1	0	-3.943544	-2.547849	0.260239
17	1	0	-2.496144	-2.136610	1.361981
18	6	0	2.565494	-0.688133	1.120185
19	6	0	3.982824	-0.372185	1.321978
20	8	0	2.979114	0.656090	1.527575
21	1	0	2.193302	-0.730588	0.100476
22	1	0	1.986019	-1.228179	1.864377
23	1	0	4.428280	-0.687182	2.262798
24	6	0	4.937512	-0.169193	0.177784
25	1	0	5.695599	0.577884	0.430245
26	1	0	5.453122	-1.108790	-0.042772
27	1	0	4.407322	0.154774	-0.720294
28	6	0	0.251975	3.471270	-1.159725
29	1	0	0.702767	4.449457	-1.354852
30	1	0	-0.218771	3.129680	-2.082205
31	6	0	1.355440	2.479600	-0.809314
32	8	0	1.676249	1.566949	-1.533098
33	8	0	1.883683	2.732603	0.387096
34	1	0	2.458082	1.967896	0.694645

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.359352	0.000000			
3	N	2.200226	1.388742	0.000000		
4	C	2.206619	2.221879	1.342310	0.000000	
5	N	1.386465	2.220714	2.178170	1.338681	0.000000
6	C	2.543351	3.644693	3.605934	2.508073	1.474170
7	H	1.075519	2.212183	3.258386	3.223878	2.156295
8	H	2.228400	1.097073	2.192252	3.263830	3.294685
9	H	3.326643	4.273144	3.973405	2.725467	2.090358
10	H	2.635513	3.929090	4.220122	3.317206	2.065901

11	Br	4.334812	3.375850	4.255132	5.413494	5.472074
12	H	3.249353	3.261625	2.153700	1.076437	2.153567
13	C	3.595354	2.524959	1.431273	2.449381	3.554888
14	C	4.299206	3.006900	2.428637	3.654377	4.593536
15	H	4.275770	3.407530	2.100165	2.608761	3.901040
16	H	5.363988	4.084069	3.393885	4.514733	5.566071
17	H	4.125992	2.780457	2.734423	4.058358	4.734372
18	C	4.144003	4.245287	5.108321	5.484342	4.975477
19	C	5.228588	5.549186	6.463685	6.702614	6.020791
20	O	3.942714	4.483432	5.456332	5.574073	4.741628
21	H	4.105010	4.146072	4.734070	5.023629	4.681970
22	H	4.038741	3.879942	4.870361	5.485983	5.073401
23	H	5.804552	6.075610	7.121018	7.464386	6.747333
24	C	6.202111	6.614787	7.344489	7.405841	6.745278
25	H	6.711034	7.285770	8.070729	8.027793	7.229738
26	H	7.043704	7.305446	7.999047	8.163314	7.615679
27	H	5.898323	6.341970	6.894968	6.829453	6.237065
28	C	3.432669	4.431698	4.328149	3.264018	2.501438
29	H	4.312841	5.421394	5.371088	4.257235	3.417087
30	H	3.956601	4.706606	4.293309	3.169281	2.856984
31	C	3.315918	4.233853	4.439348	3.755393	2.948946
32	O	3.964031	4.577908	4.662838	4.148227	3.667088
33	O	3.149181	4.248584	4.830861	4.312246	3.219090
34	H	3.417373	4.327704	5.068191	4.793228	3.798899

		6	7	8	9	10
6	C	0.000000				
7	H	2.824161	0.000000			
8	H	4.679777	2.759339	0.000000		
9	H	1.091328	3.719783	5.352283	0.000000	
10	H	1.088303	2.506682	4.862069	1.765885	0.000000
11	Br	6.771651	4.546281	2.340608	7.558635	6.895570
12	H	2.856596	4.223944	4.261045	2.729308	3.824498
13	C	4.917829	4.625214	2.865231	5.147503	5.611075
14	C	6.020342	5.212550	2.840036	6.361580	6.618315
15	H	5.097294	5.345016	3.898898	5.120565	5.910053
16	H	6.959522	6.291850	3.888072	7.219244	7.613211
17	H	6.189248	4.885603	2.236824	6.681973	6.650052
18	C	5.592414	3.913162	4.064909	6.645264	5.624271
19	C	6.374331	4.771580	5.397610	7.459169	6.249314
20	O	5.047865	3.390362	4.504568	6.138556	4.843578
21	H	5.289604	4.110478	4.129339	6.293579	5.520548
22	H	5.914155	3.850615	3.440396	6.931975	5.924112
23	H	7.151084	5.241844	5.774753	8.240687	6.916390
24	C	6.873975	5.805082	6.604785	7.927315	6.825740

25	H	7.178087	6.180264	7.327145	8.224261	7.001428
26	H	7.836721	6.711183	7.191498	8.881124	7.847115
27	H	6.287478	5.633831	6.479339	7.296233	6.370952
28	C	1.535711	3.638520	5.392672	2.175451	2.173135
29	H	2.142027	4.341747	6.375600	2.527163	2.436343
30	H	2.184472	4.390313	5.686593	2.481539	3.079888
31	C	2.551172	3.323158	4.983147	3.490535	2.868614
32	O	3.547342	4.108014	5.205992	4.408115	4.018377
33	O	2.844889	2.726173	4.866825	3.891725	2.650404
34	H	3.716551	2.914132	4.738123	4.792928	3.526065

		11	12	13	14	15
11	Br	0.000000				
12	H	6.337169	0.000000			
13	C	4.411748	2.785171	0.000000		
14	C	3.685606	4.092308	1.326607	0.000000	
15	H	5.484941	2.504606	1.083015	2.131141	0.000000
16	H	4.415815	4.771880	2.071940	1.082776	2.446513
17	H	2.615611	4.707263	2.134921	1.092092	3.115162
18	C	3.871282	6.328439	5.922819	5.923574	6.786625
19	C	5.091888	7.524805	7.356536	7.387588	8.197393
20	O	4.784510	6.439353	6.529108	6.743340	7.346039
21	H	4.172776	5.746303	5.463528	5.552741	6.227240
22	H	2.864493	6.407348	5.578016	5.393161	6.538523
23	H	5.172714	8.351162	7.994704	7.912033	8.902335
24	C	6.400374	8.089838	8.217458	8.341300	8.948482
25	H	7.231354	8.712174	9.046519	9.240958	9.765664
26	H	6.675115	8.827990	8.737988	8.734406	9.480528
27	H	6.545773	7.408885	7.756227	7.997973	8.389908
28	C	7.203561	3.427684	5.524930	6.575332	5.671217
29	H	8.175781	4.338249	6.583724	7.655759	6.686112
30	H	7.475641	3.030328	5.286838	6.388387	5.266518
31	C	6.407068	4.192123	5.627441	6.442288	6.001163
32	O	6.322277	4.500538	5.639359	6.334249	6.005831
33	O	6.191242	4.961872	6.140125	6.847102	6.667325
34	H	5.699661	5.531403	6.301942	6.831061	6.944291

		16	17	18	19	20
16	H	0.000000				
17	H	1.864918	0.000000			
18	C	6.823901	5.270363	0.000000		
19	C	8.287829	6.715045	1.466072	0.000000	
20	O	7.732694	6.148581	1.464234	1.451569	0.000000
21	H	6.402253	5.055611	1.086341	2.196112	2.139390
22	H	6.282874	4.600808	1.086859	2.239230	2.156418
23	H	8.806801	7.131617	2.185300	1.087565	2.108320

24	C	9.194452	7.780250	2.604590	1.503933	2.517608
25	H	10.134702	8.679934	3.446212	2.152072	2.930791
26	H	9.511049	8.137603	3.141309	2.137032	3.420747
27	H	8.831907	7.565987	2.736821	2.151455	2.709984
28	C	7.473183	6.734945	5.277403	5.903408	4.752274
29	H	8.553304	7.809641	5.999199	6.416574	5.280131
30	H	7.182988	6.691985	5.708163	6.442431	5.419929
31	C	7.382305	6.392075	3.901504	4.424729	3.379728
32	O	7.192335	6.285435	3.593892	4.151142	3.448890
33	O	7.864848	6.621369	3.564228	3.862656	2.610090
34	H	7.846112	6.468127	2.692046	2.862580	1.638928

		21	22	23	24	25
21	H	0.000000				
22	H	1.844427	0.000000			
23	H	3.110088	2.532993	0.000000		
24	C	2.802111	3.560528	2.207921	0.000000	
25	H	3.753256	4.368018	2.562175	1.093873	0.000000
26	H	3.284811	3.958823	2.558068	1.094231	1.768448
27	H	2.521788	3.802077	3.099704	1.092062	1.778319
28	C	4.797131	5.851232	6.815270	6.082446	6.366531
29	H	5.583237	6.651745	7.304238	6.450889	6.565365
30	H	5.048154	6.279135	7.419068	6.525133	6.914032
31	C	3.440209	4.614529	5.376684	4.563081	4.897959
32	O	2.866109	4.410389	5.202269	4.071503	4.581281
33	O	3.488798	4.228549	4.657055	4.217832	4.378970
34	H	2.775781	3.435987	3.659266	3.313890	3.533207

		26	27	28	29	30
26	H	0.000000				
27	H	1.774635	0.000000			
28	C	7.019719	5.334712	0.000000		
29	H	7.428428	5.707074	1.094595	0.000000	
30	H	7.368466	5.666181	1.090530	1.766376	0.000000
31	C	5.500466	3.837542	1.524411	2.145677	2.126263
32	O	4.862656	3.180196	2.407156	3.047670	2.516893
33	O	5.261367	3.773628	2.366591	2.715977	3.267327
34	H	4.356610	3.014797	3.250496	3.666021	4.028173

		31	32	33	34
31	C	0.000000			
32	O	1.208186	0.000000		
33	O	1.332084	2.255864	0.000000	
34	H	1.933792	2.394756	1.004638	0.000000

Stoichiometry C11H17BrN2O3

Framework group C1[X(C11H17BrN2O3)]

Deg. of freedom 96

Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.067191	1.325953	1.233899
2	6	0	-1.166692	1.236539	0.670539
3	7	0	-1.254626	2.275631	-0.246609
4	6	0	-0.105635	2.969377	-0.228448
5	7	0	0.718040	2.410994	0.667005
6	6	0	2.122022	2.789253	0.909766
7	1	0	0.544635	0.697601	1.964626
8	1	0	-1.935835	0.461804	0.779039
9	1	0	2.180738	3.878468	0.943825
10	1	0	2.379937	2.403520	1.894192
11	35	0	-3.047089	-1.543532	0.307666
12	1	0	0.117494	3.825203	-0.842038
13	6	0	-2.359677	2.579345	-1.104024
14	6	0	-3.388758	1.762151	-1.285887
15	1	0	-2.255507	3.541006	-1.591136
16	1	0	-4.179751	2.074841	-1.955931
17	1	0	-3.472176	0.780227	-0.815215
18	6	0	0.657265	-2.460428	-0.343406
19	6	0	1.642999	-3.497924	-0.025134
20	8	0	1.672142	-2.233605	0.687398
21	1	0	0.815523	-1.864785	-1.238002
22	1	0	-0.363115	-2.504544	0.028265
23	1	0	1.312665	-4.309912	0.618567
24	6	0	2.815331	-3.801168	-0.917040
25	1	0	3.684933	-4.106440	-0.327838
26	1	0	2.561601	-4.624524	-1.591611
27	1	0	3.083980	-2.930094	-1.518419
28	6	0	3.072361	2.228282	-0.158211
29	1	0	4.098348	2.427164	0.167266
30	1	0	2.925267	2.719867	-1.120481
31	6	0	2.904508	0.728716	-0.374906
32	8	0	2.755407	0.232655	-1.466422
33	8	0	2.914388	0.060154	0.777212
34	1	0	2.604475	-0.886358	0.645423

Rotational constants (GHZ): 0.3277840 0.2551505 0.1591393

Standard basis: 6-311++G(d,p) (5D, 7F)
There are 538 symmetry adapted cartesian basis functions of A symmetry.
There are 519 symmetry adapted basis functions of A symmetry.
519 basis functions, 823 primitive gaussians, 538 cartesian basis functions
78 alpha electrons 78 beta electrons
nuclear repulsion energy 1572.2579302549 Hartrees.
NAtoms= 34 NActive= 34 NUniq= 34 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 519 RedAO= T EigKep= 3.54D-06 NBF= 519
NBsUse= 519 1.00D-06 EigRej= -1.00D+00 NBFU= 519
Initial guess from the checkpoint file: "./coohpo.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999999 -0.000016 -0.000221 0.001712 Ang= -0.20 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3338.90386948 A.U. after 11 cycles
NFock= 11 Conv=0.17D-08 -V/T= 2.0019
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Atomic Forces (Hartrees/Bohr)
Number Number X Y Z
---
1 6 -0.000044968 0.000065083 0.000083643
2 6 0.000289245 0.000046989 0.000127413

3	7	0.000073079	0.000182062	-0.000011697
4	6	0.000011999	-0.000114410	0.000006697
5	7	0.000009721	-0.000058350	-0.000015108
6	6	0.000068747	0.000039072	-0.000052178
7	1	0.000012181	-0.000003583	-0.000031886
8	1	-0.000342887	-0.000149288	-0.000207427
9	1	-0.000012045	0.000003277	0.000017226
10	1	-0.000011269	0.000012924	0.000016305
11	35	0.000118216	0.000083592	0.000071208
12	1	-0.000026328	0.000021547	0.000015016
13	6	-0.000119608	-0.000154261	-0.000040578
14	6	0.000031419	0.000100789	0.000006267
15	1	0.000015316	0.000017340	0.000001000
16	1	-0.000011024	-0.000015588	0.000009593
17	1	-0.000013697	-0.000024928	0.000001578
18	6	0.000020557	0.000045924	0.000039457
19	6	0.000101219	-0.000062232	-0.000101333
20	8	-0.000162681	0.000013514	0.000019264
21	1	-0.000023372	-0.000015990	0.000019742
22	1	0.000000862	-0.000011629	-0.000012638
23	1	-0.000026321	-0.000004783	0.000018623
24	6	-0.000010867	-0.000013432	0.000065928
25	1	-0.000010919	0.000000762	-0.000001611
26	1	0.000000171	0.000000980	0.000002537
27	1	-0.000000347	-0.000005415	-0.000020183
28	6	0.000025466	-0.000069709	-0.000014865
29	1	-0.000012771	0.000025424	0.000021918
30	1	-0.000015549	0.000004175	-0.000009071
31	6	0.000034170	-0.000022739	-0.000132228
32	8	-0.000022286	0.000016007	0.000052009
33	8	-0.000064194	0.000102855	0.000108264
34	1	0.000118766	-0.000055979	-0.000052885

Cartesian Forces: Max 0.000342887 RMS 0.000075725

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000290686 RMS 0.000052243

Search for a local minimum.

Step number 32 out of a maximum of 175

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 21 22 23 24 25
26 27 28 29 30
31 32

DE= -4.87D-06 DEPred=-2.64D-06 R= 1.84D+00

TightC=F SS= 1.41D+00 RLast= 2.45D-02 DXNew= 6.5746D-01 7.3589D-02

Trust test= 1.84D+00 RLast= 2.45D-02 DXMaxT set to 3.91D-01

ITU= 1 -1 1 1 1 1 1 -1 0 1 1 1 1 1 1 1 1 1 1 0

ITU= 0 -1 1 1 1 0 1 0 -1 0 1 0

Eigenvalues ---	0.00159	0.00272	0.00351	0.00510	0.00643
Eigenvalues ---	0.00751	0.00826	0.01199	0.01264	0.01496
Eigenvalues ---	0.01929	0.02006	0.02241	0.02273	0.02393
Eigenvalues ---	0.02419	0.02703	0.02825	0.03098	0.03244
Eigenvalues ---	0.03431	0.03747	0.04047	0.04267	0.04842
Eigenvalues ---	0.04877	0.05108	0.05411	0.05640	0.05737
Eigenvalues ---	0.05946	0.06037	0.06537	0.07373	0.09349
Eigenvalues ---	0.09599	0.11791	0.12512	0.12863	0.13007
Eigenvalues ---	0.13607	0.14918	0.15617	0.15888	0.15957
Eigenvalues ---	0.16004	0.16023	0.16054	0.16065	0.16238
Eigenvalues ---	0.17104	0.17600	0.20084	0.21689	0.22072
Eigenvalues ---	0.23305	0.23806	0.23962	0.25310	0.26136
Eigenvalues ---	0.28459	0.29440	0.30848	0.31621	0.32261
Eigenvalues ---	0.33334	0.34500	0.34580	0.34629	0.34822
Eigenvalues ---	0.34886	0.34962	0.35001	0.35125	0.35291
Eigenvalues ---	0.35534	0.35727	0.35865	0.36579	0.37012
Eigenvalues ---	0.37208	0.37670	0.37994	0.39035	0.40597
Eigenvalues ---	0.43326	0.45413	0.49200	0.50769	0.51925
Eigenvalues ---	0.54250	0.55983	0.57327	0.62092	0.91429
Eigenvalues ---	1.33939				

En-DIIS/RFO-DIIS IScMMF= 0 using points: 32 31 30 29 28

RFO step: Lambda=-5.94355281D-07.

DidBck=F Rises=F RFO-DIIS coefs: 1.35776 -0.37993 -0.01973 -0.08277 0.12467

Iteration 1 RMS(Cart)= 0.00171333 RMS(Int)= 0.00000247

Iteration 2 RMS(Cart)= 0.00000253 RMS(Int)= 0.00000216

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000216

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56880	-0.00003	0.00000	-0.00004	-0.00004	2.56877
R2	2.62004	-0.00002	0.00003	0.00002	0.00005	2.62009
R3	2.03244	-0.00001	-0.00001	0.00001	-0.00001	2.03243
R4	2.62434	0.00004	-0.00010	0.00001	-0.00009	2.62425
R5	2.07317	-0.00006	-0.00009	-0.00006	-0.00014	2.07302
R6	2.53660	-0.00005	-0.00004	-0.00002	-0.00006	2.53654

R7	2.70471	0.00013	0.00006	0.00018	0.00024	2.70495
R8	2.52974	0.00002	-0.00002	0.00003	0.00001	2.52975
R9	2.03417	0.00000	0.00001	0.00002	0.00002	2.03419
R10	2.78578	0.00003	0.00014	0.00003	0.00017	2.78595
R11	2.06231	0.00001	0.00001	0.00000	0.00002	2.06233
R12	2.05659	0.00002	-0.00001	0.00004	0.00002	2.05662
R13	2.90207	-0.00002	-0.00016	0.00005	-0.00012	2.90196
R14	4.42311	0.00000	-0.00125	0.00068	-0.00056	4.42255
R15	2.50692	-0.00004	0.00001	-0.00002	-0.00001	2.50692
R16	2.04660	-0.00001	-0.00002	0.00001	-0.00001	2.04659
R17	2.04615	0.00002	-0.00002	0.00003	0.00001	2.04616
R18	2.06375	0.00000	0.00000	-0.00001	-0.00001	2.06374
R19	2.77048	0.00000	-0.00005	-0.00002	-0.00007	2.77041
R20	2.76700	-0.00001	-0.00007	0.00001	-0.00006	2.76694
R21	2.05289	-0.00001	-0.00004	0.00001	-0.00002	2.05286
R22	2.05387	-0.00001	0.00003	0.00001	0.00004	2.05391
R23	2.74307	0.00007	0.00015	0.00011	0.00026	2.74333
R24	2.05520	0.00000	0.00001	0.00001	0.00003	2.05523
R25	2.84202	-0.00004	-0.00003	-0.00009	-0.00012	2.84190
R26	3.09712	-0.00001	-0.00015	0.00002	-0.00014	3.09699
R27	2.06712	-0.00001	0.00000	-0.00001	-0.00001	2.06711
R28	2.06780	0.00000	0.00001	-0.00001	-0.00001	2.06779
R29	2.06370	0.00002	0.00000	0.00003	0.00003	2.06373
R30	2.06848	0.00001	0.00005	-0.00005	0.00000	2.06849
R31	2.06080	0.00001	0.00001	0.00000	0.00001	2.06081
R32	2.88072	-0.00004	0.00003	-0.00009	-0.00006	2.88066
R33	2.28314	-0.00005	-0.00004	0.00002	-0.00002	2.28312
R34	2.51727	0.00003	-0.00009	0.00014	0.00006	2.51733
R35	1.89849	0.00006	0.00007	0.00000	0.00006	1.89855
A1	1.88402	0.00000	-0.00006	-0.00002	-0.00008	1.88394
A2	2.27325	0.00001	-0.00008	0.00004	-0.00004	2.27321
A3	2.12542	-0.00001	0.00011	-0.00003	0.00008	2.12551
A4	1.85663	-0.00001	0.00006	-0.00001	0.00005	1.85668
A5	2.26769	-0.00005	-0.00006	0.00017	0.00011	2.26780
A6	2.15233	0.00007	0.00004	-0.00011	-0.00007	2.15226
A7	1.90030	0.00001	-0.00001	0.00006	0.00005	1.90035
A8	2.21841	-0.00001	-0.00010	-0.00013	-0.00023	2.21818
A9	2.16436	0.00000	0.00012	0.00006	0.00019	2.16454
A10	1.89668	-0.00002	0.00002	-0.00008	-0.00006	1.89662
A11	2.19029	0.00001	-0.00007	0.00006	0.00000	2.19029
A12	2.19614	0.00001	0.00005	0.00002	0.00007	2.19622
A13	1.88714	0.00002	-0.00001	0.00005	0.00005	1.88719
A14	2.19020	-0.00014	-0.00008	-0.00005	-0.00014	2.19007
A15	2.20076	0.00013	0.00003	0.00002	0.00005	2.20082

A16	1.88859	0.00008	0.00005	-0.00011	-0.00005	1.88854
A17	1.85847	-0.00004	-0.00013	0.00000	-0.00012	1.85834
A18	1.96180	-0.00009	-0.00008	0.00007	0.00000	1.96180
A19	1.88890	-0.00002	0.00000	-0.00011	-0.00011	1.88879
A20	1.93156	0.00001	-0.00001	-0.00012	-0.00013	1.93143
A21	1.93149	0.00006	0.00016	0.00025	0.00041	1.93190
A22	2.73372	-0.00006	0.00179	-0.00016	0.00163	2.73535
A23	2.15355	-0.00002	-0.00001	-0.00007	-0.00008	2.15347
A24	1.96449	-0.00001	0.00002	-0.00009	-0.00007	1.96442
A25	2.16510	0.00003	-0.00001	0.00016	0.00015	2.16525
A26	2.06420	0.00000	-0.00015	0.00004	-0.00011	2.06409
A27	2.15800	0.00003	0.00003	0.00009	0.00013	2.15812
A28	2.06071	-0.00003	0.00011	-0.00013	-0.00001	2.06070
A29	2.05877	0.00001	0.00027	0.00013	0.00039	2.05917
A30	2.12736	0.00001	-0.00031	-0.00012	-0.00042	2.12694
A31	1.97558	0.00000	0.00017	0.00000	0.00017	1.97575
A32	2.00013	0.00000	-0.00020	0.00007	-0.00013	2.00000
A33	2.02710	-0.00002	0.00002	-0.00005	-0.00004	2.02706
A34	2.04050	-0.00004	-0.00018	-0.00013	-0.00031	2.04019
A35	2.13893	0.00004	0.00031	0.00014	0.00046	2.13939
A36	1.94536	-0.00001	-0.00010	-0.00006	-0.00016	1.94520
A37	2.03877	0.00002	0.00012	-0.00003	0.00010	2.03887
A38	2.02332	0.00001	-0.00010	0.00003	-0.00007	2.02325
A39	2.09856	0.00003	0.00007	0.00049	0.00057	2.09913
A40	2.36719	-0.00001	-0.00052	-0.00022	-0.00073	2.36646
A41	1.93534	0.00000	-0.00001	-0.00005	-0.00006	1.93528
A42	1.91407	0.00000	-0.00003	-0.00002	-0.00005	1.91402
A43	1.93640	0.00001	0.00009	0.00008	0.00018	1.93657
A44	1.88221	0.00000	-0.00003	0.00002	0.00000	1.88221
A45	1.90039	-0.00001	0.00000	-0.00002	-0.00002	1.90037
A46	1.89415	-0.00001	-0.00003	-0.00002	-0.00005	1.89410
A47	1.88271	-0.00002	0.00001	-0.00010	-0.00009	1.88263
A48	1.94497	0.00004	-0.00004	-0.00005	-0.00008	1.94489
A49	1.97148	-0.00011	0.00010	-0.00014	-0.00005	1.97143
A50	1.88273	-0.00001	-0.00005	0.00000	-0.00004	1.88269
A51	1.90097	0.00011	-0.00002	0.00014	0.00013	1.90110
A52	1.87879	-0.00001	-0.00001	0.00015	0.00014	1.87893
A53	2.14826	-0.00003	-0.00003	0.00011	0.00008	2.14834
A54	1.94975	0.00008	-0.00007	0.00001	-0.00006	1.94969
A55	2.18490	-0.00006	0.00010	-0.00013	-0.00004	2.18486
A56	1.93597	-0.00029	0.00011	-0.00034	-0.00023	1.93574
A57	2.81330	-0.00021	-0.00036	-0.00053	-0.00090	2.81240
D1	0.00355	-0.00003	-0.00022	-0.00004	-0.00026	0.00329
D2	3.02338	0.00000	0.00010	0.00040	0.00050	3.02388

D3	-3.10394	0.00001	0.00060	0.00022	0.00082	-3.10312
D4	-0.08411	0.00003	0.00091	0.00066	0.00158	-0.08253
D5	-0.00271	0.00003	0.00009	0.00017	0.00026	-0.00245
D6	-3.04143	0.00003	0.00066	-0.00001	0.00065	-3.04077
D7	3.10827	0.00000	-0.00064	-0.00007	-0.00071	3.10756
D8	0.06955	-0.00001	-0.00007	-0.00024	-0.00032	0.06923
D9	-0.00318	0.00001	0.00027	-0.00010	0.00017	-0.00301
D10	3.12229	0.00002	0.00074	0.00006	0.00080	3.12310
D11	-3.03308	0.00000	-0.00001	-0.00053	-0.00054	-3.03362
D12	0.09240	0.00001	0.00046	-0.00037	0.00009	0.09249
D13	-1.51020	0.00013	-0.00038	0.00103	0.00065	-1.50955
D14	1.49148	0.00015	-0.00002	0.00155	0.00153	1.49302
D15	0.00154	0.00001	-0.00021	0.00021	-0.00001	0.00153
D16	3.13145	0.00001	0.00055	0.00048	0.00103	3.13247
D17	-3.12455	0.00000	-0.00067	0.00005	-0.00061	-3.12516
D18	0.00536	0.00000	0.00010	0.00032	0.00042	0.00578
D19	-0.19509	0.00001	0.00034	-0.00044	-0.00010	-0.19519
D20	2.95635	0.00000	0.00030	-0.00055	-0.00025	2.95609
D21	2.92810	0.00002	0.00088	-0.00025	0.00063	2.92873
D22	-0.20364	0.00001	0.00084	-0.00037	0.00047	-0.20317
D23	0.00070	-0.00002	0.00008	-0.00023	-0.00016	0.00054
D24	3.03863	-0.00004	-0.00050	-0.00006	-0.00056	3.03807
D25	-3.12916	-0.00002	-0.00069	-0.00050	-0.00119	-3.13035
D26	-0.09123	-0.00004	-0.00127	-0.00033	-0.00160	-0.09283
D27	-2.48402	0.00004	-0.00045	0.00068	0.00023	-2.48379
D28	-0.45685	0.00003	-0.00049	0.00050	0.00001	-0.45684
D29	1.66087	0.00003	-0.00042	0.00085	0.00043	1.66130
D30	0.77866	0.00004	0.00022	0.00047	0.00069	0.77934
D31	2.80582	0.00003	0.00018	0.00029	0.00047	2.80629
D32	-1.35964	0.00003	0.00025	0.00064	0.00089	-1.35875
D33	-3.00172	0.00007	0.00051	-0.00055	-0.00004	-3.00176
D34	1.21792	0.00006	0.00058	-0.00047	0.00011	1.21804
D35	-0.89976	0.00012	0.00055	-0.00053	0.00003	-0.89973
D36	1.16761	0.00002	0.00050	-0.00038	0.00012	1.16773
D37	-0.89593	0.00002	0.00058	-0.00030	0.00027	-0.89566
D38	-3.01361	0.00008	0.00055	-0.00036	0.00019	-3.01343
D39	-0.92630	0.00000	0.00041	-0.00033	0.00008	-0.92622
D40	-2.98984	0.00000	0.00048	-0.00025	0.00023	-2.98961
D41	1.17566	0.00006	0.00045	-0.00031	0.00015	1.17580
D42	-3.13927	-0.00001	0.00016	-0.00027	-0.00011	-3.13938
D43	-0.02350	-0.00001	0.00032	-0.00015	0.00017	-0.02333
D44	-0.00865	0.00000	0.00021	-0.00015	0.00006	-0.00859
D45	3.10712	0.00000	0.00036	-0.00002	0.00034	3.10746
D46	-2.75270	0.00000	0.00006	-0.00005	0.00000	-2.75270

D47	-0.04879	0.00002	0.00012	0.00007	0.00018	-0.04860
D48	-0.01945	-0.00002	0.00001	-0.00018	-0.00017	-0.01962
D49	2.68447	-0.00001	0.00007	-0.00007	0.00001	2.68448
D50	0.32317	-0.00004	-0.00090	-0.00056	-0.00146	0.32171
D51	-2.05630	-0.00001	-0.00089	-0.00055	-0.00145	-2.05774
D52	2.54985	0.00000	-0.00009	-0.00063	-0.00072	2.54913
D53	0.16787	-0.00001	0.00005	-0.00058	-0.00053	0.16734
D54	2.55785	-0.00001	-0.00021	-0.00052	-0.00073	2.55712
D55	-1.64855	-0.00001	-0.00027	-0.00053	-0.00080	-1.64935
D56	0.44369	-0.00001	-0.00027	-0.00051	-0.00078	0.44291
D57	1.33091	0.00000	-0.00031	-0.00053	-0.00084	1.33007
D58	-2.87549	0.00000	-0.00037	-0.00054	-0.00091	-2.87640
D59	-0.78325	0.00000	-0.00037	-0.00053	-0.00089	-0.78414
D60	-1.01744	-0.00001	-0.00018	-0.00044	-0.00061	-1.01805
D61	1.05934	0.00000	-0.00023	-0.00045	-0.00068	1.05866
D62	-3.13160	0.00000	-0.00023	-0.00043	-0.00066	-3.13226
D63	1.48238	-0.00003	0.00103	-0.00012	0.00092	1.48330
D64	2.82881	-0.00002	0.00089	0.00020	0.00108	2.82989
D65	2.25723	-0.00004	-0.00080	-0.00144	-0.00224	2.25499
D66	-0.86044	0.00008	-0.00068	-0.00082	-0.00150	-0.86194
D67	-1.93446	-0.00006	-0.00074	-0.00155	-0.00229	-1.93675
D68	1.23105	0.00006	-0.00062	-0.00093	-0.00155	1.22950
D69	0.10251	-0.00001	-0.00081	-0.00139	-0.00220	0.10031
D70	-3.01516	0.00011	-0.00069	-0.00077	-0.00146	-3.01662
D71	2.92378	-0.00018	-0.00058	-0.00067	-0.00125	2.92253
D72	-0.19330	-0.00006	-0.00046	-0.00003	-0.00049	-0.19379
D73	-1.88286	0.00002	0.00109	0.00167	0.00276	-1.88010

Item	Value	Threshold	Converged?
Maximum Force	0.000291	0.000450	YES
RMS Force	0.000052	0.000300	YES
Maximum Displacement	0.007182	0.001800	NO
RMS Displacement	0.001714	0.001200	NO

Predicted change in Energy=-5.990851D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.838481	1.638488	1.529840
2	6	0	-1.497877	0.450448	1.569147
3	7	0	-2.372440	0.452089	0.490439
4	6	0	-2.241665	1.611574	-0.173037

5	7	0	-1.312145	2.354043	0.440811
6	6	0	-0.778070	3.643682	-0.033572
7	1	0	-0.057572	2.021037	2.162747
8	1	0	-1.338580	-0.422337	2.214339
9	1	0	-1.616126	4.257387	-0.368307
10	1	0	-0.326021	4.127101	0.830366
11	35	0	-0.392599	-2.454467	2.887108
12	1	0	-2.787620	1.890376	-1.057878
13	6	0	-3.267045	-0.595911	0.102782
14	6	0	-3.225556	-1.818345	0.616403
15	1	0	-3.969843	-0.281561	-0.658904
16	1	0	-3.941656	-2.548503	0.260753
17	1	0	-2.494108	-2.136916	1.362155
18	6	0	2.563273	-0.688028	1.118273
19	6	0	3.980483	-0.372730	1.321673
20	8	0	2.976819	0.655953	1.526413
21	1	0	2.191800	-0.730257	0.098305
22	1	0	1.983144	-1.228118	1.861954
23	1	0	4.424479	-0.688204	2.263041
24	6	0	4.936938	-0.169636	0.179057
25	1	0	5.694469	0.577571	0.432776
26	1	0	5.453074	-1.109163	-0.040553
27	1	0	4.408298	0.154180	-0.720005
28	6	0	0.251683	3.472004	-1.159784
29	1	0	0.702351	4.450280	-1.354754
30	1	0	-0.219652	3.130877	-2.082142
31	6	0	1.355190	2.480123	-0.810238
32	8	0	1.674108	1.566333	-1.533405
33	8	0	1.885233	2.733840	0.385258
34	1	0	2.458785	1.968503	0.692926

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.359333	0.000000			
3	N	2.200210	1.388695	0.000000		
4	C	2.206681	2.221855	1.342277	0.000000	
5	N	1.386492	2.220655	2.178100	1.338685	0.000000
6	C	2.543366	3.644663	3.605949	2.508191	1.474260
7	H	1.075516	2.212145	3.258347	3.223943	2.156365
8	H	2.228371	1.096997	2.192103	3.263728	3.294599
9	H	3.326608	4.273229	3.973631	2.725757	2.090405
10	H	2.635350	3.928971	4.220082	3.317286	2.065896
11	Br	4.335121	3.375973	4.255803	5.414446	5.472815

12	H	3.249442	3.261608	2.153678	1.076448	2.153621
13	C	3.595408	2.524886	1.431398	2.449586	3.555015
14	C	4.299092	3.006663	2.428692	3.654532	4.593561
15	H	4.275818	3.407443	2.100222	2.608952	3.901173
16	H	5.363877	4.083829	3.393928	4.514907	5.566122
17	H	4.125881	2.780247	2.734527	4.058537	4.734409
18	C	4.141738	4.241739	5.104440	5.481157	4.973129
19	C	5.225968	5.545384	6.459946	6.699757	6.018564
20	O	3.939785	4.479616	5.452465	5.570810	4.738908
21	H	4.104004	4.143809	4.731173	5.021296	4.680582
22	H	4.036001	3.875672	4.865724	5.482158	5.070548
23	H	5.800848	6.070611	7.116214	7.460626	6.744230
24	C	6.200758	6.612390	7.342378	7.404663	6.744517
25	H	6.708840	7.282674	8.068091	8.026107	7.228316
26	H	7.042683	7.303371	7.997382	8.162657	7.615359
27	H	5.898615	6.341205	6.894369	6.829728	6.237816
28	C	3.432829	4.431458	4.327718	3.263687	2.501459
29	H	4.312913	5.421148	5.370717	4.256987	3.417083
30	H	3.956840	4.706428	4.292851	3.168832	2.856974
31	C	3.316098	4.233325	4.438458	3.754700	2.948846
32	O	3.962547	4.575206	4.659617	4.145591	3.665477
33	O	3.150949	4.249812	4.831690	4.313057	3.220334
34	H	3.417791	4.327519	5.067667	4.792862	3.798962

		6	7	8	9	10
6	C	0.000000				
7	H	2.824166	0.000000			
8	H	4.679721	2.759297	0.000000		
9	H	1.091338	3.719757	5.352280	0.000000	
10	H	1.088316	2.506553	4.861897	1.765833	0.000000
11	Br	6.772472	4.546105	2.340310	7.559347	6.895771
12	H	2.856848	4.224057	4.260958	2.729587	3.824641
13	C	4.918103	4.625212	2.864922	5.148005	5.611225
14	C	6.020498	5.212308	2.839528	6.361952	6.618264
15	H	5.097646	5.345048	3.898575	5.121180	5.910302
16	H	6.959746	6.291612	3.887555	7.219691	7.613210
17	H	6.189358	4.885307	2.236346	6.682249	6.649910
18	C	5.590620	3.911367	4.061578	6.643375	5.622844
19	C	6.372761	4.769006	5.393676	7.457617	6.247866
20	O	5.045718	3.387611	4.500958	6.136403	4.841704
21	H	5.288560	4.109893	4.127469	6.292426	5.519897
22	H	5.912002	3.848638	3.436177	6.929616	5.922398
23	H	7.148859	5.238209	5.769395	8.238433	6.914259
24	C	6.873713	5.803379	6.602149	7.927219	6.825313
25	H	7.177205	6.177570	7.323767	8.223599	7.000253

26	H	7.836883	6.709687	7.189077	8.881490	7.846967
27	H	6.288579	5.633774	6.478376	7.297512	6.371932
28	C	1.535649	3.638703	5.392544	2.175310	2.173383
29	H	2.141907	4.341834	6.375439	2.526978	2.436543
30	H	2.184362	4.390569	5.686570	2.481208	3.080013
31	C	2.551055	3.323447	4.982844	3.490371	2.868900
32	O	3.546556	4.106947	5.203526	4.407365	4.018142
33	O	2.845420	2.728012	4.868260	3.892117	2.651215
34	H	3.716350	2.914651	4.738227	4.792714	3.526128

		11	12	13	14	15
11	Br	0.000000				
12	H	6.338509	0.000000			
13	C	4.412385	2.785427	0.000000		
14	C	3.685973	4.092629	1.326602	0.000000	
15	H	5.485654	2.504824	1.083008	2.131215	0.000000
16	H	4.416151	4.772235	2.071876	1.082782	2.446546
17	H	2.615848	4.707631	2.134982	1.092085	3.115255
18	C	3.871210	6.325809	5.918811	5.919462	6.782712
19	C	5.089996	7.522707	7.352698	7.383373	8.193820
20	O	4.783219	6.436701	6.525315	6.739416	7.342389
21	H	4.174859	5.744484	5.460500	5.549785	6.224190
22	H	2.863394	6.403953	5.573048	5.387979	6.533664
23	H	5.168500	8.348170	7.989667	7.906432	8.897627
24	C	6.399841	8.089651	8.215405	8.338814	8.946813
25	H	7.229758	8.711563	9.044042	9.238018	9.763647
26	H	6.674799	8.828432	8.736387	8.732305	9.479380
27	H	6.547131	7.410112	7.755676	7.997035	8.389687
28	C	7.205241	3.427724	5.524803	6.575243	5.671104
29	H	8.177276	4.338334	6.583658	7.655689	6.686100
30	H	7.477929	3.030251	5.286723	6.388458	5.266334
31	C	6.409003	4.191897	5.626780	6.441690	6.000482
32	O	6.322898	4.498683	5.636258	6.331226	6.002804
33	O	6.194054	4.962824	6.141091	6.848064	6.668196
34	H	5.701534	5.531382	6.301557	6.830652	6.943882

		16	17	18	19	20
16	H	0.000000				
17	H	1.864909	0.000000			
18	C	6.819883	5.266484	0.000000		
19	C	8.283708	6.710761	1.466038	0.000000	
20	O	7.728890	6.144765	1.464201	1.451705	0.000000
21	H	6.399351	5.053092	1.086329	2.196324	2.139469
22	H	6.277780	4.595813	1.086880	2.238963	2.156317
23	H	8.801255	7.125812	2.185081	1.087580	2.108340
24	C	9.192122	7.777554	2.604831	1.503870	2.517744

25	H	10.131970	8.676691	3.446162	2.151966	2.930496
26	H	9.509123	8.135205	3.141844	2.136941	3.420943
27	H	8.831087	7.564900	2.737279	2.151536	2.710591
28	C	7.473187	6.734948	5.276254	5.902843	4.751018
29	H	8.553340	7.809615	5.998425	6.416451	5.279323
30	H	7.183163	6.692232	5.707133	6.442231	5.418888
31	C	7.381780	6.391669	3.900744	4.424474	3.378937
32	O	7.189414	6.282702	3.592235	4.150999	3.447946
33	O	7.865830	6.622478	3.564580	3.862347	2.609868
34	H	7.845748	6.467880	2.692396	2.862212	1.638855

		21	22	23	24	25
21	H	0.000000				
22	H	1.844414	0.000000			
23	H	3.110097	2.532290	0.000000		
24	C	2.802963	3.560538	2.207831	0.000000	
25	H	3.753794	4.367722	2.562212	1.093867	0.000000
26	H	3.286146	3.959052	2.557686	1.094228	1.768440
27	H	2.522840	3.802451	3.099748	1.092076	1.778313
28	C	4.796440	5.849787	6.814345	6.083228	6.366939
29	H	5.582813	6.650703	7.303883	6.451971	6.566154
30	H	5.047554	6.277662	7.418487	6.526625	6.915273
31	C	3.439754	4.613675	5.376232	4.563863	4.898380
32	O	2.864403	4.408279	5.201969	4.073349	4.583319
33	O	3.489454	4.229342	4.656633	4.217297	4.377446
34	H	2.776357	3.436750	3.658867	3.313147	3.531575

		26	27	28	29	30
26	H	0.000000				
27	H	1.774612	0.000000			
28	C	7.020985	5.336554	0.000000		
29	H	7.429933	5.709065	1.094596	0.000000	
30	H	7.370606	5.668691	1.090535	1.766354	0.000000
31	C	5.501639	3.839221	1.524382	2.145744	2.126346
32	O	4.864922	3.183015	2.407170	3.048505	2.516990
33	O	5.261128	3.773871	2.366543	2.715330	3.267451
34	H	4.356120	3.014754	3.250285	3.665689	4.028168

		31	32	33	34
31	C	0.000000			
32	O	1.208177	0.000000		
33	O	1.332113	2.255861	0.000000	
34	H	1.933696	2.394579	1.004670	0.000000

Stoichiometry C11H17BrN2O3

Framework group C1[X(C11H17BrN2O3)]

Deg. of freedom 96

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.071381	1.325015	1.233898
2	6	0	-1.162183	1.238895	0.669373
3	7	0	-1.246682	2.278411	-0.247545
4	6	0	-0.095945	2.969168	-0.228362
5	7	0	0.725560	2.408396	0.667598
6	6	0	2.130628	2.782431	0.911168
7	1	0	0.546767	0.694846	1.964396
8	1	0	-1.933658	0.466515	0.777352
9	1	0	2.192459	3.871463	0.945873
10	1	0	2.386820	2.395517	1.895595
11	35	0	-3.052379	-1.534966	0.308752
12	1	0	0.129513	3.825111	-0.840956
13	6	0	-2.350809	2.585439	-1.105179
14	6	0	-3.382106	1.771117	-1.287335
15	1	0	-2.243847	3.546975	-1.591918
16	1	0	-4.172130	2.086242	-1.957390
17	1	0	-3.468495	0.789400	-0.816782
18	6	0	0.649330	-2.459818	-0.345662
19	6	0	1.630568	-3.501150	-0.026185
20	8	0	1.664029	-2.236621	0.686062
21	1	0	0.810434	-1.864884	-1.240207
22	1	0	-0.371527	-2.500185	0.025188
23	1	0	1.296077	-4.311473	0.617495
24	6	0	2.802757	-3.809713	-0.916346
25	1	0	3.670455	-4.117660	-0.325743
26	1	0	2.546698	-4.632837	-1.590316
27	1	0	3.075525	-2.940377	-1.518412
28	6	0	3.079686	2.219561	-0.156860
29	1	0	4.106093	2.415305	0.169196
30	1	0	2.934371	2.712445	-1.118742
31	6	0	2.907501	0.720689	-0.374743
32	8	0	2.755083	0.226041	-1.466431
33	8	0	2.916846	0.051090	0.776811
34	1	0	2.603065	-0.894112	0.644530

Rotational constants (GHZ): 0.3279480 0.2550895 0.1591665

Standard basis: 6-311++G(d,p) (5D, 7F)

```
 There are      538 symmetry adapted cartesian basis functions of A      symmetry.
 There are      519 symmetry adapted basis functions of A      symmetry.
    519 basis functions,      823 primitive gaussians,      538 cartesian basis functions
     78 alpha electrons              78 beta electrons
          nuclear repulsion energy           1572.3323432367 Hartrees.
 NAtoms=       34 NActive=       34 NUniq=       34 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      519 RedAO= T EigKep=    3.53D-06    NBF=      519
 NBsUse=      519 1.00D-06 EigRej= -1.00D+00 NBFU=      519
 Initial guess from the checkpoint file:    "./coohpo.chk"
 B after Tr=          0.000000        0.000000        0.000000
             Rot=       0.999999      -0.000025        0.000004        0.001514 Ang=    -0.17 deg.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                    energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3338.90387220         A.U. after        9 cycles
                  NFock=    9    Conv=0.49D-08         -V/T= 2.0019
 Calling FoFJK, ICntrl=             2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center         Atomic                         Forces (Hartrees/Bohr)
 Number         Number                      X                      Y                      Z
 -------------------------------------------------------------------
       1              6              -0.000006023        0.000030694        0.000000082
       2              6               0.000265744        0.000088361        0.000137247
       3              7              -0.000000291        0.000110210       -0.000000726
       4              6              -0.000006437       -0.000092451        0.000015965
       5              7               0.000046167       -0.000002926       -0.000016982
       6              6              -0.000016031        0.000013419       -0.000016132
       7              1               0.000002319        0.000013121       -0.000012782
       8              1              -0.000325362       -0.000187076       -0.000169168
       9              1              -0.000012288        0.000003824        0.000020145
      10              1               0.000014386        0.000003577       -0.000007090
      11             35               0.000119029        0.000076106        0.000064842
      12              1               0.000002268        0.000011635        0.000003751
      13              6              -0.000064041       -0.000093547       -0.000024156
      14              6               0.000007119        0.000100707       -0.000011687
      15              1               0.000014179        0.000006755       -0.000006408
```

16	1	-0.000007053	-0.000018592	0.000012696
17	1	-0.000005968	-0.000021807	0.000003236
18	6	-0.000001861	0.000015783	0.000057312
19	6	0.000074900	-0.000035564	-0.000037913
20	8	-0.000104429	-0.000014549	0.000002995
21	1	-0.000004119	0.000000231	0.000001484
22	1	-0.000006689	-0.000011452	-0.000012127
23	1	-0.000018569	0.000003237	0.000006692
24	6	-0.000020840	-0.000010577	0.000027027
25	1	-0.000006056	0.000001255	-0.000000960
26	1	0.000002609	-0.000000077	-0.000000077
27	1	-0.000000947	-0.000006256	-0.000007340
28	6	0.000063895	-0.000028418	-0.000048925
29	1	-0.000009890	0.000025711	0.000023430
30	1	-0.000011829	-0.000005232	-0.000002312
31	6	-0.000016000	-0.000045971	-0.000052699
32	8	-0.000004577	0.000019968	0.000018884
33	8	-0.000052351	0.000094054	0.000078284
34	1	0.000089034	-0.000044151	-0.000046589

Cartesian Forces: Max 0.000325362 RMS 0.000063559

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000236343 RMS 0.000045835
Search for a local minimum.
Step number 33 out of a maximum of 175
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 21 22 23 24 25
26 27 28 29 30
31 32 33
DE= -2.72D-06 DEPred=-5.99D-07 R= 4.54D+00
TightC=F SS= 1.41D+00 RLast= 8.19D-03 DXNew= 6.5746D-01 2.4571D-02
Trust test= 4.54D+00 RLast= 8.19D-03 DXMaxT set to 3.91D-01
ITU= 1 1 -1 1 1 1 1 1 -1 0 1 1 1 1 1 1 1 1 1 1
ITU= 0 0 -1 1 1 1 0 1 0 -1 0 1 0
Eigenvalues --- 0.00174 0.00247 0.00386 0.00488 0.00605
Eigenvalues --- 0.00749 0.00937 0.01166 0.01284 0.01437
Eigenvalues --- 0.01785 0.02051 0.02223 0.02281 0.02376
Eigenvalues --- 0.02428 0.02802 0.02869 0.03095 0.03214

Eigenvalues --- 0.03439 0.03889 0.04096 0.04368 0.04634
Eigenvalues --- 0.04852 0.05022 0.05353 0.05613 0.05737
Eigenvalues --- 0.05954 0.06219 0.06416 0.07529 0.09366
Eigenvalues --- 0.09584 0.11800 0.12447 0.12874 0.12966
Eigenvalues --- 0.13491 0.14945 0.15606 0.15742 0.15954
Eigenvalues --- 0.16004 0.16013 0.16036 0.16067 0.16190
Eigenvalues --- 0.17143 0.17558 0.19745 0.20880 0.22016
Eigenvalues --- 0.23312 0.23835 0.24161 0.25081 0.25790
Eigenvalues --- 0.28567 0.29187 0.30330 0.31432 0.31988
Eigenvalues --- 0.33283 0.34498 0.34573 0.34633 0.34794
Eigenvalues --- 0.34828 0.34929 0.34965 0.35084 0.35303
Eigenvalues --- 0.35507 0.35717 0.35741 0.35891 0.36591
Eigenvalues --- 0.37019 0.37273 0.37738 0.38925 0.39326
Eigenvalues --- 0.41206 0.45258 0.49196 0.50735 0.51532
Eigenvalues --- 0.54336 0.55876 0.56655 0.61628 0.90889
Eigenvalues --- 1.19670
En-DIIS/RFO-DIIS IScMMF= 0 using points: 33 32 31 30 29
RFO step: Lambda=-5.79313113D-07.
DidBck=F Rises=F RFO-DIIS coefs: 1.99713 -0.87822 -0.09061 -0.14669 0.11840
Iteration 1 RMS(Cart)= 0.00198820 RMS(Int)= 0.00000184
Iteration 2 RMS(Cart)= 0.00000216 RMS(Int)= 0.00000119
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000119

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56877	-0.00001	-0.00002	0.00003	0.00001	2.56878
R2	2.62009	-0.00003	0.00005	-0.00002	0.00004	2.62013
R3	2.03243	0.00000	-0.00001	0.00002	0.00001	2.03244
R4	2.62425	0.00006	-0.00014	0.00004	-0.00010	2.62415
R5	2.07302	0.00000	-0.00023	-0.00002	-0.00025	2.07277
R6	2.53654	-0.00003	-0.00008	-0.00003	-0.00011	2.53643
R7	2.70495	0.00007	0.00030	0.00005	0.00035	2.70530
R8	2.52975	0.00001	0.00000	0.00003	0.00003	2.52978
R9	2.03419	0.00000	0.00003	-0.00002	0.00001	2.03420
R10	2.78595	-0.00001	0.00023	-0.00003	0.00020	2.78614
R11	2.06233	0.00001	0.00003	0.00002	0.00005	2.06238
R12	2.05662	0.00000	0.00002	-0.00002	0.00000	2.05662
R13	2.90196	-0.00001	-0.00021	0.00004	-0.00017	2.90178
R14	4.42255	0.00000	-0.00018	0.00000	-0.00018	4.42237
R15	2.50692	-0.00005	-0.00001	-0.00006	-0.00007	2.50684
R16	2.04659	0.00000	-0.00002	-0.00001	-0.00003	2.04656
R17	2.04616	0.00001	0.00001	0.00002	0.00002	2.04618
R18	2.06374	0.00001	-0.00002	-0.00001	-0.00003	2.06371
R19	2.77041	0.00000	-0.00009	-0.00002	-0.00010	2.77031

R20	2.76694	0.00000	-0.00009	-0.00002	-0.00011	2.76683
R21	2.05286	0.00000	-0.00005	0.00004	-0.00001	2.05286
R22	2.05391	0.00000	0.00003	0.00003	0.00006	2.05397
R23	2.74333	0.00004	0.00038	0.00005	0.00043	2.74375
R24	2.05523	-0.00001	0.00003	-0.00001	0.00002	2.05525
R25	2.84190	-0.00002	-0.00015	-0.00002	-0.00018	2.84173
R26	3.09699	0.00001	-0.00085	0.00062	-0.00024	3.09675
R27	2.06711	0.00000	-0.00001	0.00001	-0.00001	2.06710
R28	2.06779	0.00000	0.00000	0.00000	0.00000	2.06779
R29	2.06373	0.00001	0.00003	0.00001	0.00003	2.06376
R30	2.06849	0.00001	0.00002	0.00001	0.00003	2.06852
R31	2.06081	0.00001	0.00002	0.00002	0.00004	2.06085
R32	2.88066	-0.00004	-0.00008	-0.00004	-0.00013	2.88054
R33	2.28312	-0.00003	-0.00001	-0.00004	-0.00005	2.28308
R34	2.51733	0.00002	0.00003	0.00009	0.00012	2.51745
R35	1.89855	0.00006	0.00020	0.00002	0.00021	1.89877
A1	1.88394	0.00002	-0.00010	0.00001	-0.00009	1.88385
A2	2.27321	0.00001	-0.00005	0.00007	0.00002	2.27323
A3	2.12551	-0.00002	0.00011	-0.00008	0.00003	2.12553
A4	1.85668	-0.00002	0.00006	-0.00001	0.00005	1.85673
A5	2.26780	-0.00004	0.00011	0.00019	0.00031	2.26811
A6	2.15226	0.00007	-0.00009	-0.00015	-0.00024	2.15202
A7	1.90035	0.00000	0.00005	-0.00001	0.00004	1.90039
A8	2.21818	0.00001	-0.00028	-0.00002	-0.00030	2.21789
A9	2.16454	-0.00002	0.00024	0.00002	0.00027	2.16481
A10	1.89662	0.00000	-0.00005	0.00002	-0.00003	1.89659
A11	2.19029	0.00001	-0.00003	0.00004	0.00001	2.19031
A12	2.19622	-0.00001	0.00009	-0.00006	0.00003	2.19625
A13	1.88719	0.00001	0.00004	-0.00001	0.00003	1.88721
A14	2.19007	-0.00012	-0.00015	0.00001	-0.00014	2.18993
A15	2.20082	0.00012	0.00006	0.00003	0.00010	2.20091
A16	1.88854	0.00008	0.00000	-0.00002	-0.00001	1.88853
A17	1.85834	-0.00002	-0.00022	-0.00002	-0.00024	1.85810
A18	1.96180	-0.00011	0.00000	0.00004	0.00004	1.96183
A19	1.88879	-0.00002	-0.00012	-0.00001	-0.00013	1.88866
A20	1.93143	0.00003	-0.00015	0.00018	0.00004	1.93146
A21	1.93190	0.00003	0.00047	-0.00018	0.00029	1.93219
A22	2.73535	-0.00008	0.00124	-0.00085	0.00039	2.73575
A23	2.15347	-0.00001	-0.00010	-0.00006	-0.00016	2.15331
A24	1.96442	-0.00001	-0.00009	0.00000	-0.00009	1.96433
A25	2.16525	0.00002	0.00019	0.00006	0.00025	2.16550
A26	2.06409	0.00001	-0.00014	0.00011	-0.00003	2.06406
A27	2.15812	0.00002	0.00014	0.00005	0.00019	2.15831
A28	2.06070	-0.00003	0.00000	-0.00016	-0.00015	2.06055

A29	2.05917	-0.00002	0.00047	-0.00002	0.00045	2.05962
A30	2.12694	0.00002	-0.00043	-0.00004	-0.00047	2.12648
A31	1.97575	-0.00001	0.00031	-0.00015	0.00016	1.97592
A32	2.00000	0.00001	-0.00023	0.00008	-0.00015	1.99985
A33	2.02706	-0.00001	-0.00012	0.00006	-0.00006	2.02701
A34	2.04019	-0.00002	-0.00039	-0.00002	-0.00040	2.03979
A35	2.13939	0.00000	0.00060	-0.00002	0.00058	2.13996
A36	1.94520	-0.00001	-0.00026	-0.00002	-0.00029	1.94491
A37	2.03887	0.00000	0.00015	-0.00006	0.00009	2.03896
A38	2.02325	0.00002	-0.00009	0.00007	-0.00001	2.02323
A39	2.09913	0.00002	0.00030	0.00071	0.00102	2.10015
A40	2.36646	-0.00002	-0.00144	-0.00005	-0.00148	2.36498
A41	1.93528	0.00000	-0.00008	-0.00002	-0.00010	1.93518
A42	1.91402	0.00001	-0.00005	0.00003	-0.00002	1.91400
A43	1.93657	0.00000	0.00020	0.00004	0.00024	1.93681
A44	1.88221	0.00000	-0.00001	0.00000	-0.00001	1.88220
A45	1.90037	0.00000	-0.00001	-0.00002	-0.00004	1.90033
A46	1.89410	-0.00001	-0.00004	-0.00003	-0.00007	1.89402
A47	1.88263	-0.00001	-0.00010	-0.00013	-0.00024	1.88239
A48	1.94489	0.00005	-0.00008	-0.00001	-0.00010	1.94479
A49	1.97143	-0.00015	0.00002	-0.00013	-0.00011	1.97132
A50	1.88269	-0.00001	-0.00008	0.00008	-0.00001	1.88268
A51	1.90110	0.00012	0.00010	0.00012	0.00023	1.90133
A52	1.87893	0.00000	0.00015	0.00009	0.00024	1.87917
A53	2.14834	-0.00004	0.00006	-0.00006	0.00000	2.14834
A54	1.94969	0.00008	-0.00009	0.00009	0.00000	1.94969
A55	2.18486	-0.00004	0.00003	-0.00003	0.00000	2.18486
A56	1.93574	-0.00024	-0.00021	-0.00014	-0.00035	1.93538
A57	2.81240	-0.00016	-0.00066	-0.00025	-0.00091	2.81150
D1	0.00329	-0.00002	-0.00020	0.00002	-0.00017	0.00312
D2	3.02388	0.00000	0.00059	0.00033	0.00093	3.02481
D3	-3.10312	0.00000	0.00117	-0.00007	0.00110	-3.10202
D4	-0.08253	0.00001	0.00196	0.00024	0.00220	-0.08033
D5	-0.00245	0.00002	0.00019	-0.00012	0.00007	-0.00237
D6	-3.04077	0.00002	0.00069	-0.00042	0.00028	-3.04050
D7	3.10756	0.00000	-0.00104	-0.00003	-0.00107	3.10649
D8	0.06923	0.00000	-0.00053	-0.00033	-0.00087	0.06837
D9	-0.00301	0.00001	0.00013	0.00008	0.00021	-0.00280
D10	3.12310	0.00001	0.00096	-0.00017	0.00079	3.12389
D11	-3.03362	0.00001	-0.00061	-0.00023	-0.00084	-3.03446
D12	0.09249	0.00001	0.00022	-0.00048	-0.00026	0.09222
D13	-1.50955	0.00013	0.00061	0.00189	0.00250	-1.50704
D14	1.49302	0.00014	0.00153	0.00226	0.00380	1.49681
D15	0.00153	0.00000	-0.00002	-0.00016	-0.00017	0.00136

D16	3.13247	0.00000	0.00132	0.00016	0.00148	3.13396
D17	-3.12516	0.00000	-0.00080	0.00008	-0.00072	-3.12588
D18	0.00578	-0.00001	0.00054	0.00040	0.00093	0.00672
D19	-0.19519	0.00001	-0.00030	-0.00018	-0.00048	-0.19567
D20	2.95609	0.00001	-0.00046	-0.00008	-0.00054	2.95555
D21	2.92873	0.00002	0.00063	-0.00046	0.00017	2.92890
D22	-0.20317	0.00001	0.00048	-0.00036	0.00011	-0.20306
D23	0.00054	-0.00001	-0.00011	0.00017	0.00006	0.00061
D24	3.03807	-0.00003	-0.00063	0.00047	-0.00016	3.03791
D25	-3.13035	-0.00001	-0.00145	-0.00015	-0.00160	-3.13195
D26	-0.09283	-0.00002	-0.00197	0.00015	-0.00182	-0.09465
D27	-2.48379	0.00003	0.00044	0.00079	0.00123	-2.48256
D28	-0.45684	0.00004	0.00019	0.00076	0.00095	-0.45589
D29	1.66130	0.00001	0.00063	0.00054	0.00117	1.66247
D30	0.77934	0.00004	0.00104	0.00044	0.00148	0.78082
D31	2.80629	0.00005	0.00079	0.00041	0.00119	2.80749
D32	-1.35875	0.00001	0.00122	0.00020	0.00142	-1.35733
D33	-3.00176	0.00007	0.00020	-0.00006	0.00015	-3.00161
D34	1.21804	0.00006	0.00042	-0.00006	0.00036	1.21839
D35	-0.89973	0.00013	0.00028	-0.00008	0.00020	-0.89953
D36	1.16773	0.00002	0.00030	-0.00019	0.00011	1.16785
D37	-0.89566	0.00001	0.00052	-0.00019	0.00032	-0.89533
D38	-3.01343	0.00008	0.00038	-0.00021	0.00017	-3.01326
D39	-0.92622	0.00000	0.00024	-0.00018	0.00006	-0.92616
D40	-2.98961	-0.00001	0.00046	-0.00018	0.00028	-2.98934
D41	1.17580	0.00006	0.00032	-0.00020	0.00012	1.17592
D42	-3.13938	-0.00001	-0.00003	-0.00014	-0.00018	-3.13955
D43	-0.02333	-0.00001	0.00026	0.00006	0.00032	-0.02300
D44	-0.00859	0.00000	0.00014	-0.00025	-0.00011	-0.00870
D45	3.10746	0.00000	0.00044	-0.00005	0.00039	3.10785
D46	-2.75270	0.00000	0.00006	-0.00019	-0.00013	-2.75283
D47	-0.04860	0.00001	0.00036	-0.00010	0.00026	-0.04835
D48	-0.01962	-0.00001	-0.00018	-0.00016	-0.00035	-0.01997
D49	2.68448	0.00000	0.00011	-0.00007	0.00004	2.68452
D50	0.32171	-0.00002	-0.00226	-0.00031	-0.00257	0.31914
D51	-2.05774	-0.00001	-0.00216	-0.00033	-0.00250	-2.06024
D52	2.54913	-0.00001	-0.00049	-0.00103	-0.00152	2.54761
D53	0.16734	-0.00003	-0.00021	-0.00106	-0.00127	0.16607
D54	2.55712	-0.00001	-0.00093	-0.00064	-0.00157	2.55555
D55	-1.64935	-0.00001	-0.00103	-0.00064	-0.00166	-1.65101
D56	0.44291	-0.00001	-0.00099	-0.00063	-0.00161	0.44130
D57	1.33007	0.00000	-0.00107	-0.00059	-0.00166	1.32842
D58	-2.87640	0.00000	-0.00117	-0.00058	-0.00175	-2.87815
D59	-0.78414	0.00000	-0.00113	-0.00057	-0.00170	-0.78584

D60	-1.01805	-0.00001	-0.00071	-0.00057	-0.00128	-1.01933
D61	1.05866	0.00000	-0.00081	-0.00056	-0.00137	1.05729
D62	-3.13226	0.00000	-0.00077	-0.00056	-0.00132	-3.13359
D63	1.48330	-0.00003	0.00156	-0.00178	-0.00022	1.48308
D64	2.82989	-0.00003	0.00119	-0.00117	0.00001	2.82990
D65	2.25499	-0.00002	-0.00188	0.00078	-0.00109	2.25390
D66	-0.86194	0.00006	-0.00127	0.00059	-0.00068	-0.86263
D67	-1.93675	-0.00005	-0.00192	0.00062	-0.00131	-1.93806
D68	1.22950	0.00004	-0.00132	0.00042	-0.00090	1.22860
D69	0.10031	0.00001	-0.00189	0.00082	-0.00107	0.09925
D70	-3.01662	0.00009	-0.00128	0.00063	-0.00066	-3.01728
D71	2.92253	-0.00015	-0.00095	0.00018	-0.00077	2.92176
D72	-0.19379	-0.00006	-0.00034	-0.00002	-0.00035	-0.19414
D73	-1.88010	-0.00002	0.00138	0.00151	0.00290	-1.87720

Item	Value	Threshold	Converged?
Maximum Force	0.000236	0.000450	YES
RMS Force	0.000046	0.000300	YES
Maximum Displacement	0.009949	0.001800	NO
RMS Displacement	0.001989	0.001200	NO

Predicted change in Energy=-9.015805D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.838460	1.639248	1.530509
2	6	0	-1.497100	0.450766	1.569260
3	7	0	-2.370644	0.451700	0.489796
4	6	0	-2.239923	1.611042	-0.173827
5	7	0	-1.311505	2.354253	0.440825
6	6	0	-0.777476	3.644113	-0.033330
7	1	0	-0.057775	2.022011	2.163569
8	1	0	-1.338691	-0.421585	2.215033
9	1	0	-1.615613	4.257880	-0.367835
10	1	0	-0.325678	4.127261	0.830894
11	35	0	-0.391983	-2.451751	2.892373
12	1	0	-2.786161	1.889860	-1.058492
13	6	0	-3.264786	-0.596974	0.102214
14	6	0	-3.222890	-1.819045	0.616568
15	1	0	-3.967359	-0.283176	-0.659884
16	1	0	-3.938610	-2.549715	0.261168
17	1	0	-2.491861	-2.136906	1.363007

18	6	0	2.560759	-0.688967	1.116705
19	6	0	3.977873	-0.373807	1.320585
20	8	0	2.973880	0.654754	1.525927
21	1	0	2.189037	-0.730602	0.096806
22	1	0	1.980938	-1.229798	1.860135
23	1	0	4.421281	-0.689993	2.262005
24	6	0	4.935055	-0.169458	0.178924
25	1	0	5.691378	0.578683	0.433481
26	1	0	5.452614	-1.108314	-0.040201
27	1	0	4.407042	0.153733	-0.720752
28	6	0	0.252176	3.472800	-1.159565
29	1	0	0.702730	4.451248	-1.354027
30	1	0	-0.219332	3.132206	-2.082056
31	6	0	1.355497	2.480721	-0.810285
32	8	0	1.673601	1.566493	-1.533216
33	8	0	1.886091	2.734518	0.385019
34	1	0	2.458966	1.968515	0.692658

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.359337	0.000000			
3	N	2.200214	1.388641	0.000000		
4	C	2.206729	2.221796	1.342221	0.000000	
5	N	1.386512	2.220602	2.178045	1.338700	0.000000
6	C	2.543383	3.644670	3.606015	2.508359	1.474364
7	H	1.075519	2.212165	3.258336	3.223986	2.156402
8	H	2.228416	1.096865	2.191802	3.263502	3.294515
9	H	3.326396	4.273230	3.973991	2.726380	2.090504
10	H	2.634885	3.928617	4.219951	3.317402	2.065809
11	Br	4.334776	3.375872	4.256466	5.415049	5.472959
12	H	3.249503	3.261556	2.153637	1.076451	2.153653
13	C	3.595521	2.524816	1.431582	2.449874	3.555237
14	C	4.298905	3.006329	2.428720	3.654648	4.593550
15	H	4.275926	3.407335	2.100311	2.609282	3.901430
16	H	5.363727	4.083498	3.394007	4.515159	5.566225
17	H	4.125667	2.779952	2.734606	4.058626	4.734360
18	C	4.140834	4.239105	5.100281	5.477413	4.971160
19	C	5.224320	5.542300	6.455644	6.695810	6.016129
20	O	3.937409	4.475841	5.447820	5.566632	4.736061
21	H	4.103344	4.141420	4.726835	5.017193	4.678512
22	H	4.035974	3.873713	4.862256	5.479329	5.069521
23	H	5.798735	6.066998	7.111570	7.456519	6.741585
24	C	6.199329	6.609866	7.338646	7.401008	6.742198

25	H	6.705747	7.278775	8.063218	8.021229	7.224477
26	H	7.042289	7.302028	7.994867	8.160139	7.614070
27	H	5.898323	6.339659	6.891389	6.826787	6.236452
28	C	3.433351	4.431607	4.327426	3.263185	2.501499
29	H	4.313138	5.421136	5.370446	4.256624	3.417021
30	H	3.957634	4.706901	4.292746	3.168290	2.857093
31	C	3.316752	4.233233	4.437484	3.753460	2.948588
32	O	3.962594	4.574226	4.657387	4.143137	3.664459
33	O	3.151974	4.250168	4.831358	4.312597	3.220611
34	H	3.418103	4.326945	5.066262	4.791465	3.798509

		6	7	8	9	10
6	C	0.000000				
7	H	2.824102	0.000000			
8	H	4.679744	2.759449	0.000000		
9	H	1.091364	3.719405	5.352129	0.000000	
10	H	1.088318	2.505968	4.861486	1.765770	0.000000
11	Br	6.772585	4.545041	2.340217	7.559456	6.894744
12	H	2.857127	4.224125	4.260741	2.730331	3.824882
13	C	4.918527	4.625277	2.864368	5.148818	5.611393
14	C	6.020674	5.211994	2.838695	6.362500	6.618031
15	H	5.098188	5.345149	3.897973	5.122225	5.910687
16	H	6.960101	6.291318	3.886657	7.220478	7.613138
17	H	6.189431	4.884901	2.235637	6.682582	6.649457
18	C	5.589453	3.911783	4.059991	6.642081	5.622211
19	C	6.371037	4.768335	5.391491	7.455895	6.246596
20	O	5.043831	3.386283	4.497960	6.134517	4.840295
21	H	5.287275	4.110542	4.126408	6.290962	5.519195
22	H	5.911774	3.850024	3.434982	6.929188	5.922660
23	H	7.147036	5.237041	5.766414	8.236601	6.912860
24	C	6.871783	5.802561	6.600697	7.925372	6.823648
25	H	7.173622	6.174881	7.320951	8.220141	6.996807
26	H	7.835792	6.709689	7.188845	8.880496	7.845935
27	H	6.287649	5.634214	6.477907	7.296639	6.371433
28	C	1.535558	3.639242	5.393052	2.175275	2.173513
29	H	2.141663	4.342010	6.375743	2.526793	2.436487
30	H	2.184228	4.391351	5.687475	2.480987	3.080052
31	C	2.550827	3.324389	4.983431	3.490208	2.868956
32	O	3.545976	4.107478	5.203434	4.406881	4.017918
33	O	2.845517	2.729381	4.869205	3.892217	2.651501
34	H	3.716080	2.915549	4.738397	4.792498	3.526122

		11	12	13	14	15
11	Br	0.000000				
12	H	6.339638	0.000000			
13	C	4.413409	2.785797	0.000000		

14	C	3.686956	4.092986	1.326564	0.000000	
15	H	5.486762	2.505235	1.082992	2.131304	0.000000
16	H	4.417171	4.772784	2.071835	1.082793	2.446704
17	H	2.616787	4.707984	2.135041	1.092067	3.115364
18	C	3.870282	6.322292	5.913935	5.914204	6.777702
19	C	5.087633	7.519066	7.347812	7.378031	8.188845
20	O	4.779810	6.432945	6.520333	6.733987	7.337458
21	H	4.176029	5.740569	5.455463	5.544711	6.218841
22	H	2.861720	6.401241	5.568517	5.382704	6.529075
23	H	5.164171	8.344373	7.984296	7.900353	8.892256
24	C	6.399141	8.086357	8.211337	8.334551	8.942567
25	H	7.227514	8.707114	9.039070	9.232919	9.758557
26	H	6.675637	8.826289	8.733545	8.729310	9.476325
27	H	6.547814	7.407454	7.752276	7.993506	8.386011
28	C	7.206487	3.427449	5.524869	6.575284	5.671112
29	H	8.178124	4.338250	6.583797	7.655738	6.686280
30	H	7.480329	3.029805	5.287023	6.388961	5.266413
31	C	6.410354	4.190949	5.626000	6.440926	5.999545
32	O	6.324457	4.496599	5.634082	6.329223	6.000367
33	O	6.194661	4.962570	6.140875	6.847644	6.667921
34	H	5.701351	5.530287	6.300135	6.828975	6.942416

		16	17	18	19	20
16	H	0.000000				
17	H	1.864817	0.000000			
18	C	6.814405	5.261763	0.000000		
19	C	8.278142	6.705801	1.465983	0.000000	
20	O	7.723390	6.139563	1.464145	1.451931	0.000000
21	H	6.394079	5.048936	1.086326	2.196559	2.139528
22	H	6.272155	4.590851	1.086912	2.238656	2.156193
23	H	8.794867	7.119921	2.184778	1.087592	2.108347
24	C	9.187726	7.773801	2.605112	1.503778	2.517926
25	H	10.126856	8.672014	3.445941	2.151811	2.929849
26	H	9.505974	8.132753	3.142787	2.136844	3.421299
27	H	8.827384	7.562006	2.737728	2.151637	2.711557
28	C	7.473410	6.735125	5.275535	5.901555	4.749834
29	H	8.553618	7.809703	5.998217	6.415704	5.278790
30	H	7.183867	6.693010	5.706342	6.441011	5.417740
31	C	7.381115	6.391231	3.900368	4.423324	3.378047
32	O	7.187481	6.281269	3.591133	4.149532	3.446788
33	O	7.865468	6.622211	3.565220	3.861673	2.609669
34	H	7.844078	6.466416	2.693026	2.861440	1.638731

		21	22	23	24	25
21	H	0.000000				
22	H	1.844405	0.000000			

23	H	3.110088	2.531435	0.000000		
24	C	2.803969	3.560561	2.207747	0.000000	
25	H	3.754193	4.367299	2.562457	1.093864	0.000000
26	H	3.288217	3.959617	2.557106	1.094227	1.768428
27	H	2.523885	3.802777	3.099825	1.092093	1.778301
28	C	4.795674	5.849926	6.813034	6.081691	6.363853
29	H	5.582615	6.651236	7.303128	6.450848	6.563425
30	H	5.046679	6.277670	7.417234	6.525391	6.912662
31	C	3.439506	4.614138	5.375075	4.562370	4.895362
32	O	2.863440	4.407781	5.200498	4.072105	4.581070
33	O	3.490258	4.230929	4.655915	4.215654	4.373807
34	H	2.777253	3.438127	3.658031	3.311475	3.528071

		26	27	28	29	30
26	H	0.000000				
27	H	1.774580	0.000000			
28	C	7.020266	5.335886	0.000000		
29	H	7.429418	5.708905	1.094612	0.000000	
30	H	7.370356	5.668138	1.090556	1.766380	0.000000
31	C	5.500960	3.838595	1.524315	2.145865	2.126481
32	O	4.864630	3.182403	2.407088	3.049018	2.517117
33	O	5.260062	3.773377	2.366533	2.715103	3.267632
34	H	4.354983	3.014326	3.250159	3.665686	4.028213

		31	32	33	34
31	C	0.000000			
32	O	1.208152	0.000000		
33	O	1.332176	2.255894	0.000000	
34	H	1.933608	2.394355	1.004783	0.000000

Stoichiometry C11H17BrN2O3
Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.075138	1.324680	1.234242
2	6	0	-1.157925	1.242252	0.668063
3	7	0	-1.237824	2.281424	-0.249575
4	6	0	-0.084854	2.968312	-0.229497
5	7	0	0.733629	2.405477	0.667956
6	6	0	2.139802	2.774771	0.913006

7	1	0	0.547813	0.692899	1.965113
8	1	0	-1.932536	0.473190	0.775930
9	1	0	2.205176	3.863602	0.948369
10	1	0	2.393509	2.386630	1.897595
11	35	0	-3.057698	-1.525363	0.310726
12	1	0	0.143710	3.823886	-0.841460
13	6	0	-2.340501	2.591730	-1.108203
14	6	0	-3.374202	1.780577	-1.290595
15	1	0	-2.230024	3.552738	-1.595162
16	1	0	-4.162896	2.097952	-1.961174
17	1	0	-3.464277	0.799476	-0.819494
18	6	0	0.639731	-2.459649	-0.348982
19	6	0	1.616873	-3.504533	-0.028801
20	8	0	1.653539	-2.240356	0.684373
21	1	0	0.803736	-1.864470	-1.242833
22	1	0	-0.381761	-2.497252	0.020502
23	1	0	1.278314	-4.313852	0.614034
24	6	0	2.789592	-3.816978	-0.916751
25	1	0	3.655404	-4.126868	-0.324403
26	1	0	2.532377	-4.639957	-1.590455
27	1	0	3.065917	-2.948986	-1.519164
28	6	0	3.087954	2.209355	-0.154351
29	1	0	4.114619	2.401547	0.173058
30	1	0	2.945334	2.703510	-1.116007
31	6	0	2.910744	0.711279	-0.373215
32	8	0	2.756587	0.217889	-1.465201
33	8	0	2.917442	0.040907	0.777980
34	1	0	2.599725	-0.902969	0.644777

Rotational constants (GHZ): 0.3281596 0.2550461 0.1592318

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 538 symmetry adapted cartesian basis functions of A symmetry.

There are 519 symmetry adapted basis functions of A symmetry.

519 basis functions, 823 primitive gaussians, 538 cartesian basis functions

78 alpha electrons 78 beta electrons

nuclear repulsion energy 1572.4671800277 Hartrees.

NAtoms= 34 NActive= 34 NUniq= 34 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 519 RedAO= T EigKep= 3.53D-06 NBF= 519

NBsUse= 519 1.00D-06 EigRej= -1.00D+00 NBFU= 519

Initial guess from the checkpoint file: "./coohpo.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999999 -0.000014 0.000077 0.001670 Ang= -0.19 deg.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3338.90387512 A.U. after 11 cycles
NFock= 11 Conv=0.15D-08 -V/T= 2.0019
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000029482	-0.000018888	-0.000070602
2	6	0.000221904	0.000153589	0.000145881
3	7	-0.000079324	0.000012218	0.000009346
4	6	-0.000056671	-0.000026531	0.000026822
5	7	0.000085200	0.000026109	-0.000035329
6	6	-0.000110694	-0.000014372	0.000042471
7	1	-0.000020508	0.000023958	0.000012191
8	1	-0.000265386	-0.000227632	-0.000124091
9	1	-0.000003238	-0.000004804	0.000016806
10	1	0.000037572	0.000000794	-0.000024396
11	35	0.000106031	0.000059372	0.000055416
12	1	0.000034447	-0.000003717	-0.000020147
13	6	0.000026534	0.000021335	-0.000012850
14	6	-0.000034889	0.000057249	-0.000006082
15	1	0.000007561	-0.000006954	-0.000016542
16	1	-0.000002204	-0.000014691	0.000008926
17	1	0.000013781	-0.000011655	0.000002074
18	6	-0.000042359	-0.000019602	0.000071298
19	6	0.000030310	0.000018967	0.000048977
20	8	-0.000014808	-0.000058873	-0.000021914
21	1	0.000022376	0.000012924	-0.000013344
22	1	-0.000021728	0.000005411	-0.000018146
23	1	-0.000001963	0.000009228	-0.000007399
24	6	-0.000022204	-0.000005525	-0.000028424
25	1	0.000001740	-0.000001227	0.000000083
26	1	0.000003451	-0.000001862	0.000000155
27	1	-0.000004020	-0.000003263	0.000010397
28	6	0.000057695	0.000030840	-0.000069767

29	1	0.000002363	0.000008738	0.000014785
30	1	0.000007926	-0.000012899	0.000008846
31	6	-0.000021411	-0.000021394	0.000027457
32	8	0.000017804	-0.000010440	-0.000015967
33	8	-0.000023778	0.000037289	0.000023095
34	1	0.000019007	-0.000013692	-0.000040028

Cartesian Forces: Max 0.000265386 RMS 0.000057524

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000142079 RMS 0.000037592

Search for a local minimum.

Step number 34 out of a maximum of 175

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 21 22 23 24 25
26 27 28 29 30
31 32 33 34

DE= -2.92D-06 DEPred=-9.02D-07 R= 3.24D+00

TightC=F SS= 1.41D+00 RLast= 1.06D-02 DXNew= 6.5746D-01 3.1744D-02

Trust test= 3.24D+00 RLast= 1.06D-02 DXMaxT set to 3.91D-01

ITU= 1 1 1 -1 1 1 1 1 1 -1 0 1 1 1 1 1 1 1 1 1

ITU= 1 0 0 -1 1 1 1 0 1 0 -1 0 1 0

Eigenvalues ---	0.00174	0.00262	0.00381	0.00456	0.00573
Eigenvalues ---	0.00744	0.00932	0.01147	0.01280	0.01347
Eigenvalues ---	0.01711	0.02108	0.02200	0.02284	0.02363
Eigenvalues ---	0.02440	0.02766	0.02925	0.03058	0.03148
Eigenvalues ---	0.03438	0.03845	0.04001	0.04351	0.04650
Eigenvalues ---	0.04850	0.05015	0.05327	0.05611	0.05737
Eigenvalues ---	0.05941	0.06189	0.06415	0.07723	0.09281
Eigenvalues ---	0.09701	0.11746	0.12551	0.12871	0.13262
Eigenvalues ---	0.13552	0.14915	0.15246	0.15663	0.15945
Eigenvalues ---	0.16004	0.16013	0.16035	0.16063	0.16174
Eigenvalues ---	0.17014	0.17667	0.19301	0.20352	0.21947
Eigenvalues ---	0.23314	0.23645	0.24092	0.25289	0.26126
Eigenvalues ---	0.28387	0.28765	0.29912	0.31821	0.31991
Eigenvalues ---	0.32944	0.34358	0.34508	0.34607	0.34668
Eigenvalues ---	0.34837	0.34902	0.34965	0.35053	0.35188
Eigenvalues ---	0.35309	0.35590	0.35741	0.35901	0.36590
Eigenvalues ---	0.37025	0.37261	0.37753	0.38905	0.39548

Eigenvalues --- 0.42001 0.45380 0.49222 0.50613 0.51086
Eigenvalues --- 0.54126 0.55913 0.56311 0.61075 0.90974
Eigenvalues --- 1.14667
En-DIIS/RFO-DIIS IScMMF= 0 using points: 34 33 32 31 30
RFO step: Lambda=-4.10094873D-07.
DidBck=F Rises=F RFO-DIIS coefs: 2.05728 -1.52676 0.27160 0.18184 0.01604
Iteration 1 RMS(Cart)= 0.00372062 RMS(Int)= 0.00000381
Iteration 2 RMS(Cart)= 0.00000555 RMS(Int)= 0.00000031
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000031

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56878	-0.00001	0.00003	-0.00001	0.00002	2.56880
R2	2.62013	-0.00002	0.00000	0.00004	0.00003	2.62016
R3	2.03244	0.00000	0.00000	-0.00001	-0.00001	2.03243
R4	2.62415	0.00007	-0.00003	0.00006	0.00002	2.62417
R5	2.07277	0.00007	-0.00019	0.00010	-0.00009	2.07268
R6	2.53643	0.00000	-0.00010	-0.00001	-0.00011	2.53632
R7	2.70530	-0.00003	0.00028	-0.00005	0.00023	2.70553
R8	2.52978	0.00001	0.00004	0.00000	0.00004	2.52982
R9	2.03420	0.00000	0.00000	0.00002	0.00001	2.03421
R10	2.78614	-0.00005	0.00011	-0.00002	0.00008	2.78623
R11	2.06238	-0.00001	0.00004	-0.00003	0.00002	2.06240
R12	2.05662	0.00000	-0.00001	0.00001	0.00000	2.05662
R13	2.90178	0.00003	-0.00010	0.00012	0.00003	2.90181
R14	4.42237	0.00001	0.00036	-0.00058	-0.00022	4.42215
R15	2.50684	-0.00002	-0.00010	0.00002	-0.00008	2.50677
R16	2.04656	0.00000	-0.00002	0.00001	-0.00001	2.04655
R17	2.04618	0.00001	0.00003	0.00000	0.00004	2.04622
R18	2.06371	0.00002	-0.00003	0.00004	0.00000	2.06371
R19	2.77031	0.00002	-0.00007	0.00008	0.00001	2.77032
R20	2.76683	0.00000	-0.00005	-0.00005	-0.00010	2.76673
R21	2.05286	0.00001	0.00001	-0.00002	-0.00001	2.05285
R22	2.05397	-0.00001	0.00001	-0.00004	-0.00003	2.05394
R23	2.74375	-0.00003	0.00038	-0.00006	0.00032	2.74407
R24	2.05525	-0.00001	0.00000	-0.00001	-0.00001	2.05525
R25	2.84173	0.00001	-0.00014	0.00004	-0.00010	2.84163
R26	3.09675	0.00002	-0.00103	0.00035	-0.00068	3.09607
R27	2.06710	0.00000	0.00000	0.00001	0.00001	2.06711
R28	2.06779	0.00000	0.00000	0.00001	0.00001	2.06779
R29	2.06376	0.00000	0.00002	-0.00001	0.00001	2.06377
R30	2.06852	0.00001	0.00003	-0.00003	0.00000	2.06852
R31	2.06085	-0.00001	0.00004	-0.00004	0.00000	2.06085
R32	2.88054	-0.00002	-0.00011	-0.00001	-0.00012	2.88042

R33	2.28308	0.00002	-0.00003	0.00004	0.00001	2.28309
R34	2.51745	-0.00002	0.00011	-0.00004	0.00007	2.51752
R35	1.89877	0.00001	0.00034	-0.00014	0.00021	1.89897
A1	1.88385	0.00003	-0.00005	0.00001	-0.00003	1.88382
A2	2.27323	0.00000	0.00008	0.00000	0.00008	2.27331
A3	2.12553	-0.00003	-0.00006	0.00000	-0.00006	2.12547
A4	1.85673	-0.00003	0.00001	-0.00005	-0.00004	1.85669
A5	2.26811	-0.00002	0.00026	0.00022	0.00048	2.26858
A6	2.15202	0.00005	-0.00020	-0.00019	-0.00039	2.15163
A7	1.90039	0.00000	0.00003	0.00006	0.00008	1.90047
A8	2.21789	0.00003	-0.00018	-0.00005	-0.00023	2.21766
A9	2.16481	-0.00004	0.00015	-0.00001	0.00014	2.16495
A10	1.89659	0.00000	-0.00001	-0.00004	-0.00005	1.89654
A11	2.19031	0.00001	0.00005	0.00005	0.00010	2.19040
A12	2.19625	-0.00001	-0.00003	-0.00001	-0.00004	2.19621
A13	1.88721	0.00000	0.00001	0.00002	0.00003	1.88725
A14	2.18993	-0.00007	-0.00005	0.00011	0.00006	2.18998
A15	2.20091	0.00007	0.00007	-0.00009	-0.00002	2.20090
A16	1.88853	0.00007	-0.00002	-0.00001	-0.00003	1.88850
A17	1.85810	0.00001	-0.00019	0.00006	-0.00013	1.85798
A18	1.96183	-0.00011	0.00010	0.00007	0.00017	1.96200
A19	1.88866	-0.00001	-0.00010	0.00003	-0.00007	1.88859
A20	1.93146	0.00004	0.00012	-0.00004	0.00008	1.93155
A21	1.93219	0.00000	0.00007	-0.00011	-0.00004	1.93215
A22	2.73575	-0.00009	-0.00121	-0.00001	-0.00122	2.73452
A23	2.15331	-0.00001	-0.00017	-0.00005	-0.00022	2.15309
A24	1.96433	0.00001	-0.00007	0.00004	-0.00003	1.96430
A25	2.16550	0.00000	0.00024	0.00001	0.00025	2.16575
A26	2.06406	0.00002	0.00008	0.00005	0.00013	2.06419
A27	2.15831	0.00000	0.00015	-0.00002	0.00012	2.15844
A28	2.06055	-0.00002	-0.00022	-0.00003	-0.00025	2.06029
A29	2.05962	-0.00004	0.00017	-0.00025	-0.00008	2.05954
A30	2.12648	0.00005	-0.00010	0.00034	0.00025	2.12672
A31	1.97592	-0.00002	0.00005	0.00003	0.00009	1.97600
A32	1.99985	0.00002	0.00003	-0.00016	-0.00013	1.99972
A33	2.02701	0.00000	-0.00015	-0.00001	-0.00016	2.02685
A34	2.03979	0.00001	-0.00026	0.00009	-0.00016	2.03963
A35	2.13996	-0.00004	0.00031	-0.00011	0.00019	2.14015
A36	1.94491	0.00000	-0.00027	0.00002	-0.00024	1.94467
A37	2.03896	-0.00002	0.00000	-0.00002	-0.00002	2.03894
A38	2.02323	0.00002	0.00010	0.00003	0.00013	2.02336
A39	2.10015	-0.00001	0.00031	0.00040	0.00071	2.10086
A40	2.36498	-0.00004	-0.00167	-0.00046	-0.00212	2.36285
A41	1.93518	0.00001	-0.00008	0.00003	-0.00005	1.93513

A42	1.91400	0.00001	0.00001	0.00003	0.00005	1.91405
A43	1.93681	-0.00001	0.00015	-0.00008	0.00007	1.93688
A44	1.88220	-0.00001	-0.00001	-0.00002	-0.00003	1.88217
A45	1.90033	0.00000	-0.00004	0.00000	-0.00003	1.90029
A46	1.89402	0.00000	-0.00004	0.00003	0.00000	1.89402
A47	1.88239	0.00002	-0.00028	0.00006	-0.00022	1.88217
A48	1.94479	0.00005	-0.00002	0.00006	0.00004	1.94483
A49	1.97132	-0.00014	-0.00004	-0.00010	-0.00015	1.97117
A50	1.88268	-0.00001	-0.00003	0.00007	0.00004	1.88273
A51	1.90133	0.00009	0.00016	-0.00001	0.00015	1.90147
A52	1.87917	0.00000	0.00022	-0.00008	0.00014	1.87931
A53	2.14834	-0.00002	-0.00004	0.00012	0.00008	2.14842
A54	1.94969	0.00004	0.00006	-0.00012	-0.00006	1.94963
A55	2.18486	-0.00002	-0.00002	-0.00001	-0.00003	2.18483
A56	1.93538	-0.00014	-0.00031	-0.00012	-0.00042	1.93496
A57	2.81150	-0.00011	0.00002	-0.00004	-0.00002	2.81147
D1	0.00312	-0.00001	-0.00007	0.00004	-0.00003	0.00309
D2	3.02481	-0.00001	0.00054	-0.00015	0.00040	3.02521
D3	-3.10202	-0.00001	0.00069	-0.00027	0.00042	-3.10160
D4	-0.08033	-0.00001	0.00131	-0.00047	0.00084	-0.07949
D5	-0.00237	0.00001	-0.00001	0.00009	0.00008	-0.00229
D6	-3.04050	0.00001	-0.00039	-0.00027	-0.00067	-3.04117
D7	3.10649	0.00001	-0.00069	0.00038	-0.00032	3.10618
D8	0.06837	0.00001	-0.00108	0.00001	-0.00107	0.06730
D9	-0.00280	0.00000	0.00013	-0.00017	-0.00004	-0.00283
D10	3.12389	0.00000	0.00030	-0.00039	-0.00009	3.12379
D11	-3.03446	0.00001	-0.00047	-0.00002	-0.00050	-3.03496
D12	0.09222	0.00000	-0.00031	-0.00025	-0.00055	0.09167
D13	-1.50704	0.00012	0.00212	0.00269	0.00481	-1.50223
D14	1.49681	0.00011	0.00285	0.00249	0.00533	1.50214
D15	0.00136	0.00000	-0.00014	0.00023	0.00009	0.00145
D16	3.13396	-0.00002	0.00100	-0.00024	0.00076	3.13472
D17	-3.12588	0.00001	-0.00029	0.00044	0.00015	-3.12573
D18	0.00672	-0.00001	0.00085	-0.00002	0.00082	0.00754
D19	-0.19567	0.00002	-0.00056	-0.00025	-0.00080	-0.19648
D20	2.95555	0.00002	-0.00055	-0.00029	-0.00084	2.95471
D21	2.92890	0.00001	-0.00037	-0.00050	-0.00087	2.92803
D22	-0.20306	0.00001	-0.00036	-0.00055	-0.00091	-0.20397
D23	0.00061	-0.00001	0.00009	-0.00020	-0.00011	0.00050
D24	3.03791	-0.00002	0.00047	0.00019	0.00066	3.03856
D25	-3.13195	0.00002	-0.00105	0.00027	-0.00078	-3.13274
D26	-0.09465	0.00001	-0.00067	0.00066	-0.00002	-0.09467
D27	-2.48256	0.00002	0.00204	0.00098	0.00303	-2.47953
D28	-0.45589	0.00005	0.00181	0.00105	0.00287	-0.45303

D29	1.66247	0.00000	0.00184	0.00099	0.00283	1.66530
D30	0.78082	0.00003	0.00160	0.00054	0.00214	0.78296
D31	2.80749	0.00005	0.00137	0.00061	0.00198	2.80946
D32	-1.35733	0.00000	0.00139	0.00055	0.00194	-1.35539
D33	-3.00161	0.00006	0.00002	0.00008	0.00010	-3.00152
D34	1.21839	0.00003	0.00024	-0.00009	0.00015	1.21855
D35	-0.89953	0.00010	0.00000	0.00004	0.00004	-0.89950
D36	1.16785	0.00002	-0.00011	0.00007	-0.00004	1.16780
D37	-0.89533	0.00000	0.00011	-0.00009	0.00001	-0.89532
D38	-3.01326	0.00006	-0.00013	0.00003	-0.00010	-3.01336
D39	-0.92616	0.00001	-0.00011	0.00013	0.00002	-0.92614
D40	-2.98934	-0.00002	0.00011	-0.00004	0.00007	-2.98926
D41	1.17592	0.00005	-0.00013	0.00009	-0.00004	1.17588
D42	-3.13955	0.00000	-0.00024	0.00005	-0.00018	-3.13974
D43	-0.02300	-0.00001	0.00010	-0.00012	-0.00002	-0.02302
D44	-0.00870	0.00000	-0.00025	0.00010	-0.00014	-0.00884
D45	3.10785	-0.00001	0.00009	-0.00007	0.00002	3.10788
D46	-2.75283	-0.00001	-0.00017	0.00012	-0.00006	-2.75288
D47	-0.04835	0.00000	0.00023	0.00014	0.00037	-0.04798
D48	-0.01997	0.00000	-0.00041	0.00035	-0.00006	-0.02003
D49	2.68452	0.00001	-0.00001	0.00037	0.00036	2.68488
D50	0.31914	0.00001	-0.00232	-0.00031	-0.00263	0.31651
D51	-2.06024	0.00001	-0.00218	-0.00016	-0.00234	-2.06258
D52	2.54761	-0.00002	-0.00071	-0.00088	-0.00159	2.54602
D53	0.16607	-0.00004	-0.00057	-0.00092	-0.00149	0.16458
D54	2.55555	-0.00001	-0.00135	-0.00026	-0.00161	2.55394
D55	-1.65101	-0.00001	-0.00140	-0.00024	-0.00165	-1.65266
D56	0.44130	-0.00001	-0.00135	-0.00023	-0.00158	0.43972
D57	1.32842	0.00001	-0.00134	-0.00018	-0.00152	1.32689
D58	-2.87815	0.00001	-0.00140	-0.00017	-0.00156	-2.87971
D59	-0.78584	0.00001	-0.00135	-0.00015	-0.00150	-0.78733
D60	-1.01933	-0.00001	-0.00104	-0.00022	-0.00125	-1.02059
D61	1.05729	0.00000	-0.00109	-0.00020	-0.00129	1.05599
D62	-3.13359	0.00000	-0.00104	-0.00019	-0.00123	-3.13481
D63	1.48308	-0.00004	-0.00031	-0.00136	-0.00167	1.48141
D64	2.82990	-0.00004	-0.00079	-0.00108	-0.00187	2.82802
D65	2.25390	-0.00002	0.00107	-0.00098	0.00008	2.25398
D66	-0.86263	0.00003	0.00121	-0.00070	0.00052	-0.86211
D67	-1.93806	-0.00003	0.00079	-0.00098	-0.00019	-1.93824
D68	1.22860	0.00002	0.00094	-0.00069	0.00025	1.22885
D69	0.09925	0.00001	0.00097	-0.00094	0.00002	0.09927
D70	-3.01728	0.00006	0.00111	-0.00066	0.00046	-3.01682
D71	2.92176	-0.00012	-0.00004	-0.00027	-0.00031	2.92144
D72	-0.19414	-0.00007	0.00011	0.00002	0.00013	-0.19401

D73	-1.87720	-0.00006	-0.00161	0.00179	0.00019	-1.87701

Item	Value	Threshold	Converged?
Maximum Force	0.000142	0.000450	YES
RMS Force	0.000038	0.000300	YES
Maximum Displacement	0.014519	0.001800	NO
RMS Displacement	0.003722	0.001200	NO

Predicted change in Energy=-6.589916D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.840212	1.640495	1.532431
2	6	0	-1.498450	0.451758	1.570652
3	7	0	-2.369019	0.451201	0.488772
4	6	0	-2.237060	1.609835	-0.175723
5	7	0	-1.310578	2.354085	0.440641
6	6	0	-0.776382	3.644087	-0.033073
7	1	0	-0.061197	2.024208	2.166965
8	1	0	-1.342067	-0.419905	2.217764
9	1	0	-1.614428	4.257861	-0.367821
10	1	0	-0.325151	4.127065	0.831543
11	35	0	-0.392579	-2.446976	2.900057
12	1	0	-2.781452	1.887789	-1.061804
13	6	0	-3.261555	-0.598560	0.099980
14	6	0	-3.219486	-1.820144	0.615371
15	1	0	-3.962809	-0.285803	-0.663750
16	1	0	-3.933833	-2.551865	0.259312
17	1	0	-2.489695	-2.136816	1.363525
18	6	0	2.558547	-0.689555	1.118742
19	6	0	3.976218	-0.374440	1.318818
20	8	0	2.972534	0.653993	1.527472
21	1	0	2.184097	-0.730865	0.099832
22	1	0	1.980573	-1.230601	1.863431
23	1	0	4.422047	-0.690929	2.258988
24	6	0	4.930334	-0.169237	0.174814
25	1	0	5.686291	0.579965	0.427344
26	1	0	5.448622	-1.107466	-0.045278
27	1	0	4.399792	0.153019	-0.723718
28	6	0	0.253999	3.473255	-1.158733
29	1	0	0.704393	4.451924	-1.352459
30	1	0	-0.216857	3.132918	-2.081651

31	6	0	1.357154	2.481298	-0.808846
32	8	0	1.676022	1.567257	-1.531684
33	8	0	1.886385	2.734640	0.387199
34	1	0	2.458875	1.968221	0.694879

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.359350	0.000000			
3	N	2.200204	1.388653	0.000000		
4	C	2.206789	2.221827	1.342163	0.000000	
5	N	1.386528	2.220600	2.177976	1.338723	0.000000
6	C	2.543474	3.644760	3.606014	2.508408	1.474407
7	H	1.075515	2.212212	3.258332	3.224015	2.156378
8	H	2.228629	1.096817	2.191545	3.263379	3.294568
9	H	3.325804	4.272885	3.974144	2.727015	2.090526
10	H	2.634305	3.928204	4.219818	3.317593	2.065752
11	Br	4.333381	3.375341	4.256764	5.414818	5.471895
12	H	3.249558	3.261611	2.153642	1.076457	2.153658
13	C	3.595578	2.524794	1.431704	2.450022	3.555343
14	C	4.298600	3.006006	2.428647	3.654551	4.593326
15	H	4.276032	3.407289	2.100392	2.609564	3.901668
16	H	5.363507	4.083192	3.394068	4.515312	5.566209
17	H	4.125215	2.779602	2.734517	4.058387	4.733943
18	C	4.141477	4.238636	5.096969	5.473635	4.969275
19	C	5.225284	5.542383	6.452340	6.691474	6.013839
20	O	3.938304	4.475763	5.445384	5.563666	4.734613
21	H	4.101479	4.138002	4.720108	5.010134	4.673951
22	H	4.038512	3.875520	4.861800	5.478564	5.070107
23	H	5.801275	6.068923	7.110324	7.454197	6.741030
24	C	6.198181	6.607818	7.332398	7.393207	6.736972
25	H	6.703818	7.276269	8.056573	8.012729	7.218300
26	H	7.042009	7.300973	7.989378	8.152941	7.609549
27	H	5.895798	6.335821	6.883011	6.816921	6.229667
28	C	3.434920	4.432839	4.327506	3.262517	2.501688
29	H	4.314224	5.422030	5.370454	4.256092	3.417052
30	H	3.959481	4.708547	4.293074	3.167580	2.857406
31	C	3.319179	4.235034	4.437282	3.752155	2.948592
32	O	3.965552	4.576691	4.657272	4.141577	3.664553
33	O	3.153259	4.250790	4.830411	4.311017	3.219977
34	H	3.419485	4.327477	5.064819	4.789384	3.797671

		6	7	8	9	10
6	C	0.000000				
7	H	2.824122	0.000000			

8	H	4.679989	2.759872	0.000000		
9	H	1.091373	3.718450	5.351722	0.000000	
10	H	1.088319	2.505001	4.861138	1.765734	0.000000
11	Br	6.771381	4.542986	2.340100	7.558226	6.892119
12	H	2.857127	4.224139	4.260616	2.731446	3.825249
13	C	4.918723	4.625324	2.863802	5.149435	5.611522
14	C	6.020553	5.211648	2.837788	6.362784	6.617643
15	H	5.098539	5.345248	3.897358	5.123216	5.911164
16	H	6.960230	6.291017	3.885620	7.221170	7.613024
17	H	6.189085	4.884387	2.234851	6.682480	6.648643
18	C	5.588281	3.914887	4.061446	6.640822	5.621212
19	C	6.368938	4.772168	5.393916	7.453743	6.245219
20	O	5.042850	3.389685	4.499504	6.133532	4.839553
21	H	5.284156	4.111546	4.125065	6.287676	5.516449
22	H	5.912708	3.854185	3.438418	6.930060	5.923322
23	H	7.146298	5.242129	5.770629	8.235878	6.912782
24	C	6.866678	5.804761	6.601476	7.920073	6.819796
25	H	7.167076	6.176223	7.321418	8.213386	6.991619
26	H	7.831225	6.712638	7.190796	8.875666	7.842550
27	H	6.281507	5.635407	6.476843	7.290215	6.366864
28	C	1.535572	3.641339	5.394891	2.175355	2.173495
29	H	2.141512	4.343532	6.377241	2.526678	2.436259
30	H	2.184270	4.393655	5.689782	2.481112	3.080058
31	C	2.550663	3.328078	4.986295	3.490126	2.868724
32	O	3.545891	4.111781	5.207306	4.406925	4.017730
33	O	2.845005	2.732280	4.870834	3.891780	2.650883
34	H	3.715553	2.919064	4.740199	4.792033	3.525633

		11	12	13	14	15
11	Br	0.000000				
12	H	6.339814	0.000000			
13	C	4.414532	2.786068	0.000000		
14	C	3.688376	4.093111	1.326523	0.000000	
15	H	5.487981	2.505704	1.082986	2.131404	0.000000
16	H	4.418711	4.773244	2.071894	1.082813	2.447023
17	H	2.618210	4.707950	2.135075	1.092068	3.115471
18	C	3.869206	6.317679	5.909292	5.909084	6.772620
19	C	5.087447	7.513398	7.343102	7.373131	8.183312
20	O	4.777445	6.429227	6.516938	6.730111	7.333734
21	H	4.174393	5.732663	5.447259	5.536337	6.210120
22	H	2.861120	6.399863	5.566789	5.380133	6.527104
23	H	5.164813	8.340735	7.981703	7.897445	8.888889
24	C	6.399097	8.076647	8.203472	8.327013	8.933351
25	H	7.226987	8.696588	9.031059	9.225440	9.749112
26	H	6.677493	8.816972	8.726240	8.722412	9.467453

27	H	6.546643	7.395539	7.742065	7.983729	8.374321
28	C	7.207009	3.425939	5.524776	6.575151	5.670714
29	H	8.178145	4.337093	6.583745	7.655587	6.686041
30	H	7.482213	3.027802	5.287119	6.389251	5.265952
31	C	6.411350	4.188592	5.625296	6.440220	5.998325
32	O	6.327204	4.493618	5.633184	6.328533	5.998630
33	O	6.193325	4.960390	6.139543	6.846023	6.666381
34	H	5.699787	5.527516	6.298062	6.826553	6.940067

		16	17	18	19	20
16	H	0.000000				
17	H	1.864695	0.000000			
18	C	6.808657	5.257302	0.000000		
19	C	8.272402	6.701940	1.465988	0.000000	
20	O	7.719045	6.136077	1.464092	1.452099	0.000000
21	H	6.385181	5.041622	1.086323	2.196512	2.139537
22	H	6.268902	4.588510	1.086898	2.238798	2.156050
23	H	8.791048	7.117908	2.184673	1.087589	2.108322
24	C	9.179189	7.767962	2.605207	1.503725	2.518009
25	H	10.118467	8.666261	3.445649	2.151735	2.929204
26	H	9.497869	8.127802	3.143585	2.136834	3.421592
27	H	8.816578	7.554135	2.737658	2.151645	2.712175
28	C	7.473343	6.735172	5.275113	5.898977	4.749144
29	H	8.553596	7.809626	5.998293	6.413606	5.278517
30	H	7.184204	6.693663	5.705846	6.437905	5.416923
31	C	7.380260	6.390964	3.900417	4.420598	3.377407
32	O	7.186467	6.281369	3.591213	4.145655	3.445784
33	O	7.863741	6.620753	3.565398	3.860271	2.609412
34	H	7.841404	6.464268	2.693208	2.860016	1.638369

		21	22	23	24	25
21	H	0.000000				
22	H	1.844300	0.000000			
23	H	3.109980	2.531503	0.000000		
24	C	2.804080	3.560760	2.207782	0.000000	
25	H	3.753785	4.367247	2.562890	1.093868	0.000000
26	H	3.289378	3.960517	2.556756	1.094229	1.768413
27	H	2.523646	3.802679	3.099883	1.092100	1.778288
28	C	4.794151	5.851564	6.811305	6.075705	6.355829
29	H	5.582111	6.652945	7.301537	6.445639	6.555843
30	H	5.045023	6.279544	7.415011	6.518392	6.903606
31	C	3.439116	4.616050	5.372914	4.556373	4.887194
32	O	2.863800	4.409941	5.197043	4.064245	4.571083
33	O	3.490119	4.232171	4.654858	4.212271	4.368469
34	H	2.777526	3.439005	3.656715	3.308671	3.523499

		26	27	28	29	30

26	H	0.000000				
27	H	1.774584	0.000000			
28	C	7.014762	5.329240	0.000000		
29	H	7.424503	5.703672	1.094613	0.000000	
30	H	7.363784	5.660144	1.090556	1.766408	0.000000
31	C	5.495669	3.832203	1.524254	2.145921	2.126535
32	O	4.857577	3.173610	2.407087	3.049178	2.517290
33	O	5.257219	3.770426	2.366462	2.715249	3.267640
34	H	4.352731	3.012396	3.249997	3.665867	4.028049

		31	32	33	34
31	C	0.000000			
32	O	1.208157	0.000000		
33	O	1.332213	2.255914	0.000000	
34	H	1.933449	2.393995	1.004893	0.000000

Stoichiometry C11H17BrN2O3
Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.075792	1.325339	1.235443
2	6	0	-1.156552	1.245751	0.667266
3	7	0	-1.231391	2.283263	-0.252693
4	6	0	-0.076304	2.966453	-0.232047
5	7	0	0.738800	2.402776	0.667983
6	6	0	2.145549	2.768546	0.915259
7	1	0	0.545309	0.693414	1.968217
8	1	0	-1.934277	0.479937	0.775332
9	1	0	2.213497	3.857211	0.951158
10	1	0	2.396680	2.379481	1.900144
11	35	0	-3.061648	-1.518008	0.313467
12	1	0	0.155931	3.820399	-0.844911
13	6	0	-2.331731	2.595115	-1.113957
14	6	0	-3.367038	1.786192	-1.296848
15	1	0	-2.217831	3.555089	-1.602153
16	1	0	-4.153927	2.104323	-1.969219
17	1	0	-3.460448	0.806072	-0.824354
18	6	0	0.631999	-2.459872	-0.350320
19	6	0	1.608276	-3.506445	-0.033002

20	8	0	1.645751	-2.244132	0.683765
21	1	0	0.796543	-1.862461	-1.242577
22	1	0	-0.389552	-2.497386	0.018967
23	1	0	1.268912	-4.317108	0.607707
24	6	0	2.781000	-3.817361	-0.921393
25	1	0	3.646805	-4.128108	-0.329476
26	1	0	2.523934	-4.639318	-1.596404
27	1	0	3.057334	-2.948413	-1.522434
28	6	0	3.094132	2.201121	-0.150668
29	1	0	4.120625	2.390810	0.178737
30	1	0	2.954426	2.695922	-1.112419
31	6	0	2.913525	0.703591	-0.370063
32	8	0	2.760006	0.210667	-1.462354
33	8	0	2.916017	0.033141	0.781146
34	1	0	2.595787	-0.909846	0.646840

Rotational constants (GHZ): 0.3284108 0.2549576 0.1593275

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 538 symmetry adapted cartesian basis functions of A symmetry.

There are 519 symmetry adapted basis functions of A symmetry.

519 basis functions, 823 primitive gaussians, 538 cartesian basis functions

78 alpha electrons 78 beta electrons

nuclear repulsion energy 1572.6024552496 Hartrees.

NAtoms= 34 NActive= 34 NUniq= 34 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 519 RedAO= T EigKep= 3.53D-06 NBF= 519

NBsUse= 519 1.00D-06 EigRej= -1.00D+00 NBFU= 519

Initial guess from the checkpoint file: "./coohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999999 -0.000009 0.000172 0.001185 Ang= -0.14 deg.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3338.90387747 A.U. after 11 cycles

NFock= 11 Conv=0.18D-08 -V/T= 2.0019

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000046264	-0.000036597	-0.000110834
2	6	0.000161681	0.000169819	0.000113802
3	7	-0.000125826	-0.000065235	0.000017520
4	6	-0.000048361	0.000028717	0.000027691
5	7	0.000081464	0.000038586	-0.000037725
6	6	-0.000128150	-0.000018033	0.000059594
7	1	-0.000024169	0.000021822	0.000028547
8	1	-0.000193855	-0.000207818	-0.000100289
9	1	0.000003424	-0.000003626	0.000006297
10	1	0.000040500	-0.000006281	-0.000030938
11	35	0.000086148	0.000040570	0.000043395
12	1	0.000049320	-0.000019039	-0.000030444
13	6	0.000084164	0.000110650	0.000007312
14	6	-0.000054434	-0.000017597	0.000005130
15	1	0.000002178	-0.000020659	-0.000017034
16	1	0.000002401	0.000001847	0.000001454
17	1	0.000015249	0.000009475	0.000001079
18	6	-0.000056304	-0.000009873	0.000050855
19	6	-0.000025238	0.000048404	0.000128279
20	8	0.000056086	-0.000086457	-0.000053611
21	1	0.000025909	0.000020424	-0.000021787
22	1	-0.000014921	-0.000000496	-0.000008868
23	1	0.000013657	0.000007708	-0.000014613
24	6	-0.000016645	-0.000004726	-0.000061229
25	1	0.000005547	-0.000005971	0.000004602
26	1	0.000000234	-0.000003073	0.000003853
27	1	-0.000005540	0.000002041	0.000017966
28	6	0.000023803	0.000055366	-0.000054516
29	1	0.000011051	0.000001515	0.000001266
30	1	0.000013097	-0.000012403	0.000006138
31	6	-0.000030655	-0.000017117	0.000111259
32	8	0.000026571	-0.000012385	-0.000040873
33	8	-0.000001532	-0.000016099	-0.000041906
34	1	-0.000023119	0.000006540	-0.000011376

Cartesian Forces: Max 0.000207818 RMS 0.000058011

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000157720 RMS 0.000036477
Search for a local minimum.
Step number 35 out of a maximum of 175
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 21 22 23 24 25
26 27 28 29 30
31 32 33 34 35
DE= -2.35D-06 DEPred=-6.59D-07 R= 3.56D+00
TightC=F SS= 1.41D+00 RLast= 1.23D-02 DXNew= 6.5746D-01 3.6809D-02
Trust test= 3.56D+00 RLast= 1.23D-02 DXMaxT set to 3.91D-01
ITU= 1 1 1 1 -1 1 1 1 1 1 -1 0 1 1 1 1 1 1 1 1
ITU= 1 1 0 0 -1 1 1 1 0 1 0 -1 0 1 0
Eigenvalues --- 0.00173 0.00257 0.00367 0.00439 0.00546
Eigenvalues --- 0.00738 0.00915 0.01034 0.01184 0.01305
Eigenvalues --- 0.01655 0.02112 0.02180 0.02281 0.02323
Eigenvalues --- 0.02459 0.02538 0.02866 0.03058 0.03128
Eigenvalues --- 0.03456 0.03696 0.03964 0.04360 0.04657
Eigenvalues --- 0.04854 0.05027 0.05335 0.05634 0.05736
Eigenvalues --- 0.05889 0.06054 0.06159 0.07496 0.09349
Eigenvalues --- 0.09737 0.11741 0.12594 0.12863 0.13147
Eigenvalues --- 0.13663 0.14804 0.15588 0.15908 0.15939
Eigenvalues --- 0.16003 0.16022 0.16040 0.16151 0.16212
Eigenvalues --- 0.16633 0.17683 0.19763 0.20881 0.21902
Eigenvalues --- 0.23314 0.23531 0.24114 0.25271 0.26983
Eigenvalues --- 0.27895 0.29218 0.29765 0.31772 0.32210
Eigenvalues --- 0.32979 0.34290 0.34505 0.34607 0.34722
Eigenvalues --- 0.34872 0.34900 0.34965 0.35049 0.35163
Eigenvalues --- 0.35310 0.35592 0.35765 0.35882 0.36598
Eigenvalues --- 0.37035 0.37257 0.37820 0.39072 0.39653
Eigenvalues --- 0.42670 0.45607 0.49228 0.50327 0.50696
Eigenvalues --- 0.54310 0.56049 0.56487 0.61308 0.91057
Eigenvalues --- 1.10483
En-DIIS/RFO-DIIS IScMMF= 0 using points: 35 34 33 32 31
RFO step: Lambda=-3.99079464D-07.
DidBck=F Rises=F RFO-DIIS coefs: 2.54406 -1.62350 -0.87481 1.06399 -0.10974
Iteration 1 RMS(Cart)= 0.00607849 RMS(Int)= 0.00000947
Iteration 2 RMS(Cart)= 0.00001442 RMS(Int)= 0.00000020
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000020

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56880	-0.00001	0.00007	-0.00004	0.00003	2.56883

R2	2.62016	-0.00002	0.00001	-0.00001	0.00000	2.62016
R3	2.03243	0.00001	0.00000	-0.00001	-0.00001	2.03242
R4	2.62417	0.00005	0.00011	-0.00002	0.00010	2.62427
R5	2.07268	0.00009	0.00002	0.00009	0.00011	2.07279
R6	2.53632	0.00003	-0.00010	0.00002	-0.00007	2.53625
R7	2.70553	-0.00009	0.00009	-0.00012	-0.00004	2.70549
R8	2.52982	0.00000	0.00005	0.00000	0.00005	2.52987
R9	2.03421	-0.00001	0.00000	0.00000	0.00000	2.03421
R10	2.78623	-0.00007	-0.00004	-0.00002	-0.00006	2.78616
R11	2.06240	-0.00001	0.00000	-0.00001	-0.00001	2.06239
R12	2.05662	-0.00001	-0.00002	0.00000	-0.00002	2.05660
R13	2.90181	0.00000	0.00016	-0.00005	0.00010	2.90191
R14	4.42215	0.00002	0.00002	-0.00095	-0.00093	4.42122
R15	2.50677	0.00001	-0.00009	0.00006	-0.00003	2.50674
R16	2.04655	0.00000	0.00000	-0.00001	-0.00001	2.04653
R17	2.04622	0.00000	0.00004	-0.00002	0.00002	2.04624
R18	2.06371	0.00001	0.00002	-0.00006	-0.00004	2.06367
R19	2.77032	0.00001	0.00008	0.00001	0.00009	2.77041
R20	2.76673	-0.00001	-0.00010	-0.00007	-0.00017	2.76656
R21	2.05285	0.00001	0.00001	0.00003	0.00004	2.05289
R22	2.05394	0.00000	-0.00007	0.00001	-0.00006	2.05388
R23	2.74407	-0.00007	0.00018	-0.00010	0.00009	2.74416
R24	2.05525	-0.00001	-0.00003	0.00000	-0.00003	2.05522
R25	2.84163	0.00003	-0.00002	0.00002	0.00000	2.84163
R26	3.09607	0.00002	-0.00047	-0.00011	-0.00058	3.09549
R27	2.06711	0.00000	0.00002	-0.00001	0.00002	2.06713
R28	2.06779	0.00000	0.00001	-0.00001	0.00000	2.06779
R29	2.06377	-0.00001	-0.00001	0.00003	0.00002	2.06379
R30	2.06852	0.00001	0.00000	0.00001	0.00001	2.06853
R31	2.06085	-0.00001	-0.00002	0.00002	0.00000	2.06086
R32	2.88042	0.00001	-0.00011	0.00011	0.00000	2.88042
R33	2.28309	0.00004	0.00003	-0.00001	0.00002	2.28311
R34	2.51752	-0.00005	0.00004	-0.00006	-0.00002	2.51750
R35	1.89897	-0.00001	0.00016	0.00001	0.00018	1.89915
A1	1.88382	0.00003	0.00003	-0.00001	0.00002	1.88384
A2	2.27331	-0.00002	0.00013	-0.00006	0.00007	2.27339
A3	2.12547	-0.00002	-0.00015	0.00007	-0.00008	2.12539
A4	1.85669	-0.00002	-0.00009	0.00002	-0.00008	1.85662
A5	2.26858	-0.00001	0.00061	0.00016	0.00077	2.26935
A6	2.15163	0.00003	-0.00052	-0.00019	-0.00071	2.15092
A7	1.90047	-0.00001	0.00007	0.00000	0.00007	1.90054
A8	2.21766	0.00003	-0.00012	-0.00010	-0.00022	2.21744
A9	2.16495	-0.00002	0.00004	0.00010	0.00014	2.16509
A10	1.89654	0.00000	-0.00001	-0.00002	-0.00003	1.89651

A11	2.19040	0.00001	0.00014	-0.00002	0.00012	2.19052
A12	2.19621	-0.00001	-0.00013	0.00004	-0.00009	2.19612
A13	1.88725	0.00000	0.00000	0.00001	0.00002	1.88726
A14	2.18998	-0.00006	0.00021	-0.00002	0.00019	2.19018
A15	2.20090	0.00006	-0.00008	0.00002	-0.00006	2.20083
A16	1.88850	0.00008	0.00002	0.00002	0.00004	1.88853
A17	1.85798	0.00003	-0.00006	0.00005	-0.00001	1.85796
A18	1.96200	-0.00015	0.00023	-0.00018	0.00006	1.96206
A19	1.88859	-0.00001	0.00001	0.00003	0.00004	1.88863
A20	1.93155	0.00005	0.00024	0.00000	0.00024	1.93178
A21	1.93215	0.00000	-0.00045	0.00009	-0.00036	1.93178
A22	2.73452	-0.00008	-0.00297	0.00136	-0.00161	2.73291
A23	2.15309	0.00000	-0.00023	0.00008	-0.00015	2.15294
A24	1.96430	0.00002	0.00003	0.00006	0.00009	1.96438
A25	2.16575	-0.00002	0.00020	-0.00014	0.00006	2.16582
A26	2.06419	0.00001	0.00027	-0.00005	0.00022	2.06441
A27	2.15844	-0.00002	0.00006	-0.00001	0.00005	2.15849
A28	2.06029	0.00001	-0.00033	0.00006	-0.00027	2.06003
A29	2.05954	-0.00003	-0.00048	-0.00002	-0.00050	2.05904
A30	2.12672	0.00003	0.00072	-0.00014	0.00058	2.12730
A31	1.97600	-0.00002	-0.00003	-0.00013	-0.00016	1.97584
A32	1.99972	0.00003	-0.00012	0.00028	0.00016	1.99988
A33	2.02685	0.00001	-0.00015	0.00007	-0.00008	2.02677
A34	2.03963	0.00004	0.00006	0.00008	0.00014	2.03977
A35	2.14015	-0.00006	-0.00014	-0.00019	-0.00033	2.13983
A36	1.94467	0.00002	-0.00018	0.00022	0.00004	1.94471
A37	2.03894	-0.00003	-0.00010	-0.00011	-0.00022	2.03873
A38	2.02336	0.00002	0.00022	0.00004	0.00026	2.02362
A39	2.10086	-0.00003	0.00073	0.00007	0.00080	2.10167
A40	2.36285	-0.00002	-0.00222	0.00006	-0.00216	2.36070
A41	1.93513	0.00000	0.00000	-0.00002	-0.00002	1.93511
A42	1.91405	0.00001	0.00011	-0.00001	0.00010	1.91415
A43	1.93688	-0.00002	-0.00007	-0.00001	-0.00008	1.93680
A44	1.88217	0.00000	-0.00005	0.00000	-0.00005	1.88212
A45	1.90029	0.00001	-0.00003	0.00000	-0.00003	1.90026
A46	1.89402	0.00001	0.00004	0.00005	0.00009	1.89411
A47	1.88217	0.00004	-0.00020	0.00007	-0.00013	1.88204
A48	1.94483	0.00005	0.00013	0.00007	0.00020	1.94504
A49	1.97117	-0.00016	-0.00020	-0.00005	-0.00026	1.97091
A50	1.88273	-0.00002	0.00013	-0.00009	0.00004	1.88277
A51	1.90147	0.00008	0.00010	-0.00004	0.00007	1.90154
A52	1.87931	0.00001	0.00005	0.00004	0.00009	1.87940
A53	2.14842	-0.00002	0.00006	-0.00007	-0.00001	2.14841
A54	1.94963	0.00003	-0.00006	0.00008	0.00002	1.94965

A55	2.18483	-0.00001	0.00000	-0.00002	-0.00001	2.18482
A56	1.93496	-0.00003	-0.00040	0.00017	-0.00024	1.93472
A57	2.81147	-0.00008	0.00058	-0.00039	0.00019	2.81166
D1	0.00309	-0.00001	0.00022	-0.00008	0.00014	0.00323
D2	3.02521	-0.00002	0.00016	-0.00021	-0.00005	3.02516
D3	-3.10160	-0.00001	-0.00018	-0.00021	-0.00039	-3.10199
D4	-0.07949	-0.00003	-0.00024	-0.00033	-0.00057	-0.08006
D5	-0.00229	0.00001	-0.00015	-0.00005	-0.00020	-0.00249
D6	-3.04117	0.00001	-0.00149	-0.00016	-0.00165	-3.04282
D7	3.10618	0.00001	0.00022	0.00006	0.00028	3.10645
D8	0.06730	0.00002	-0.00113	-0.00005	-0.00118	0.06612
D9	-0.00283	0.00001	-0.00022	0.00019	-0.00003	-0.00286
D10	3.12379	-0.00001	-0.00088	0.00006	-0.00082	3.12297
D11	-3.03496	0.00002	-0.00026	0.00027	0.00002	-3.03494
D12	0.09167	0.00001	-0.00092	0.00015	-0.00077	0.09090
D13	-1.50223	0.00010	0.00669	0.00129	0.00798	-1.49425
D14	1.50214	0.00008	0.00666	0.00117	0.00783	1.50997
D15	0.00145	0.00000	0.00013	-0.00023	-0.00009	0.00135
D16	3.13472	-0.00003	0.00012	-0.00037	-0.00024	3.13447
D17	-3.12573	0.00001	0.00077	-0.00010	0.00067	-3.12506
D18	0.00754	-0.00002	0.00076	-0.00024	0.00052	0.00806
D19	-0.19648	0.00002	-0.00101	0.00143	0.00042	-0.19606
D20	2.95471	0.00002	-0.00093	0.00130	0.00038	2.95508
D21	2.92803	0.00001	-0.00177	0.00129	-0.00048	2.92755
D22	-0.20397	0.00001	-0.00168	0.00116	-0.00053	-0.20450
D23	0.00050	0.00000	0.00001	0.00017	0.00018	0.00068
D24	3.03856	-0.00002	0.00139	0.00028	0.00166	3.04023
D25	-3.13274	0.00003	0.00002	0.00031	0.00033	-3.13241
D26	-0.09467	0.00001	0.00139	0.00042	0.00181	-0.09286
D27	-2.47953	0.00000	0.00392	0.00075	0.00467	-2.47486
D28	-0.45303	0.00004	0.00391	0.00082	0.00474	-0.44829
D29	1.66530	-0.00002	0.00345	0.00086	0.00431	1.66961
D30	0.78296	0.00001	0.00233	0.00063	0.00295	0.78591
D31	2.80946	0.00006	0.00232	0.00070	0.00302	2.81248
D32	-1.35539	-0.00001	0.00186	0.00073	0.00259	-1.35280
D33	-3.00152	0.00006	0.00028	0.00025	0.00053	-3.00099
D34	1.21855	0.00002	0.00016	0.00028	0.00045	1.21899
D35	-0.89950	0.00009	0.00014	0.00022	0.00036	-0.89913
D36	1.16780	0.00003	-0.00008	0.00036	0.00028	1.16808
D37	-0.89532	-0.00001	-0.00019	0.00039	0.00019	-0.89513
D38	-3.01336	0.00005	-0.00021	0.00032	0.00011	-3.01325
D39	-0.92614	0.00000	0.00004	0.00026	0.00031	-0.92584
D40	-2.98926	-0.00003	-0.00007	0.00029	0.00022	-2.98904
D41	1.17588	0.00003	-0.00009	0.00023	0.00014	1.17602

D42	-3.13974	0.00000	-0.00012	-0.00012	-0.00024	-3.13998
D43	-0.02302	-0.00001	-0.00014	-0.00013	-0.00027	-0.02329
D44	-0.00884	0.00000	-0.00021	0.00002	-0.00019	-0.00903
D45	3.10788	-0.00001	-0.00024	0.00002	-0.00022	3.10765
D46	-2.75288	-0.00001	-0.00006	0.00007	0.00001	-2.75288
D47	-0.04798	-0.00001	0.00035	-0.00009	0.00026	-0.04771
D48	-0.02003	0.00001	0.00016	-0.00018	-0.00001	-0.02004
D49	2.68488	0.00001	0.00058	-0.00034	0.00024	2.68512
D50	0.31651	0.00003	-0.00229	0.00004	-0.00226	0.31425
D51	-2.06258	0.00001	-0.00189	-0.00023	-0.00213	-2.06471
D52	2.54602	-0.00002	-0.00194	-0.00011	-0.00205	2.54397
D53	0.16458	-0.00004	-0.00196	-0.00030	-0.00226	0.16233
D54	2.55394	-0.00001	-0.00164	0.00035	-0.00129	2.55265
D55	-1.65266	-0.00001	-0.00163	0.00033	-0.00130	-1.65396
D56	0.43972	-0.00001	-0.00156	0.00038	-0.00118	0.43854
D57	1.32689	0.00002	-0.00142	0.00048	-0.00094	1.32595
D58	-2.87971	0.00002	-0.00141	0.00046	-0.00095	-2.88067
D59	-0.78733	0.00002	-0.00134	0.00050	-0.00083	-0.78817
D60	-1.02059	0.00000	-0.00127	0.00021	-0.00106	-1.02165
D61	1.05599	0.00000	-0.00125	0.00018	-0.00107	1.05492
D62	-3.13481	0.00000	-0.00118	0.00023	-0.00095	-3.13576
D63	1.48141	-0.00004	-0.00354	-0.00039	-0.00393	1.47748
D64	2.82802	-0.00004	-0.00368	-0.00025	-0.00392	2.82410
D65	2.25398	-0.00002	0.00174	0.00001	0.00175	2.25573
D66	-0.86211	0.00000	0.00166	0.00013	0.00178	-0.86033
D67	-1.93824	-0.00001	0.00143	0.00003	0.00146	-1.93678
D68	1.22885	0.00001	0.00135	0.00015	0.00150	1.23034
D69	0.09927	0.00001	0.00167	-0.00008	0.00159	0.10086
D70	-3.01682	0.00004	0.00159	0.00004	0.00163	-3.01519
D71	2.92144	-0.00009	0.00063	-0.00032	0.00032	2.92176
D72	-0.19401	-0.00007	0.00054	-0.00019	0.00035	-0.19366
D73	-1.87701	-0.00008	-0.00085	-0.00042	-0.00127	-1.87829

Item	Value	Threshold	Converged?
Maximum Force	0.000158	0.000450	YES
RMS Force	0.000036	0.000300	YES
Maximum Displacement	0.023111	0.001800	NO
RMS Displacement	0.006080	0.001200	NO

Predicted change in Energy=-7.634787D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.842830	1.642452	1.535115
2	6	0	-1.500480	0.453355	1.572754
3	7	0	-2.366515	0.450363	0.487177
4	6	0	-2.232533	1.607853	-0.178828
5	7	0	-1.309184	2.353851	0.440176
6	6	0	-0.775337	3.644291	-0.032636
7	1	0	-0.066940	2.028010	2.172343
8	1	0	-1.346779	-0.417535	2.221648
9	1	0	-1.613435	4.257774	-0.367774
10	1	0	-0.324953	4.127131	0.832483
11	35	0	-0.392805	-2.439504	2.911098
12	1	0	-2.773175	1.883878	-1.067800
13	6	0	-3.256005	-0.601143	0.096201
14	6	0	-3.214558	-1.821740	0.613934
15	1	0	-3.954314	-0.290613	-0.671119
16	1	0	-3.926410	-2.555162	0.256347
17	1	0	-2.487514	-2.136215	1.365654
18	6	0	2.555541	-0.690258	1.122875
19	6	0	3.974207	-0.375407	1.316579
20	8	0	2.971496	0.653047	1.530075
21	1	0	2.176942	-0.731164	0.105463
22	1	0	1.980381	-1.231338	1.869668
23	1	0	4.424384	-0.692116	2.254584
24	6	0	4.922706	-0.169867	0.167973
25	1	0	5.679210	0.580092	0.416627
26	1	0	5.440807	-1.107694	-0.054264
27	1	0	4.387562	0.151672	-0.728094
28	6	0	0.256388	3.474495	-1.157295
29	1	0	0.706624	4.453488	-1.349775
30	1	0	-0.213125	3.134538	-2.081039
31	6	0	1.359411	2.482754	-0.806383
32	8	0	1.680691	1.570144	-1.529979
33	8	0	1.885539	2.734436	0.391369
34	1	0	2.458077	1.967843	0.698836

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.359365	0.000000			
3	N	2.200196	1.388705	0.000000		
4	C	2.206824	2.221893	1.342124	0.000000	
5	N	1.386530	2.220634	2.177940	1.338751	0.000000
6	C	2.543572	3.644885	3.605999	2.508361	1.474375

7	H	1.075509	2.212257	3.258343	3.224024	2.156326
8	H	2.229089	1.096876	2.191232	3.263287	3.294789
9	H	3.324865	4.272238	3.974223	2.727832	2.090520
10	H	2.633537	3.927658	4.219696	3.317887	2.065705
11	Br	4.331076	3.374424	4.257024	5.414180	5.470051
12	H	3.249567	3.261699	2.153670	1.076455	2.153634
13	C	3.595498	2.524686	1.431684	2.450061	3.555337
14	C	4.298174	3.005571	2.428518	3.654443	4.593060
15	H	4.276159	3.407309	2.100429	2.609799	3.901907
16	H	5.363178	4.082798	3.394074	4.515450	5.566155
17	H	4.124564	2.779029	2.734365	4.058139	4.733463
18	C	4.142512	4.238107	5.092324	5.468217	4.966767
19	C	5.227175	5.542984	6.447834	6.685296	6.010919
20	O	3.940563	4.476636	5.442709	5.560029	4.733374
21	H	4.098412	4.132730	4.710065	4.999529	4.667164
22	H	4.042415	3.878497	4.861574	5.477772	5.071318
23	H	5.806152	6.072974	7.109522	7.451571	6.741201
24	C	6.196369	6.604479	7.322522	7.380922	6.729019
25	H	6.701988	7.273283	8.047081	8.000410	7.210023
26	H	7.040847	7.298324	7.979660	8.140630	7.601917
27	H	5.890802	6.328820	6.869036	6.800575	6.218308
28	C	3.437111	4.434754	4.327734	3.261362	2.501753
29	H	4.315707	5.423427	5.370623	4.255280	3.416999
30	H	3.962249	4.711288	4.293905	3.166573	2.857856
31	C	3.322437	4.237656	4.436940	3.749845	2.948206
32	O	3.970918	4.581923	4.658617	4.140091	3.665386
33	O	3.153503	4.250192	4.827643	4.307301	3.217683
34	H	3.420707	4.327538	5.062039	4.785574	3.795809

		6	7	8	9	10
6	C	0.000000				
7	H	2.824203	0.000000			
8	H	4.680468	2.760636	0.000000		
9	H	1.091369	3.716946	5.351142	0.000000	
10	H	1.088306	2.503619	4.860854	1.765749	0.000000
11	Br	6.769377	4.539893	2.339608	7.556088	6.888102
12	H	2.856917	4.224099	4.260467	2.733206	3.825840
13	C	4.918742	4.625251	2.862931	5.149989	5.611573
14	C	6.020411	5.211210	2.836395	6.363005	6.617148
15	H	5.098728	5.345368	3.896594	5.124408	5.911814
16	H	6.960316	6.290629	3.884116	7.221875	7.612849
17	H	6.188782	4.883718	2.233353	6.682207	6.647590
18	C	5.587331	3.920175	4.063223	6.639685	5.620393
19	C	6.366830	4.779081	5.397575	7.451520	6.244196
20	O	5.042654	3.396340	4.502435	6.133309	4.839677

21	H	5.280117	4.113398	4.122282	6.283344	5.512810
22	H	5.914770	3.860892	3.443277	6.931956	5.924822
23	H	7.146531	5.251461	5.777786	8.236105	6.914024
24	C	6.859719	5.809022	6.601921	7.912785	6.814961
25	H	7.159074	6.180393	7.322424	8.205078	6.986016
26	H	7.824467	6.717567	7.192178	8.868419	7.837966
27	H	6.271967	5.637000	6.473611	7.280238	6.359833
28	C	1.535625	3.644632	5.397712	2.175571	2.173271
29	H	2.141463	4.345879	6.379529	2.526916	2.435757
30	H	2.184464	4.397389	5.693462	2.481492	3.079993
31	C	2.550490	3.333778	4.990402	3.490112	2.868264
32	O	3.546293	4.119593	5.214513	4.407418	4.017713
33	O	2.843920	2.735522	4.871624	3.890974	2.649615
34	H	3.714902	2.924134	4.741932	4.791519	3.525003

		11	12	13	14	15
11	Br	0.000000				
12	H	6.339513	0.000000			
13	C	4.416008	2.786280	0.000000		
14	C	3.690649	4.093245	1.326507	0.000000	
15	H	5.489476	2.506164	1.082979	2.131419	0.000000
16	H	4.421249	4.773720	2.072023	1.082825	2.447274
17	H	2.620723	4.707915	2.135073	1.092049	3.115476
18	C	3.866568	6.310345	5.902208	5.901975	6.764343
19	C	5.086628	7.504452	7.335955	7.366406	8.174324
20	O	4.773848	6.423795	6.512354	6.725411	7.328205
21	H	4.170565	5.720022	5.434510	5.524144	6.195923
22	H	2.859415	6.397624	5.564356	5.377065	6.523891
23	H	5.166207	8.335397	7.978425	7.894379	8.883891
24	C	6.397707	8.060496	8.190388	8.315205	8.917406
25	H	7.225629	8.680220	9.018651	9.214491	9.733761
26	H	6.678183	8.800356	8.712851	8.710436	9.450736
27	H	6.542922	7.375100	7.724656	7.967912	8.353787
28	C	7.207541	3.422912	5.524399	6.575319	5.669428
29	H	8.177844	4.334906	6.583508	7.655738	6.685164
30	H	7.484896	3.024014	5.287231	6.390319	5.264602
31	C	6.412375	4.183928	5.623801	6.439500	5.995459
32	O	6.332443	4.488760	5.632932	6.329669	5.996110
33	O	6.189470	4.955426	6.135853	6.842461	6.662108
34	H	5.696169	5.522142	6.293933	6.822532	6.935139

		16	17	18	19	20
16	H	0.000000				
17	H	1.864538	0.000000			
18	C	6.800325	5.251870	0.000000		
19	C	8.264089	6.697514	1.466038	0.000000	

20	O	7.713372	6.132521	1.464001	1.452146	0.000000
21	H	6.371863	5.031839	1.086342	2.196253	2.139364
22	H	6.264622	4.586384	1.086865	2.239167	2.156048
23	H	8.786334	7.116879	2.184799	1.087574	2.108379
24	C	9.165386	7.759661	2.605018	1.503727	2.517882
25	H	10.105615	8.658774	3.445270	2.151727	2.928618
26	H	9.483480	8.119871	3.143990	2.136907	3.421672
27	H	8.798762	7.542207	2.737012	2.151596	2.712185
28	C	7.473349	6.736048	5.275456	5.896098	4.749140
29	H	8.553702	7.810267	5.999218	6.411300	5.278876
30	H	7.185023	6.695774	5.706105	6.434071	5.416618
31	C	7.379018	6.391515	3.901381	4.417376	3.377230
32	O	7.186703	6.284563	3.593385	4.141048	3.445457
33	O	7.859824	6.617860	3.565464	3.858713	2.609240
34	H	7.836776	6.461178	2.693475	2.858509	1.638061

		21	22	23	24	25
21	H	0.000000				
22	H	1.844242	0.000000			
23	H	3.109863	2.532208	0.000000		
24	C	2.803246	3.560866	2.207944	0.000000	
25	H	3.752613	4.367373	2.563432	1.093876	0.000000
26	H	3.289393	3.961231	2.556677	1.094230	1.768388
27	H	2.522114	3.802053	3.099952	1.092109	1.778282
28	C	4.792770	5.854871	6.809827	6.067308	6.345219
29	H	5.582130	6.656164	7.300027	6.438503	6.545991
30	H	5.043497	6.283345	7.412651	6.507988	6.890802
31	C	3.439345	4.619668	5.370604	4.547839	4.876121
32	O	2.866524	4.415396	5.193129	4.052325	4.556055
33	O	3.489562	4.233406	4.653876	4.208237	4.362772
34	H	2.777727	3.440029	3.655420	3.305452	3.518692

		26	27	28	29	30
26	H	0.000000				
27	H	1.774648	0.000000			
28	C	7.006520	5.319018	0.000000		
29	H	7.417384	5.695736	1.094619	0.000000	
30	H	7.353319	5.647501	1.090558	1.766441	0.000000
31	C	5.487695	3.822273	1.524252	2.145972	2.126602
32	O	4.846342	3.159467	2.407090	3.048762	2.517446
33	O	5.253616	3.766163	2.366470	2.715983	3.267610
34	H	4.350030	3.009570	3.250024	3.666446	4.027928

		31	32	33	34
31	C	0.000000			
32	O	1.208168	0.000000		
33	O	1.332203	2.255907	0.000000	

34 H 1.933361 2.393764 1.004988 0.000000

Stoichiometry C11H17BrN2O3

Framework group C1[X(C11H17BrN2O3)]

Deg. of freedom 96

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.077160	1.326483	1.237058
2	6	0	-1.154221	1.251474	0.666139
3	7	0	-1.221265	2.286335	-0.257480
4	6	0	-0.062688	2.963496	-0.236273
5	7	0	0.747175	2.398603	0.667758
6	6	0	2.154595	2.759180	0.918624
7	1	0	0.541505	0.694792	1.973312
8	1	0	-1.936709	0.490444	0.774226
9	1	0	2.226428	3.847571	0.955123
10	1	0	2.401901	2.368775	1.903933
11	35	0	-3.067434	-1.506203	0.317473
12	1	0	0.175729	3.814022	-0.851510
13	6	0	-2.317589	2.600352	-1.123035
14	6	0	-3.356215	1.795691	-1.305791
15	1	0	-2.197711	3.557948	-1.614444
16	1	0	-4.139933	2.114928	-1.981352
17	1	0	-3.455547	0.817719	-0.830107
18	6	0	0.619271	-2.460810	-0.351316
19	6	0	1.594177	-3.510225	-0.038981
20	8	0	1.633761	-2.250973	0.683130
21	1	0	0.784680	-1.860125	-1.241234
22	1	0	-0.402235	-2.497824	0.018052
23	1	0	1.254086	-4.323155	0.598437
24	6	0	2.765991	-3.818543	-0.929479
25	1	0	3.632125	-4.131874	-0.339394
26	1	0	2.508028	-4.637928	-1.607271
27	1	0	3.042279	-2.947488	-1.527500
28	6	0	3.103895	2.188327	-0.144908
29	1	0	4.130172	2.373836	0.187552
30	1	0	2.968958	2.683857	-1.106968
31	6	0	2.917770	0.691568	-0.364942
32	8	0	2.766918	0.199186	-1.457862

```
      33        8        0        2.912252        0.021238        0.786315
      34        1        0        2.588754       -0.920500        0.650377
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.3287477           0.2548589           0.1594782
 Standard basis: 6-311++G(d,p) (5D, 7F)
 There are     538 symmetry adapted cartesian basis functions of A      symmetry.
 There are     519 symmetry adapted basis functions of A      symmetry.
    519 basis functions,      823 primitive gaussians,      538 cartesian basis functions
     78 alpha electrons              78 beta electrons
          nuclear repulsion energy           1572.8193178675 Hartrees.
 NAtoms=       34 NActive=       34 NUniq=       34 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      519 RedAO= T EigKep=    3.53D-06    NBF=      519
 NBsUse=      519 1.00D-06 EigRej= -1.00D+00 NBFU=      519
 Initial guess from the checkpoint file:    "./coohpo.chk"
 B after Tr=          0.000000        0.000000        0.000000
             Rot=        0.999998       -0.000006        0.000271        0.001907 Ang=    -0.22 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn=                5 AccDes=
0.00D+00
 Harris functional with IExCor=    402 and IRadAn=             5 diagonalized for initial guess.
 HarFok:    IExCor=    402 AccDes= 0.00D+00 IRadAn=                5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=    3500011 ScaDFX=    1.000000    1.000000    1.000000    1.000000
 FoFCou: FMM=F IPFlag=                  0 FMFlag=           100000 FMFlg1=                  0
             NFxFlg=                    0 DoJE=T BraDBF=F KetDBF=T FulRan=T
             wScrn=      0.000000 ICntrl=             500 IOpCl=      0 I1Cent=        200000004 NGrid=
0
             NMat0=        1 NMatS0=            1 NMatT0=        0 NMatD0=        1 NMtDS0=        0
NMtDT0=        0
 Petite list used in FoFCou.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                    energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3338.90388098          A.U. after      11 cycles
                  NFock= 11    Conv=0.22D-08         -V/T= 2.0019
 Calling FoFJK, ICntrl=             2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 ---------------------------------------------------------------------
 Center          Atomic                             Forces (Hartrees/Bohr)
```

Number	Number	X	Y	Z
1	6	0.000027040	-0.000032202	-0.000083462
2	6	0.000081257	0.000118565	0.000065824
3	7	-0.000081315	-0.000092309	0.000002585
4	6	-0.000037417	0.000080106	0.000027118
5	7	0.000040086	0.000007848	-0.000028657
6	6	-0.000074612	-0.000011507	0.000030116
7	1	-0.000014438	0.000007319	0.000032668
8	1	-0.000106011	-0.000109588	-0.000079925
9	1	0.000009921	0.000004874	-0.000007332
10	1	0.000021345	-0.000017371	-0.000018432
11	35	0.000050212	0.000009716	0.000029266
12	1	0.000037054	-0.000024067	-0.000029749
13	6	0.000085173	0.000127405	0.000023279
14	6	-0.000055489	-0.000075029	0.000023070
15	1	-0.000003050	-0.000022375	-0.000015411
16	1	0.000006412	0.000019140	-0.000011671
17	1	0.000015139	0.000026845	-0.000001227
18	6	-0.000034165	0.000013585	-0.000006672
19	6	-0.000071877	0.000048729	0.000118809
20	8	0.000099389	-0.000075395	-0.000037481
21	1	0.000015961	0.000004478	-0.000011641
22	1	-0.000012228	0.000007161	0.000013248
23	1	0.000017547	0.000008500	-0.000010079
24	6	0.000001074	0.000000231	-0.000061848
25	1	0.000009653	-0.000009932	0.000007499
26	1	-0.000002888	-0.000005995	0.000006117
27	1	-0.000000231	0.000004874	0.000025366
28	6	-0.000007841	0.000058742	-0.000001522
29	1	0.000015005	-0.000008575	-0.000015552
30	1	0.000015500	-0.000007546	0.000006348
31	6	-0.000017265	0.000009208	0.000133555
32	8	0.000024742	-0.000028915	-0.000055036
33	8	0.000012986	-0.000044501	-0.000085679
34	1	-0.000066666	0.000007983	0.000016509

Cartesian Forces: Max 0.000133555 RMS 0.000047284

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000116118 RMS 0.000026507

Search for a local minimum.
Step number 36 out of a maximum of 175
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 21 22 23 24 25
26 27 28 29 30
31 32 33 34 35
36
DE= -3.51D-06 DEPred=-7.63D-07 R= 4.59D+00
TightC=F SS= 1.41D+00 RLast= 1.78D-02 DXNew= 6.5746D-01 5.3432D-02
Trust test= 4.59D+00 RLast= 1.78D-02 DXMaxT set to 3.91D-01
ITU= 1 1 1 1 1 -1 1 1 1 1 1 -1 0 1 1 1 1 1 1 1
ITU= 1 1 1 0 0 -1 1 1 1 0 1 0 -1 0 1 0
Eigenvalues --- 0.00166 0.00248 0.00361 0.00429 0.00539
Eigenvalues --- 0.00733 0.00842 0.00947 0.01181 0.01348
Eigenvalues --- 0.01639 0.01995 0.02174 0.02273 0.02288
Eigenvalues --- 0.02430 0.02471 0.02889 0.02974 0.03144
Eigenvalues --- 0.03458 0.03663 0.03965 0.04311 0.04636
Eigenvalues --- 0.04865 0.05031 0.05344 0.05672 0.05737
Eigenvalues --- 0.05775 0.05981 0.06160 0.07510 0.09409
Eigenvalues --- 0.09679 0.11784 0.12508 0.12861 0.13022
Eigenvalues --- 0.13590 0.14909 0.15632 0.15944 0.15978
Eigenvalues --- 0.16002 0.16032 0.16045 0.16133 0.16449
Eigenvalues --- 0.16807 0.17667 0.19799 0.21648 0.22071
Eigenvalues --- 0.23319 0.23673 0.24131 0.25278 0.26753
Eigenvalues --- 0.28298 0.29477 0.30007 0.31707 0.32145
Eigenvalues --- 0.33306 0.34456 0.34511 0.34613 0.34773
Eigenvalues --- 0.34890 0.34951 0.34970 0.35103 0.35306
Eigenvalues --- 0.35540 0.35625 0.35877 0.35940 0.36631
Eigenvalues --- 0.37047 0.37258 0.38053 0.39188 0.39653
Eigenvalues --- 0.41489 0.45567 0.49243 0.50314 0.50883
Eigenvalues --- 0.54536 0.55981 0.57009 0.61973 0.91419
Eigenvalues --- 1.03763
En-DIIS/RFO-DIIS IScMMF= 0 using points: 36 35 34 33 32
RFO step: Lambda=-2.05856678D-07.
DidBck=F Rises=F RFO-DIIS coefs: 1.61940 -0.41360 -0.75661 0.56139 -0.01058
Iteration 1 RMS(Cart)= 0.00509428 RMS(Int)= 0.00000792
Iteration 2 RMS(Cart)= 0.00001164 RMS(Int)= 0.00000028
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000028

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56883	-0.00002	0.00002	-0.00002	0.00000	2.56882

R2	2.62016	-0.00001	-0.00001	0.00000	-0.00001	2.62015
R3	2.03242	0.00001	-0.00001	0.00002	0.00001	2.03243
R4	2.62427	0.00000	0.00012	-0.00007	0.00005	2.62432
R5	2.07279	0.00005	0.00019	-0.00011	0.00007	2.07287
R6	2.53625	0.00004	-0.00001	0.00003	0.00002	2.53627
R7	2.70549	-0.00009	-0.00016	-0.00005	-0.00021	2.70528
R8	2.52987	-0.00001	0.00003	-0.00002	0.00000	2.52988
R9	2.03421	0.00000	0.00000	0.00000	0.00000	2.03420
R10	2.78616	-0.00004	-0.00013	0.00006	-0.00007	2.78610
R11	2.06239	0.00000	-0.00003	0.00002	-0.00001	2.06238
R12	2.05660	-0.00001	-0.00002	-0.00002	-0.00004	2.05657
R13	2.90191	-0.00001	0.00016	-0.00016	0.00000	2.90191
R14	4.42122	0.00002	-0.00053	0.00041	-0.00012	4.42110
R15	2.50674	0.00004	0.00001	0.00004	0.00004	2.50678
R16	2.04653	0.00000	0.00001	0.00000	0.00001	2.04654
R17	2.04624	-0.00001	0.00001	-0.00003	-0.00002	2.04622
R18	2.06367	0.00000	0.00000	-0.00002	-0.00003	2.06365
R19	2.77041	0.00001	0.00012	-0.00003	0.00009	2.77050
R20	2.76656	-0.00003	-0.00007	-0.00007	-0.00013	2.76643
R21	2.05289	0.00001	0.00002	-0.00001	0.00001	2.05290
R22	2.05388	0.00001	-0.00008	0.00001	-0.00006	2.05381
R23	2.74416	-0.00008	-0.00011	-0.00004	-0.00015	2.74401
R24	2.05522	-0.00001	-0.00003	0.00001	-0.00002	2.05519
R25	2.84163	0.00004	0.00008	0.00003	0.00011	2.84174
R26	3.09549	0.00000	-0.00037	-0.00026	-0.00064	3.09485
R27	2.06713	0.00000	0.00001	0.00000	0.00002	2.06714
R28	2.06779	0.00000	0.00000	0.00000	0.00000	2.06780
R29	2.06379	-0.00002	0.00000	-0.00002	-0.00002	2.06377
R30	2.06853	0.00000	-0.00001	0.00002	0.00001	2.06854
R31	2.06086	-0.00001	-0.00002	0.00002	0.00000	2.06085
R32	2.88042	0.00002	0.00004	0.00004	0.00009	2.88050
R33	2.28311	0.00006	0.00004	0.00002	0.00006	2.28317
R34	2.51750	-0.00007	-0.00006	-0.00012	-0.00019	2.51731
R35	1.89915	-0.00003	0.00004	0.00005	0.00009	1.89924
A1	1.88384	0.00002	0.00006	-0.00004	0.00001	1.88385
A2	2.27339	-0.00002	0.00005	-0.00007	-0.00003	2.27336
A3	2.12539	0.00001	-0.00008	0.00011	0.00004	2.12543
A4	1.85662	0.00000	-0.00008	0.00004	-0.00004	1.85658
A5	2.26935	0.00000	0.00041	0.00015	0.00056	2.26991
A6	2.15092	0.00000	-0.00039	-0.00019	-0.00058	2.15034
A7	1.90054	-0.00001	0.00004	0.00000	0.00004	1.90058
A8	2.21744	0.00000	-0.00002	-0.00018	-0.00020	2.21724
A9	2.16509	0.00001	-0.00003	0.00018	0.00015	2.16524
A10	1.89651	-0.00001	-0.00002	-0.00004	-0.00005	1.89645

A11	2.19052	0.00000	0.00009	-0.00004	0.00004	2.19056
A12	2.19612	0.00001	-0.00008	0.00008	0.00000	2.19612
A13	1.88726	0.00000	0.00000	0.00004	0.00004	1.88730
A14	2.19018	-0.00002	0.00021	-0.00008	0.00013	2.19030
A15	2.20083	0.00002	-0.00010	0.00002	-0.00007	2.20076
A16	1.88853	0.00006	0.00002	0.00013	0.00015	1.88868
A17	1.85796	0.00003	0.00010	-0.00016	-0.00006	1.85790
A18	1.96206	-0.00012	0.00005	-0.00013	-0.00008	1.96198
A19	1.88863	-0.00001	0.00009	0.00003	0.00011	1.88875
A20	1.93178	0.00003	0.00014	0.00004	0.00018	1.93196
A21	1.93178	0.00001	-0.00039	0.00010	-0.00029	1.93149
A22	2.73291	-0.00004	-0.00145	-0.00027	-0.00172	2.73119
A23	2.15294	0.00000	-0.00005	-0.00002	-0.00007	2.15287
A24	1.96438	0.00002	0.00010	0.00010	0.00020	1.96458
A25	2.16582	-0.00003	-0.00004	-0.00008	-0.00013	2.16569
A26	2.06441	0.00000	0.00018	-0.00010	0.00007	2.06449
A27	2.15849	-0.00003	-0.00005	-0.00007	-0.00012	2.15837
A28	2.06003	0.00003	-0.00013	0.00018	0.00004	2.06007
A29	2.05904	0.00000	-0.00057	0.00014	-0.00042	2.05862
A30	2.12730	0.00000	0.00066	-0.00010	0.00056	2.12786
A31	1.97584	0.00000	-0.00017	0.00014	-0.00003	1.97582
A32	1.99988	0.00000	0.00015	-0.00009	0.00006	1.99994
A33	2.02677	0.00001	-0.00005	-0.00005	-0.00010	2.02667
A34	2.03977	0.00004	0.00027	0.00002	0.00030	2.04006
A35	2.13983	-0.00004	-0.00048	0.00006	-0.00041	2.13941
A36	1.94471	0.00001	0.00013	0.00001	0.00014	1.94485
A37	2.03873	-0.00001	-0.00019	0.00005	-0.00014	2.03859
A38	2.02362	0.00000	0.00019	-0.00008	0.00011	2.02373
A39	2.10167	-0.00003	0.00009	-0.00030	-0.00022	2.10145
A40	2.36070	0.00001	-0.00096	-0.00017	-0.00114	2.35956
A41	1.93511	0.00001	0.00003	0.00000	0.00003	1.93514
A42	1.91415	0.00000	0.00008	-0.00003	0.00005	1.91420
A43	1.93680	-0.00002	-0.00017	0.00001	-0.00016	1.93664
A44	1.88212	0.00000	-0.00003	-0.00002	-0.00005	1.88207
A45	1.90026	0.00000	-0.00001	0.00001	0.00001	1.90027
A46	1.89411	0.00001	0.00009	0.00003	0.00012	1.89423
A47	1.88204	0.00005	0.00000	0.00013	0.00013	1.88217
A48	1.94504	0.00002	0.00019	-0.00005	0.00014	1.94518
A49	1.97091	-0.00009	-0.00013	0.00003	-0.00010	1.97081
A50	1.88277	-0.00001	0.00004	-0.00008	-0.00004	1.88273
A51	1.90154	0.00003	-0.00005	-0.00003	-0.00008	1.90146
A52	1.87940	0.00001	-0.00004	-0.00001	-0.00005	1.87935
A53	2.14841	-0.00001	0.00001	-0.00008	-0.00006	2.14834
A54	1.94965	-0.00002	0.00000	-0.00004	-0.00004	1.94961

A55	2.18482	0.00003	-0.00001	0.00012	0.00011	2.18492
A56	1.93472	0.00008	-0.00004	0.00030	0.00025	1.93498
A57	2.81166	-0.00002	0.00061	0.00024	0.00085	2.81251
D1	0.00323	-0.00001	0.00017	0.00006	0.00023	0.00346
D2	3.02516	-0.00002	-0.00045	0.00011	-0.00035	3.02481
D3	-3.10199	-0.00001	-0.00075	0.00019	-0.00056	-3.10255
D4	-0.08006	-0.00002	-0.00138	0.00023	-0.00114	-0.08120
D5	-0.00249	0.00001	-0.00014	0.00000	-0.00014	-0.00263
D6	-3.04282	0.00002	-0.00131	0.00019	-0.00111	-3.04393
D7	3.10645	0.00001	0.00069	-0.00012	0.00057	3.10702
D8	0.06612	0.00002	-0.00047	0.00007	-0.00040	0.06572
D9	-0.00286	0.00000	-0.00014	-0.00011	-0.00025	-0.00311
D10	3.12297	0.00000	-0.00095	0.00007	-0.00088	3.12209
D11	-3.03494	0.00002	0.00037	-0.00017	0.00019	-3.03475
D12	0.09090	0.00001	-0.00045	0.00000	-0.00044	0.09046
D13	-1.49425	0.00006	0.00456	0.00164	0.00620	-1.48805
D14	1.50997	0.00004	0.00387	0.00171	0.00558	1.51555
D15	0.00135	0.00000	0.00006	0.00011	0.00016	0.00152
D16	3.13447	-0.00003	-0.00080	-0.00006	-0.00086	3.13361
D17	-3.12506	0.00001	0.00084	-0.00006	0.00078	-3.12428
D18	0.00806	-0.00002	-0.00002	-0.00023	-0.00025	0.00781
D19	-0.19606	0.00002	0.00036	-0.00016	0.00020	-0.19586
D20	2.95508	0.00002	0.00036	-0.00013	0.00023	2.95531
D21	2.92755	0.00001	-0.00057	0.00004	-0.00053	2.92702
D22	-0.20450	0.00001	-0.00057	0.00008	-0.00049	-0.20500
D23	0.00068	0.00000	0.00005	-0.00007	-0.00002	0.00066
D24	3.04023	-0.00002	0.00125	-0.00027	0.00098	3.04121
D25	-3.13241	0.00002	0.00091	0.00010	0.00101	-3.13140
D26	-0.09286	0.00001	0.00211	-0.00010	0.00201	-0.09085
D27	-2.47486	-0.00001	0.00284	0.00074	0.00358	-2.47128
D28	-0.44829	0.00002	0.00300	0.00075	0.00376	-0.44453
D29	1.66961	-0.00001	0.00261	0.00069	0.00330	1.67291
D30	0.78591	0.00000	0.00146	0.00096	0.00243	0.78834
D31	2.81248	0.00003	0.00162	0.00098	0.00260	2.81508
D32	-1.35280	0.00000	0.00123	0.00091	0.00214	-1.35066
D33	-3.00099	0.00003	0.00027	-0.00013	0.00013	-3.00085
D34	1.21899	0.00000	0.00011	-0.00009	0.00002	1.21902
D35	-0.89913	0.00004	0.00012	-0.00006	0.00006	-0.89907
D36	1.16808	0.00001	0.00010	-0.00024	-0.00013	1.16795
D37	-0.89513	-0.00001	-0.00005	-0.00019	-0.00024	-0.89537
D38	-3.01325	0.00003	-0.00004	-0.00016	-0.00021	-3.01346
D39	-0.92584	-0.00001	0.00016	-0.00036	-0.00020	-0.92604
D40	-2.98904	-0.00003	0.00000	-0.00031	-0.00031	-2.98935
D41	1.17602	0.00001	0.00001	-0.00029	-0.00027	1.17575

D42	-3.13998	0.00001	-0.00009	0.00011	0.00002	-3.13995
D43	-0.02329	0.00000	-0.00035	0.00008	-0.00027	-0.02356
D44	-0.00903	0.00001	-0.00009	0.00007	-0.00001	-0.00904
D45	3.10765	0.00000	-0.00035	0.00004	-0.00030	3.10735
D46	-2.75288	-0.00001	0.00006	0.00010	0.00016	-2.75272
D47	-0.04771	-0.00001	0.00010	0.00008	0.00018	-0.04754
D48	-0.02004	0.00001	0.00017	0.00006	0.00022	-0.01982
D49	2.68512	0.00001	0.00020	0.00004	0.00024	2.68536
D50	0.31425	0.00004	-0.00054	-0.00022	-0.00076	0.31349
D51	-2.06471	0.00001	-0.00044	-0.00020	-0.00064	-2.06535
D52	2.54397	-0.00001	-0.00077	0.00036	-0.00041	2.54356
D53	0.16233	-0.00001	-0.00101	0.00043	-0.00059	0.16174
D54	2.55265	0.00000	-0.00027	0.00049	0.00022	2.55287
D55	-1.65396	0.00000	-0.00024	0.00045	0.00021	-1.65375
D56	0.43854	0.00000	-0.00017	0.00047	0.00029	0.43883
D57	1.32595	0.00001	0.00001	0.00046	0.00047	1.32642
D58	-2.88067	0.00001	0.00004	0.00042	0.00046	-2.88020
D59	-0.78817	0.00001	0.00010	0.00044	0.00054	-0.78762
D60	-1.02165	0.00000	-0.00022	0.00049	0.00028	-1.02137
D61	1.05492	0.00000	-0.00018	0.00045	0.00027	1.05520
D62	-3.13576	0.00000	-0.00012	0.00047	0.00035	-3.13541
D63	1.47748	-0.00003	-0.00265	-0.00065	-0.00330	1.47418
D64	2.82410	-0.00002	-0.00281	-0.00097	-0.00378	2.82033
D65	2.25573	-0.00002	0.00168	-0.00021	0.00147	2.25720
D66	-0.86033	-0.00003	0.00157	-0.00034	0.00123	-0.85909
D67	-1.93678	0.00000	0.00156	-0.00004	0.00152	-1.93526
D68	1.23034	-0.00001	0.00146	-0.00017	0.00128	1.23163
D69	0.10086	0.00001	0.00156	-0.00016	0.00140	0.10226
D70	-3.01519	0.00000	0.00145	-0.00029	0.00116	-3.01403
D71	2.92176	-0.00004	0.00054	0.00029	0.00084	2.92260
D72	-0.19366	-0.00005	0.00043	0.00016	0.00060	-0.19306
D73	-1.87829	-0.00007	-0.00232	-0.00041	-0.00272	-1.88101

Item	Value	Threshold	Converged?
Maximum Force	0.000116	0.000450	YES
RMS Force	0.000027	0.000300	YES
Maximum Displacement	0.019976	0.001800	NO
RMS Displacement	0.005095	0.001200	NO

Predicted change in Energy=-4.822146D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	-0.845615	1.643865	1.537254
2	6	0	-1.503009	0.454608	1.574269
3	7	0	-2.365329	0.449907	0.485713
4	6	0	-2.229668	1.606670	-0.181238
5	7	0	-1.308660	2.353757	0.439943
6	6	0	-0.774696	3.644391	-0.032095
7	1	0	-0.072344	2.030705	2.176893
8	1	0	-1.351384	-0.415856	2.224286
9	1	0	-1.612556	4.258014	-0.367552
10	1	0	-0.324746	4.126841	0.833443
11	35	0	-0.393330	-2.434405	2.917865
12	1	0	-2.766848	1.881072	-1.072806
13	6	0	-3.252274	-0.602861	0.092774
14	6	0	-3.211285	-1.822863	0.612004
15	1	0	-3.948291	-0.294080	-0.677334
16	1	0	-3.921032	-2.557516	0.252794
17	1	0	-2.486313	-2.135652	1.366404
18	6	0	2.554531	-0.689733	1.128315
19	6	0	3.974269	-0.375393	1.315225
20	8	0	2.973025	0.653513	1.532844
21	1	0	2.171609	-0.731042	0.112530
22	1	0	1.982107	-1.229949	1.877781
23	1	0	4.428968	-0.691688	2.251172
24	6	0	4.917040	-0.170931	0.161645
25	1	0	5.675277	0.578685	0.406056
26	1	0	5.433469	-1.109146	-0.062853
27	1	0	4.377381	0.150592	-0.731702
28	6	0	0.257990	3.474957	-1.155927
29	1	0	0.708423	4.453975	-1.347862
30	1	0	-0.210573	3.135127	-2.080197
31	6	0	1.360790	2.483199	-0.804172
32	8	0	1.683746	1.571612	-1.528364
33	8	0	1.884707	2.733810	0.394665
34	1	0	2.457694	1.967527	0.702217

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.359363	0.000000			
3	N	2.200182	1.388730	0.000000		
4	C	2.206853	2.221955	1.342136	0.000000	
5	N	1.386524	2.220638	2.177909	1.338753	0.000000
6	C	2.543618	3.644936	3.605963	2.508285	1.474339

7	H	1.075514	2.212247	3.258341	3.224071	2.156347
8	H	2.229409	1.096914	2.190951	3.263210	3.294914
9	H	3.324193	4.271834	3.974469	2.728583	2.090597
10	H	2.632836	3.927139	4.219566	3.318067	2.065613
11	Br	4.329311	3.373876	4.257159	5.413582	5.468494
12	H	3.249587	3.261763	2.153702	1.076453	2.153637
13	C	3.595317	2.524480	1.431570	2.450068	3.555243
14	C	4.297753	3.005168	2.428389	3.654381	4.592792
15	H	4.276286	3.407295	2.100468	2.610101	3.902179
16	H	5.362801	4.082405	3.393974	4.515478	5.565979
17	H	4.123812	2.778407	2.734112	4.057837	4.732863
18	C	4.144141	4.239342	5.090849	5.465981	4.965977
19	C	5.230486	5.545861	6.446682	6.682575	6.010301
20	O	3.944974	4.480642	5.443892	5.560089	4.734774
21	H	4.095566	4.128591	4.702947	4.992237	4.662130
22	H	4.046082	3.882768	4.864151	5.479508	5.073408
23	H	5.812548	6.079518	7.112141	7.452281	6.743564
24	C	6.196288	6.603320	7.315966	7.372440	6.723901
25	H	6.703450	7.273782	8.042032	7.993111	7.206067
26	H	7.040334	7.296590	7.972002	8.131011	7.596104
27	H	5.887080	6.323679	6.858267	6.787950	6.209489
28	C	3.438614	4.435943	4.327553	3.260208	2.501656
29	H	4.316903	5.424409	5.370523	4.254473	3.416985
30	H	3.963975	4.712823	4.293865	3.165276	2.857874
31	C	3.324903	4.239517	4.436445	3.748031	2.947972
32	O	3.975035	4.585786	4.659371	4.138935	3.666125
33	O	3.154068	4.250040	4.825692	4.304670	3.216222
34	H	3.422557	4.328576	5.060791	4.783521	3.795179

		6	7	8	9	10
6	C	0.000000				
7	H	2.824342	0.000000			
8	H	4.680751	2.761131	0.000000		
9	H	1.091363	3.715825	5.350784	0.000000	
10	H	1.088288	2.502469	4.860507	1.765800	0.000000
11	Br	6.767531	4.537541	2.339543	7.554400	6.884728
12	H	2.856754	4.224131	4.260309	2.734890	3.826373
13	C	4.918652	4.625059	2.862114	5.150600	5.611515
14	C	6.020191	5.210740	2.835199	6.363373	6.616655
15	H	5.098979	5.345484	3.895915	5.125737	5.912450
16	H	6.960190	6.290177	3.882858	7.222558	7.612560
17	H	6.188241	4.882895	2.231977	6.681992	6.646446
18	C	5.587033	3.924382	4.065997	6.639460	5.619304
19	C	6.366051	4.786111	5.402833	7.450692	6.243697
20	O	5.043788	3.403781	4.508009	6.134450	4.840295

21	H	5.276935	4.113899	4.119506	6.280212	5.509132
22	H	5.916653	3.865501	3.448909	6.934037	5.925151
23	H	7.147938	5.261060	5.786991	8.237553	6.915633
24	C	6.854932	5.813982	6.603606	7.907669	6.811644
25	H	7.154906	6.187033	7.325915	8.200515	6.983720
26	H	7.819103	6.722284	7.193461	8.862602	7.834280
27	H	6.264182	5.638688	6.471281	7.272061	6.353757
28	C	1.535626	3.647283	5.399477	2.175697	2.173046
29	H	2.141567	4.348072	6.381089	2.527124	2.435682
30	H	2.184561	4.400190	5.695569	2.481851	3.079908
31	C	2.550445	3.338469	4.993192	3.490185	2.867817
32	O	3.546713	4.125960	5.219619	4.407930	4.017632
33	O	2.843186	2.738748	4.872390	3.890376	2.648536
34	H	3.714759	2.929122	4.744079	4.791417	3.524462

		11	12	13	14	15
11	Br	0.000000				
12	H	6.338958	0.000000			
13	C	4.416928	2.786421	0.000000		
14	C	3.692134	4.093317	1.326531	0.000000	
15	H	5.490373	2.506689	1.082983	2.131372	0.000000
16	H	4.422945	4.773932	2.072081	1.082815	2.447249
17	H	2.622377	4.707709	2.135013	1.092036	3.115387
18	C	3.864745	6.306429	5.899058	5.898745	6.760444
19	C	5.087623	7.499132	7.332739	7.363551	8.169692
20	O	4.773454	6.422028	6.512037	6.725033	7.327170
21	H	4.165364	5.711087	5.425433	5.515169	6.186113
22	H	2.859228	6.398202	5.565809	5.378202	6.524882
23	H	5.170696	8.333528	7.979226	7.895561	8.883282
24	C	6.396882	8.048399	8.181015	8.306707	8.905793
25	H	7.226056	8.669067	9.010847	9.207651	9.723606
26	H	6.677767	8.786729	8.701878	8.700379	9.437125
27	H	6.539207	7.358731	7.710972	7.955371	8.337716
28	C	7.206980	3.420091	5.523569	6.574827	5.668111
29	H	8.176801	4.332781	6.582868	7.655317	6.684207
30	H	7.485567	3.020270	5.286427	6.390140	5.262891
31	C	6.411968	4.179966	5.622156	6.438291	5.992971
32	O	6.334933	4.484538	5.632115	6.329689	5.993738
33	O	6.185987	4.951524	6.132951	6.839564	6.658916
34	H	5.693369	5.518517	6.291428	6.820009	6.932148

		16	17	18	19	20
16	H	0.000000				
17	H	1.864542	0.000000			
18	C	6.796181	5.249521	0.000000		
19	C	8.259916	6.696286	1.466084	0.000000	

20	O	7.712150	6.132822	1.463930	1.452066	0.000000
21	H	6.362072	5.024078	1.086349	2.196030	2.139288
22	H	6.264988	4.587873	1.086832	2.239519	2.155999
23	H	8.786201	7.119617	2.185023	1.087561	2.108396
24	C	9.155087	7.753787	2.604814	1.503786	2.517756
25	H	10.096950	8.654562	3.445228	2.151809	2.928723
26	H	9.471225	8.112918	3.143735	2.136997	3.421550
27	H	8.784461	7.532546	2.736529	2.151528	2.711700
28	C	7.472580	6.735895	5.276031	5.894279	4.749889
29	H	8.553068	7.810043	5.999775	6.409413	5.279242
30	H	7.184466	6.696206	5.707005	6.431605	5.417358
31	C	7.377237	6.391039	3.902182	4.415164	3.377676
32	O	7.185803	6.285927	3.595816	4.138034	3.446178
33	O	7.856517	6.615266	3.564765	3.857570	2.609123
34	H	7.833655	6.459136	2.692948	2.857456	1.637724

		21	22	23	24	25
21	H	0.000000				
22	H	1.844161	0.000000			
23	H	3.109825	2.533037	0.000000		
24	C	2.802415	3.560966	2.208060	0.000000	
25	H	3.751964	4.367681	2.563511	1.093885	0.000000
26	H	3.288382	3.961383	2.556952	1.094232	1.768367
27	H	2.521000	3.801662	3.099941	1.092098	1.778283
28	C	4.791801	5.857654	6.809282	6.060961	6.338390
29	H	5.581941	6.658381	7.298860	6.432793	6.539399
30	H	5.042827	6.287076	7.411519	6.499869	6.881866
31	C	3.439349	4.622378	5.369242	4.541380	4.868945
32	O	2.869279	4.420361	5.190729	4.043115	4.545350
33	O	3.488139	4.233262	4.653377	4.205576	4.360403
34	H	2.777023	3.439766	3.654669	3.303575	3.517020

		26	27	28	29	30
26	H	0.000000				
27	H	1.774717	0.000000			
28	C	6.999600	5.310438	0.000000		
29	H	7.411182	5.688586	1.094626	0.000000	
30	H	7.344300	5.636950	1.090555	1.766417	0.000000
31	C	5.480986	3.813939	1.524298	2.145959	2.126601
32	O	4.836798	3.147958	2.407117	3.048254	2.517447
33	O	5.250842	3.762332	2.366399	2.716434	3.267445
34	H	4.348159	3.007087	3.250192	3.666769	4.027998

		31	32	33	34
31	C	0.000000			
32	O	1.208199	0.000000		
33	O	1.332105	2.255910	0.000000	

34 H 1.933475 2.394001 1.005033 0.000000

Stoichiometry C11H17BrN2O3

Framework group C1[X(C11H17BrN2O3)]

Deg. of freedom 96

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.075864	1.328005	1.238540
2	6	0	-1.154759	1.254768	0.665765
3	7	0	-1.217430	2.287352	-0.260742
4	6	0	-0.057179	2.961654	-0.239192
5	7	0	0.749607	2.396968	0.667719
6	6	0	2.157109	2.755429	0.920935
7	1	0	0.537089	0.697298	1.977601
8	1	0	-1.939664	0.496172	0.773819
9	1	0	2.230605	3.843684	0.957984
10	1	0	2.402285	2.364129	1.906401
11	35	0	-3.069301	-1.501677	0.319971
12	1	0	0.184840	3.809467	-0.856761
13	6	0	-2.311110	2.601173	-1.129519
14	6	0	-3.351010	1.798101	-1.312191
15	1	0	-2.188313	3.557066	-1.623525
16	1	0	-4.132638	2.116906	-1.990357
17	1	0	-3.453140	0.821640	-0.834032
18	6	0	0.613951	-2.461851	-0.349336
19	6	0	1.590335	-3.511672	-0.042819
20	8	0	1.630242	-2.255161	0.683874
21	1	0	0.777467	-1.858016	-1.237481
22	1	0	-0.406845	-2.500458	0.021727
23	1	0	1.252423	-4.327400	0.592156
24	6	0	2.760559	-3.815226	-0.937136
25	1	0	3.628260	-4.130245	-0.350244
26	1	0	2.501928	-4.632009	-1.617812
27	1	0	3.034710	-2.941330	-1.531968
28	6	0	3.107217	2.183231	-0.141153
29	1	0	4.133307	2.366960	0.192895
30	1	0	2.974680	2.678986	-1.103427
31	6	0	2.918986	0.686749	-0.361592
32	8	0	2.770534	0.194578	-1.454970

```
      33        8        0        2.909044        0.016622        0.789640
      34        1        0        2.584973       -0.924869        0.653025
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.3288778           0.2548144           0.1595775
 Standard basis: 6-311++G(d,p) (5D, 7F)
 There are     538 symmetry adapted cartesian basis functions of A      symmetry.
 There are     519 symmetry adapted basis functions of A      symmetry.
    519 basis functions,      823 primitive gaussians,      538 cartesian basis functions
     78 alpha electrons              78 beta electrons
          nuclear repulsion energy           1572.9244102830 Hartrees.
 NAtoms=       34 NActive=       34 NUniq=       34 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      519 RedAO= T EigKep=    3.53D-06    NBF=      519
 NBsUse=      519 1.00D-06 EigRej= -1.00D+00 NBFU=      519
 Initial guess from the checkpoint file:    "./coohpo.chk"
 B after Tr=          0.000000        0.000000        0.000000
              Rot=        1.000000      -0.000006        0.000172        0.000666 Ang=    -0.08 deg.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                    energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3338.90388232         A.U. after      11 cycles
                  NFock= 11    Conv=0.13D-08         -V/T= 2.0019
 Calling FoFJK, ICntrl=              2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 ---------------------------------------------------------------------
 Center         Atomic                             Forces (Hartrees/Bohr)
 Number         Number                       X                      Y                      Z
 ---------------------------------------------------------------------
        1              6                 0.000004132     -0.000013508     -0.000038064
        2              6                 0.000038472      0.000048442      0.000020322
        3              7                -0.000039030     -0.000049164     -0.000001827
        4              6                -0.000006512      0.000054332      0.000015604
        5              7                -0.000000389      0.000002315     -0.000014460
        6              6                -0.000012465     -0.000004168      0.000011515
        7              1                -0.000004333      0.000000296      0.000017749
        8              1                -0.000040659     -0.000030764     -0.000058468
        9              1                 0.000008571      0.000005489     -0.000010685
       10              1                 0.000004757     -0.000010096     -0.000006115
```

11	35	0.000022558	-0.000000948	0.000019317
12	1	0.000017726	-0.000015947	-0.000017846
13	6	0.000037101	0.000071437	0.000018339
14	6	-0.000032873	-0.000061812	0.000019385
15	1	0.000001621	-0.000010950	-0.000010684
16	1	0.000004946	0.000017237	-0.000009969
17	1	0.000002636	0.000018655	-0.000001609
18	6	-0.000017805	0.000021993	-0.000028290
19	6	-0.000058045	0.000023230	0.000072977
20	8	0.000089974	-0.000022135	-0.000023087
21	1	0.000003431	-0.000004933	-0.000001659
22	1	-0.000002529	-0.000001131	0.000013406
23	1	0.000008554	0.000003480	-0.000000258
24	6	0.000009854	-0.000001354	-0.000028412
25	1	0.000005828	-0.000010779	0.000009096
26	1	-0.000005660	-0.000006510	0.000006705
27	1	0.000000494	0.000004457	0.000016704
28	6	-0.000007312	0.000036430	0.000007785
29	1	0.000007061	-0.000010964	-0.000014067
30	1	0.000010160	-0.000001699	0.000002145
31	6	-0.000020157	0.000017882	0.000082125
32	8	0.000018747	-0.000027516	-0.000034635
33	8	0.000024521	-0.000034928	-0.000053621
34	1	-0.000073374	-0.000006366	0.000020582

Cartesian Forces: Max 0.000089974 RMS 0.000027877

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000073461 RMS 0.000016572
Search for a local minimum.
Step number 37 out of a maximum of 175
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 21 22 23 24 25
26 27 28 29 30
31 32 33 34 35
36 37
DE= -1.34D-06 DEPred=-4.82D-07 R= 2.78D+00
TightC=F SS= 1.41D+00 RLast= 1.39D-02 DXNew= 6.5746D-01 4.1661D-02
Trust test= 2.78D+00 RLast= 1.39D-02 DXMaxT set to 3.91D-01

ITU= 1 1 1 1 1 1 -1 1 1 1 1 1 -1 0 1 1 1 1 1 1

ITU= 1 1 1 1 0 0 -1 1 1 1 0 1 0 -1 0 1 0

Eigenvalues --- 0.00167 0.00263 0.00395 0.00450 0.00524

Eigenvalues --- 0.00653 0.00869 0.00926 0.01183 0.01329

Eigenvalues --- 0.01532 0.01929 0.02166 0.02244 0.02284

Eigenvalues --- 0.02396 0.02467 0.02850 0.03033 0.03143

Eigenvalues --- 0.03460 0.03633 0.03971 0.04263 0.04628

Eigenvalues --- 0.04869 0.05037 0.05334 0.05536 0.05733

Eigenvalues --- 0.05837 0.05963 0.06182 0.07469 0.09384

Eigenvalues --- 0.09608 0.11795 0.12510 0.12869 0.13019

Eigenvalues --- 0.13556 0.14897 0.15629 0.15909 0.15959

Eigenvalues --- 0.16004 0.16021 0.16044 0.16069 0.16323

Eigenvalues --- 0.17182 0.17557 0.19742 0.21351 0.22082

Eigenvalues --- 0.23334 0.23826 0.24112 0.25276 0.26202

Eigenvalues --- 0.28382 0.29119 0.29979 0.31348 0.31979

Eigenvalues --- 0.33172 0.34442 0.34511 0.34617 0.34755

Eigenvalues --- 0.34871 0.34908 0.34967 0.35082 0.35313

Eigenvalues --- 0.35449 0.35645 0.35816 0.35925 0.36624

Eigenvalues --- 0.37040 0.37261 0.37827 0.38281 0.39384

Eigenvalues --- 0.40411 0.45329 0.49230 0.50339 0.50865

Eigenvalues --- 0.54466 0.55909 0.56691 0.61589 0.91066

Eigenvalues --- 0.96871

En-DIIS/RFO-DIIS IScMMF= 0 using points: 37 36 35 34 33

RFO step: Lambda=-9.27129495D-08.

DidBck=F Rises=F RFO-DIIS coefs: 1.68603 -0.63402 -0.86749 1.06527 -0.24980

Iteration 1 RMS(Cart)= 0.00153362 RMS(Int)= 0.00000108

Iteration 2 RMS(Cart)= 0.00000160 RMS(Int)= 0.00000018

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000018

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56882	-0.00002	-0.00002	-0.00002	-0.00004	2.56878
R2	2.62015	-0.00001	-0.00002	0.00000	-0.00002	2.62013
R3	2.03243	0.00001	0.00001	0.00000	0.00001	2.03244
R4	2.62432	-0.00001	-0.00001	0.00001	0.00000	2.62432
R5	2.07287	0.00000	0.00007	-0.00001	0.00006	2.07293
R6	2.53627	0.00003	0.00007	0.00001	0.00008	2.53635
R7	2.70528	-0.00004	-0.00025	0.00003	-0.00022	2.70505
R8	2.52988	-0.00001	-0.00002	0.00001	-0.00001	2.52987
R9	2.03420	0.00000	-0.00001	0.00001	0.00000	2.03420
R10	2.78610	-0.00002	-0.00007	0.00003	-0.00003	2.78606
R11	2.06238	0.00000	-0.00001	0.00000	-0.00001	2.06237
R12	2.05657	-0.00001	-0.00003	0.00000	-0.00002	2.05654
R13	2.90191	-0.00002	-0.00006	0.00004	-0.00002	2.90189

R14	4.42110	0.00002	0.00000	-0.00034	-0.00034	4.42076
R15	2.50678	0.00003	0.00007	0.00001	0.00008	2.50686
R16	2.04654	0.00000	0.00000	0.00000	0.00001	2.04655
R17	2.04622	-0.00001	-0.00004	0.00000	-0.00004	2.04619
R18	2.06365	0.00000	-0.00003	0.00000	-0.00003	2.06362
R19	2.77050	0.00000	0.00003	0.00000	0.00003	2.77052
R20	2.76643	-0.00001	-0.00005	0.00001	-0.00004	2.76639
R21	2.05290	0.00000	0.00002	0.00000	0.00002	2.05292
R22	2.05381	0.00001	-0.00001	0.00002	0.00001	2.05383
R23	2.74401	-0.00004	-0.00025	-0.00002	-0.00027	2.74374
R24	2.05519	0.00000	-0.00001	0.00000	-0.00001	2.05518
R25	2.84174	0.00002	0.00011	0.00000	0.00011	2.84186
R26	3.09485	0.00000	0.00003	-0.00008	-0.00005	3.09480
R27	2.06714	0.00000	0.00000	0.00000	0.00000	2.06714
R28	2.06780	0.00000	0.00000	0.00000	0.00000	2.06780
R29	2.06377	-0.00001	-0.00002	0.00000	-0.00002	2.06375
R30	2.06854	-0.00001	0.00002	-0.00002	-0.00001	2.06854
R31	2.06085	-0.00001	0.00001	-0.00001	-0.00001	2.06085
R32	2.88050	0.00001	0.00012	-0.00004	0.00009	2.88059
R33	2.28317	0.00004	0.00002	0.00002	0.00005	2.28321
R34	2.51731	-0.00004	-0.00016	0.00001	-0.00015	2.51717
R35	1.89924	-0.00002	-0.00005	-0.00005	-0.00009	1.89914
A1	1.88385	0.00001	0.00001	0.00002	0.00003	1.88389
A2	2.27336	-0.00002	-0.00007	-0.00002	-0.00009	2.27327
A3	2.12543	0.00001	0.00008	0.00000	0.00008	2.12551
A4	1.85658	0.00001	0.00001	-0.00001	0.00000	1.85658
A5	2.26991	-0.00001	0.00011	0.00001	0.00013	2.27004
A6	2.15034	0.00000	-0.00017	0.00000	-0.00017	2.15017
A7	1.90058	-0.00001	-0.00003	0.00001	-0.00002	1.90056
A8	2.21724	-0.00001	-0.00004	-0.00004	-0.00008	2.21716
A9	2.16524	0.00002	0.00006	0.00004	0.00010	2.16534
A10	1.89645	0.00000	0.00000	-0.00001	-0.00002	1.89644
A11	2.19056	0.00000	-0.00004	0.00000	-0.00004	2.19052
A12	2.19612	0.00001	0.00004	0.00001	0.00005	2.19617
A13	1.88730	0.00000	0.00001	-0.00001	0.00000	1.88730
A14	2.19030	-0.00002	0.00002	-0.00004	-0.00003	2.19028
A15	2.20076	0.00002	-0.00002	0.00005	0.00004	2.20080
A16	1.88868	0.00003	0.00013	0.00001	0.00014	1.88882
A17	1.85790	0.00002	0.00000	-0.00004	-0.00004	1.85786
A18	1.96198	-0.00007	-0.00018	0.00002	-0.00017	1.96181
A19	1.88875	-0.00001	0.00010	-0.00001	0.00009	1.88884
A20	1.93196	0.00001	0.00008	0.00000	0.00007	1.93204
A21	1.93149	0.00001	-0.00011	0.00002	-0.00009	1.93140
A22	2.73119	-0.00001	-0.00017	0.00079	0.00062	2.73182

A23	2.15287	0.00001	0.00008	0.00001	0.00009	2.15296
A24	1.96458	0.00000	0.00014	-0.00003	0.00011	1.96469
A25	2.16569	-0.00002	-0.00023	0.00003	-0.00020	2.16549
A26	2.06449	-0.00001	-0.00005	0.00000	-0.00005	2.06443
A27	2.15837	-0.00001	-0.00014	0.00004	-0.00010	2.15827
A28	2.06007	0.00002	0.00018	-0.00004	0.00014	2.06021
A29	2.05862	0.00002	-0.00014	-0.00007	-0.00021	2.05841
A30	2.12786	-0.00002	0.00010	0.00002	0.00012	2.12798
A31	1.97582	0.00001	-0.00006	0.00007	0.00001	1.97583
A32	1.99994	0.00000	0.00012	-0.00002	0.00009	2.00003
A33	2.02667	0.00000	0.00004	0.00002	0.00006	2.02673
A34	2.04006	0.00002	0.00024	-0.00002	0.00023	2.04029
A35	2.13941	-0.00002	-0.00031	0.00000	-0.00032	2.13909
A36	1.94485	0.00001	0.00022	-0.00004	0.00019	1.94503
A37	2.03859	0.00000	-0.00007	0.00003	-0.00004	2.03854
A38	2.02373	-0.00001	-0.00002	0.00002	0.00000	2.02373
A39	2.10145	-0.00002	-0.00043	-0.00019	-0.00063	2.10082
A40	2.35956	0.00003	0.00047	0.00072	0.00119	2.36075
A41	1.93514	0.00000	0.00003	0.00003	0.00006	1.93520
A42	1.91420	-0.00001	0.00000	0.00001	0.00001	1.91421
A43	1.93664	-0.00001	-0.00011	-0.00004	-0.00015	1.93649
A44	1.88207	0.00000	-0.00001	0.00001	0.00000	1.88207
A45	1.90027	0.00000	0.00002	0.00000	0.00002	1.90028
A46	1.89423	0.00001	0.00007	0.00000	0.00007	1.89430
A47	1.88217	0.00003	0.00020	0.00005	0.00025	1.88242
A48	1.94518	0.00001	0.00005	0.00000	0.00005	1.94523
A49	1.97081	-0.00005	0.00001	-0.00003	-0.00002	1.97080
A50	1.88273	-0.00001	-0.00007	-0.00003	-0.00009	1.88263
A51	1.90146	0.00001	-0.00012	0.00003	-0.00009	1.90137
A52	1.87935	0.00001	-0.00009	-0.00002	-0.00011	1.87924
A53	2.14834	0.00000	-0.00011	0.00007	-0.00004	2.14831
A54	1.94961	-0.00002	0.00002	-0.00006	-0.00004	1.94957
A55	2.18492	0.00001	0.00010	-0.00002	0.00008	2.18500
A56	1.93498	0.00007	0.00042	-0.00008	0.00034	1.93532
A57	2.81251	0.00001	0.00038	-0.00009	0.00030	2.81281
D1	0.00346	-0.00001	0.00015	-0.00007	0.00008	0.00354
D2	3.02481	-0.00001	-0.00033	-0.00002	-0.00036	3.02445
D3	-3.10255	0.00000	-0.00047	0.00000	-0.00047	-3.10302
D4	-0.08120	-0.00001	-0.00095	0.00004	-0.00091	-0.08211
D5	-0.00263	0.00001	-0.00016	0.00008	-0.00007	-0.00270
D6	-3.04393	0.00001	-0.00024	0.00007	-0.00017	-3.04410
D7	3.10702	0.00000	0.00040	0.00002	0.00042	3.10744
D8	0.06572	0.00001	0.00032	0.00001	0.00032	0.06604
D9	-0.00311	0.00001	-0.00009	0.00003	-0.00006	-0.00317

D10	3.12209	0.00000	-0.00037	0.00007	-0.00031	3.12179
D11	-3.03475	0.00001	0.00033	-0.00001	0.00032	-3.03443
D12	0.09046	0.00001	0.00004	0.00002	0.00007	0.09052
D13	-1.48805	0.00003	0.00137	0.00036	0.00173	-1.48631
D14	1.51555	0.00002	0.00084	0.00041	0.00125	1.51680
D15	0.00152	0.00000	-0.00001	0.00002	0.00001	0.00153
D16	3.13361	-0.00002	-0.00085	-0.00012	-0.00097	3.13264
D17	-3.12428	0.00000	0.00027	-0.00001	0.00025	-3.12403
D18	0.00781	-0.00001	-0.00058	-0.00015	-0.00073	0.00708
D19	-0.19586	0.00001	0.00069	0.00059	0.00128	-0.19457
D20	2.95531	0.00001	0.00073	0.00067	0.00140	2.95671
D21	2.92702	0.00001	0.00037	0.00063	0.00100	2.92802
D22	-0.20500	0.00001	0.00040	0.00071	0.00111	-0.20388
D23	0.00066	0.00000	0.00010	-0.00006	0.00004	0.00070
D24	3.04121	-0.00001	0.00018	-0.00005	0.00013	3.04134
D25	-3.13140	0.00001	0.00095	0.00008	0.00103	-3.13037
D26	-0.09085	0.00000	0.00103	0.00009	0.00112	-0.08973
D27	-2.47128	-0.00002	0.00054	0.00047	0.00101	-2.47026
D28	-0.44453	0.00000	0.00072	0.00045	0.00117	-0.44337
D29	1.67291	-0.00001	0.00047	0.00046	0.00093	1.67385
D30	0.78834	0.00000	0.00044	0.00046	0.00091	0.78924
D31	2.81508	0.00001	0.00063	0.00043	0.00106	2.81614
D32	-1.35066	0.00000	0.00038	0.00045	0.00082	-1.34983
D33	-3.00085	0.00001	0.00008	0.00010	0.00018	-3.00067
D34	1.21902	0.00000	0.00000	0.00010	0.00011	1.21913
D35	-0.89907	0.00002	0.00008	0.00015	0.00023	-0.89884
D36	1.16795	0.00001	-0.00002	0.00008	0.00006	1.16801
D37	-0.89537	-0.00001	-0.00009	0.00008	-0.00001	-0.89538
D38	-3.01346	0.00001	-0.00001	0.00013	0.00012	-3.01334
D39	-0.92604	-0.00001	-0.00012	0.00008	-0.00004	-0.92608
D40	-2.98935	-0.00002	-0.00019	0.00008	-0.00011	-2.98946
D41	1.17575	0.00000	-0.00012	0.00013	0.00001	1.17576
D42	-3.13995	0.00001	0.00011	0.00010	0.00021	-3.13975
D43	-0.02356	0.00000	-0.00010	-0.00006	-0.00016	-0.02373
D44	-0.00904	0.00001	0.00007	0.00001	0.00008	-0.00896
D45	3.10735	0.00000	-0.00014	-0.00015	-0.00029	3.10706
D46	-2.75272	0.00000	0.00012	0.00009	0.00021	-2.75251
D47	-0.04754	-0.00001	-0.00010	0.00007	-0.00003	-0.04757
D48	-0.01982	0.00000	0.00012	0.00002	0.00013	-0.01969
D49	2.68536	-0.00001	-0.00011	0.00000	-0.00010	2.68526
D50	0.31349	0.00003	0.00086	0.00103	0.00189	0.31539
D51	-2.06535	0.00002	0.00074	0.00095	0.00168	-2.06367
D52	2.54356	0.00001	0.00053	0.00052	0.00105	2.54461
D53	0.16174	0.00001	0.00038	0.00050	0.00088	0.16262

D54	2.55287	0.00000	0.00100	0.00050	0.00150	2.55437
D55	-1.65375	0.00000	0.00100	0.00054	0.00154	-1.65221
D56	0.43883	0.00000	0.00102	0.00051	0.00154	0.44037
D57	1.32642	0.00001	0.00110	0.00048	0.00158	1.32799
D58	-2.88020	0.00001	0.00111	0.00051	0.00162	-2.87859
D59	-0.78762	0.00001	0.00113	0.00049	0.00162	-0.78600
D60	-1.02137	0.00000	0.00084	0.00048	0.00132	-1.02005
D61	1.05520	0.00000	0.00084	0.00052	0.00136	1.05655
D62	-3.13541	0.00000	0.00086	0.00049	0.00136	-3.13405
D63	1.47418	-0.00001	-0.00116	0.00078	-0.00038	1.47380
D64	2.82033	0.00000	-0.00127	0.00088	-0.00039	2.81994
D65	2.25720	-0.00001	0.00076	-0.00015	0.00061	2.25781
D66	-0.85909	-0.00002	0.00035	0.00001	0.00036	-0.85873
D67	-1.93526	0.00001	0.00094	-0.00009	0.00086	-1.93441
D68	1.23163	0.00000	0.00053	0.00007	0.00061	1.23223
D69	0.10226	0.00001	0.00076	-0.00011	0.00064	0.10290
D70	-3.01403	0.00000	0.00034	0.00005	0.00039	-3.01364
D71	2.92260	-0.00001	0.00065	-0.00013	0.00052	2.92312
D72	-0.19306	-0.00002	0.00023	0.00003	0.00027	-0.19280
D73	-1.88101	-0.00003	-0.00136	-0.00092	-0.00229	-1.88330

Item	Value	Threshold	Converged?
Maximum Force	0.000073	0.000450	YES
RMS Force	0.000017	0.000300	YES
Maximum Displacement	0.006396	0.001800	NO
RMS Displacement	0.001533	0.001200	NO

Predicted change in Energy=-1.249335D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.846218	1.644364	1.537690
2	6	0	-1.503144	0.454863	1.574381
3	7	0	-2.364722	0.449698	0.485238
4	6	0	-2.229108	1.606520	-0.181706
5	7	0	-1.308847	2.354025	0.440070
6	6	0	-0.775197	3.644927	-0.031534
7	1	0	-0.073807	2.031658	2.178105
8	1	0	-1.351469	-0.415700	2.224305
9	1	0	-1.613121	4.258643	-0.366644
10	1	0	-0.325067	4.127002	0.834103
11	35	0	-0.392851	-2.433117	2.919791

12	1	0	-2.765202	1.880248	-1.074133
13	6	0	-3.250610	-0.603588	0.091732
14	6	0	-3.210120	-1.823249	0.611911
15	1	0	-3.945480	-0.295778	-0.679804
16	1	0	-3.918964	-2.558357	0.251907
17	1	0	-2.486154	-2.135244	1.367583
18	6	0	2.554199	-0.688916	1.129208
19	6	0	3.974276	-0.375546	1.315284
20	8	0	2.974061	0.654219	1.532613
21	1	0	2.171025	-0.730652	0.113526
22	1	0	1.981574	-1.228164	1.879227
23	1	0	4.429382	-0.691562	2.251120
24	6	0	4.916409	-0.172816	0.160796
25	1	0	5.676353	0.575301	0.404502
26	1	0	5.430782	-1.112020	-0.064288
27	1	0	4.376414	0.149856	-0.731920
28	6	0	0.257383	3.475869	-1.155505
29	1	0	0.707996	4.454827	-1.347309
30	1	0	-0.211208	3.136332	-2.079865
31	6	0	1.360153	2.483850	-0.804200
32	8	0	1.683381	1.572882	-1.529089
33	8	0	1.883803	2.733698	0.394828
34	1	0	2.457172	1.967640	0.702068

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.359342	0.000000			
3	N	2.200166	1.388731	0.000000		
4	C	2.206839	2.221976	1.342178	0.000000	
5	N	1.386511	2.220637	2.177928	1.338749	0.000000
6	C	2.543572	3.644911	3.605985	2.508288	1.474320
7	H	1.075522	2.212186	3.258325	3.224092	2.156388
8	H	2.229481	1.096945	2.190879	3.263207	3.294950
9	H	3.324016	4.271816	3.974754	2.728992	2.090679
10	H	2.632513	3.926892	4.219533	3.318142	2.065559
11	Br	4.329157	3.373916	4.257458	5.413852	5.468528
12	H	3.249578	3.261769	2.153716	1.076452	2.153658
13	C	3.595160	2.524322	1.431452	2.450064	3.555173
14	C	4.297608	3.004981	2.428381	3.654522	4.592819
15	H	4.276313	3.407318	2.100442	2.610129	3.902231
16	H	5.362636	4.082232	3.393893	4.515511	5.565933
17	H	4.123562	2.778081	2.734083	4.057977	4.732851
18	C	4.144140	4.238920	5.089884	5.465122	4.965635

19	C	5.231316	5.546066	6.446154	6.682181	6.010653
20	O	3.946511	4.481836	5.444394	5.560462	4.735641
21	H	4.095449	4.127840	4.701531	4.991063	4.661692
22	H	4.045303	3.881852	4.862995	5.478387	5.072487
23	H	5.813561	6.080060	7.112008	7.452201	6.744092
24	C	6.197245	6.603246	7.314892	7.371686	6.724339
25	H	6.706038	7.275183	8.042460	7.993958	7.208200
26	H	7.040221	7.295182	7.969367	8.128847	7.595422
27	H	5.887323	6.323073	6.856696	6.786569	6.209196
28	C	3.438844	4.436013	4.327260	3.259661	2.501494
29	H	4.317118	5.424493	5.370371	4.254182	3.416980
30	H	3.964329	4.713054	4.293643	3.164687	2.857776
31	C	3.325245	4.239446	4.435663	3.746998	2.947647
32	O	3.976068	4.586440	4.658990	4.138133	3.666224
33	O	3.153695	4.249216	4.824395	4.303365	3.215464
34	H	3.422741	4.328224	5.059824	4.782539	3.794843

		6	7	8	9	10
6	C	0.000000				
7	H	2.824374	0.000000			
8	H	4.680769	2.761181	0.000000		
9	H	1.091358	3.715467	5.350791	0.000000	
10	H	1.088275	2.501987	4.860279	1.765844	0.000000
11	Br	6.767506	4.537191	2.339363	7.554427	6.884029
12	H	2.856785	4.224166	4.260248	2.735799	3.826687
13	C	4.918611	4.624883	2.861801	5.150997	5.611452
14	C	6.020284	5.210540	2.834711	6.363756	6.616524
15	H	5.099030	5.345508	3.895783	5.126473	5.912723
16	H	6.960197	6.289969	3.882443	7.222950	7.612429
17	H	6.188319	4.882565	2.231214	6.682180	6.646099
18	C	5.586985	3.925319	4.065481	6.639464	5.618749
19	C	6.366759	4.788118	5.402916	7.451416	6.244104
20	O	5.044584	3.406391	4.509255	6.135250	4.840701
21	H	5.277022	4.114865	4.118562	6.280398	5.508767
22	H	5.915895	3.865277	3.447950	6.933313	5.923740
23	H	7.148656	5.263076	5.787492	8.238268	6.916016
24	C	6.856131	5.816485	6.603284	7.908905	6.812844
25	H	7.157879	6.191202	7.326940	8.203542	6.986858
26	H	7.819449	6.723953	7.191763	8.862957	7.834810
27	H	6.264595	5.640381	6.470531	7.272557	6.354057
28	C	1.535615	3.648067	5.399615	2.175735	2.172962
29	H	2.141743	4.348737	6.381212	2.527405	2.435826
30	H	2.184585	4.401078	5.695877	2.481949	3.079871
31	C	2.550457	3.339889	4.993208	3.490230	2.867744
32	O	3.546921	4.128132	5.220416	4.408120	4.017720

33	O	2.842957	2.739557	4.871620	3.890215	2.648276
34	H	3.714791	2.930638	4.743761	4.791464	3.524363
		11	12	13	14	15
11	Br	0.000000				
12	H	6.339132	0.000000			
13	C	4.417225	2.786450	0.000000		
14	C	3.692594	4.093481	1.326574	0.000000	
15	H	5.490580	2.506719	1.082987	2.131303	0.000000
16	H	4.423433	4.773967	2.072070	1.082796	2.447049
17	H	2.622974	4.707868	2.134985	1.092020	3.115295
18	C	3.864393	6.304867	5.897410	5.897600	6.758174
19	C	5.087224	7.497899	7.331307	7.362481	8.167575
20	O	4.774097	6.421636	6.511892	6.725298	7.326482
21	H	4.164969	5.709086	5.423167	5.513517	6.183051
22	H	2.858773	6.396596	5.564259	5.377165	6.522880
23	H	5.170500	8.332679	7.978280	7.894916	8.881738
24	C	6.396034	8.046568	8.178663	8.304692	8.902517
25	H	7.225821	8.668857	9.009898	9.206816	9.721840
26	H	6.675681	8.783370	8.697666	8.696452	9.431829
27	H	6.538550	7.356224	7.708279	7.953271	8.333980
28	C	7.207424	3.418867	5.523005	6.574800	5.667070
29	H	8.177028	4.331996	6.582474	7.655352	6.683461
30	H	7.486542	3.018630	5.285905	6.390350	5.261591
31	C	6.412308	4.178008	5.620862	6.437691	5.990956
32	O	6.336505	4.482337	5.631016	6.329608	5.991432
33	O	6.185028	4.949693	6.131193	6.838197	6.656808
34	H	5.692766	5.516857	6.289872	6.818883	6.930122
		16	17	18	19	20
16	H	0.000000				
17	H	1.864592	0.000000			
18	C	6.794580	5.249177	0.000000		
19	C	8.258249	6.696002	1.466098	0.000000	
20	O	7.711981	6.133702	1.463910	1.451922	0.000000
21	H	6.359844	5.023431	1.086359	2.195914	2.139286
22	H	6.263700	4.587502	1.086838	2.239610	2.156047
23	H	8.785024	7.119655	2.185177	1.087555	2.108397
24	C	9.152209	7.752768	2.604653	1.503846	2.517654
25	H	10.095207	8.654542	3.445473	2.151905	2.929376
26	H	9.466235	8.110186	3.142956	2.137059	3.421282
27	H	8.781550	7.531563	2.736385	2.151466	2.710919
28	C	7.472253	6.736288	5.276431	5.895209	4.750582
29	H	8.552836	7.810396	5.999975	6.410186	5.279548
30	H	7.184294	6.696999	5.707727	6.432620	5.418193
31	C	7.376197	6.391146	3.902596	4.416106	3.378304

32	O	7.185078	6.286966	3.597305	4.139448	3.447291
33	O	7.854831	6.614331	3.564131	3.858071	2.609109
34	H	7.832139	6.458564	2.692425	2.857999	1.637698

		21	22	23	24	25
21	H	0.000000				
22	H	1.844210	0.000000			
23	H	3.109825	2.533379	0.000000		
24	C	2.801883	3.560901	2.208109	0.000000	
25	H	3.752000	4.367916	2.563177	1.093885	0.000000
26	H	3.286803	3.960779	2.557479	1.094233	1.768367
27	H	2.520677	3.801616	3.099890	1.092087	1.778285
28	C	4.792420	5.857505	6.810151	6.062349	6.341305
29	H	5.582445	6.657997	7.299502	6.434299	6.542487
30	H	5.043765	6.287410	7.412508	6.501037	6.884354
31	C	3.439877	4.622336	5.370138	4.542691	4.871663
32	O	2.870932	4.421696	5.192129	4.044211	4.547281
33	O	3.487599	4.231944	4.653837	4.207053	4.363738
34	H	2.776517	3.438759	3.655206	3.304901	3.519983

		26	27	28	29	30
26	H	0.000000				
27	H	1.774755	0.000000			
28	C	7.000252	5.311139	0.000000		
29	H	7.412195	5.689356	1.094623	0.000000	
30	H	7.344596	5.637576	1.090552	1.766354	0.000000
31	C	5.481584	3.814522	1.524343	2.145933	2.126554
32	O	4.837081	3.148477	2.407155	3.047955	2.517379
33	O	5.251799	3.762833	2.366346	2.716588	3.267306
34	H	4.349019	3.007349	3.250293	3.666833	4.028057

		31	32	33	34
31	C	0.000000			
32	O	1.208223	0.000000		
33	O	1.332029	2.255908	0.000000	
34	H	1.933589	2.394295	1.004984	0.000000

Stoichiometry C11H17BrN2O3
Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.076943	1.328377	1.238839
2	6	0	-1.153384	1.256449	0.665313
3	7	0	-1.214072	2.288571	-0.261841
4	6	0	-0.052917	2.961385	-0.239863
5	7	0	0.752478	2.396148	0.667934
6	6	0	2.160213	2.752953	0.922084
7	1	0	0.536619	0.697653	1.978860
8	1	0	-1.939333	0.498829	0.772939
9	1	0	2.235037	3.841095	0.959626
10	1	0	2.404403	2.360850	1.907462
11	35	0	-3.071179	-1.497940	0.320767
12	1	0	0.190921	3.807995	-0.858365
13	6	0	-2.306606	2.603012	-1.131642
14	6	0	-3.347974	1.801632	-1.313692
15	1	0	-2.181817	3.557826	-1.627240
16	1	0	-4.128453	2.120846	-1.992957
17	1	0	-3.452096	0.826072	-0.834163
18	6	0	0.610589	-2.462216	-0.348775
19	6	0	1.585353	-3.513874	-0.043334
20	8	0	1.628063	-2.257817	0.683697
21	1	0	0.774663	-1.858538	-1.236935
22	1	0	-0.410027	-2.499028	0.022982
23	1	0	1.246659	-4.329379	0.591501
24	6	0	2.754202	-3.818954	-0.939030
25	1	0	3.621568	-4.137110	-0.353336
26	1	0	2.493009	-4.633959	-1.620860
27	1	0	3.030026	-2.944708	-1.532553
28	6	0	3.110101	2.179924	-0.139737
29	1	0	4.136355	2.362028	0.194688
30	1	0	2.978710	2.676163	-1.101916
31	6	0	2.919915	0.683753	-0.360918
32	8	0	2.771979	0.192210	-1.454675
33	8	0	2.908000	0.013286	0.790008
34	1	0	2.583217	-0.927856	0.653041

Rotational constants (GHZ): 0.3288448 0.2548041 0.1595911

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 538 symmetry adapted cartesian basis functions of A symmetry.

There are 519 symmetry adapted basis functions of A symmetry.

519 basis functions, 823 primitive gaussians, 538 cartesian basis functions

78 alpha electrons 78 beta electrons

nuclear repulsion energy 1572.9161977284 Hartrees.

NAtoms= 34 NActive= 34 NUniq= 34 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 519 RedAO= T EigKep= 3.53D-06 NBF= 519
NBsUse= 519 1.00D-06 EigRej= -1.00D+00 NBFU= 519
Initial guess from the checkpoint file: "./coohpo.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 0.000010 0.000037 0.000633 Ang= 0.07 deg.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3338.90388357 A.U. after 9 cycles
NFock= 9 Conv=0.41D-08 -V/T= 2.0019
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000006628	0.000002806	0.000004358
2	6	0.000033009	0.000010310	0.000005819
3	7	0.000006538	0.000007586	-0.000008069
4	6	0.000003335	0.000006398	0.000004569
5	7	-0.000016986	0.000001632	-0.000005890
6	6	0.000020145	-0.000004952	-0.000005762
7	1	0.000001245	-0.000000719	0.000002160
8	1	-0.000037902	-0.000004447	-0.000038311
9	1	0.000004675	0.000003724	-0.000007085
10	1	-0.000002138	-0.000003136	0.000000837
11	35	0.000015726	0.000001857	0.000014161
12	1	-0.000001158	-0.000000959	-0.000003453
13	6	-0.000009672	-0.000003616	0.000002277
14	6	-0.000007082	-0.000005589	0.000001242
15	1	0.000004199	0.000001469	-0.000005975
16	1	-0.000000707	0.000005772	-0.000003219
17	1	-0.000004430	0.000003950	0.000000211
18	6	-0.000001334	0.000008004	-0.000020054
19	6	-0.000016220	-0.000008127	0.000007078
20	8	0.000042099	0.000020073	-0.000002429
21	1	-0.000007901	-0.000004330	0.000005915
22	1	0.000003698	-0.000003935	0.000010364

23	1	-0.000003137	0.000000622	0.000007997
24	6	0.000007036	-0.000000590	0.000007762
25	1	0.000000407	-0.000007198	0.000007584
26	1	-0.000004626	-0.000005114	0.000005277
27	1	0.000003402	-0.000000249	0.000005990
28	6	0.000009119	0.000007565	-0.000004885
29	1	-0.000001569	-0.000003998	-0.000002174
30	1	0.000001327	0.000000298	-0.000000021
31	6	-0.000014819	0.000011841	0.000013014
32	8	0.000006128	-0.000013023	-0.000004914
33	8	0.000019428	-0.000003018	-0.000010146
34	1	-0.000045203	-0.000020907	0.000015772

Cartesian Forces: Max 0.000045203 RMS 0.000011725

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000037512 RMS 0.000007725
Search for a local minimum.
Step number 38 out of a maximum of 175
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 21 22 23 24 25
26 27 28 29 30
31 32 33 34 35
36 37 38
DE= -1.25D-06 DEPred=-1.25D-07 R= 1.00D+01
TightC=F SS= 1.41D+00 RLast= 7.88D-03 DXNew= 6.5746D-01 2.3636D-02
Trust test= 1.00D+01 RLast= 7.88D-03 DXMaxT set to 3.91D-01
ITU= 1 1 1 1 1 1 1 -1 1 1 1 1 1 -1 0 1 1 1 1 1
ITU= 1 1 1 1 1 0 0 -1 1 1 1 0 1 0 -1 0 1 0

Eigenvalues ---	0.00168	0.00277	0.00344	0.00426	0.00480
Eigenvalues ---	0.00563	0.00875	0.00980	0.01169	0.01311
Eigenvalues ---	0.01432	0.01995	0.02145	0.02202	0.02285
Eigenvalues ---	0.02377	0.02473	0.02715	0.02975	0.03136
Eigenvalues ---	0.03435	0.03631	0.03927	0.04296	0.04612
Eigenvalues ---	0.04860	0.05035	0.05235	0.05394	0.05743
Eigenvalues ---	0.05866	0.05959	0.06247	0.07422	0.09328
Eigenvalues ---	0.09628	0.11750	0.12565	0.12876	0.13353
Eigenvalues ---	0.13533	0.14250	0.15139	0.15666	0.15965
Eigenvalues ---	0.16006	0.16010	0.16043	0.16062	0.16227

Eigenvalues --- 0.16694 0.17797 0.19368 0.20868 0.22052
Eigenvalues --- 0.23323 0.23690 0.23936 0.25350 0.26279
Eigenvalues --- 0.28225 0.28861 0.29834 0.31447 0.32083
Eigenvalues --- 0.33329 0.34346 0.34507 0.34608 0.34721
Eigenvalues --- 0.34862 0.34896 0.34967 0.35074 0.35240
Eigenvalues --- 0.35322 0.35650 0.35764 0.35915 0.36604
Eigenvalues --- 0.37051 0.37263 0.37807 0.38515 0.39529
Eigenvalues --- 0.40796 0.45457 0.49288 0.50353 0.50904
Eigenvalues --- 0.54534 0.56019 0.56616 0.61242 0.90608
Eigenvalues --- 0.96948
En-DIIS/RFO-DIIS IScMMF= 0 using points: 38 37 36 35 34
RFO step: Lambda=-3.49321468D-08.
DidBck=F Rises=F RFO-DIIS coefs: 1.42732 -0.07284 -0.65526 0.47011 -0.16934
Iteration 1 RMS(Cart)= 0.00142386 RMS(Int)= 0.00000099
Iteration 2 RMS(Cart)= 0.00000130 RMS(Int)= 0.00000010
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000010

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56878	-0.00001	-0.00002	-0.00001	-0.00003	2.56876
R2	2.62013	0.00000	-0.00001	0.00000	-0.00001	2.62011
R3	2.03244	0.00000	0.00001	0.00000	0.00001	2.03245
R4	2.62432	0.00000	-0.00001	-0.00002	-0.00003	2.62429
R5	2.07293	-0.00001	0.00000	-0.00006	-0.00006	2.07287
R6	2.53635	0.00000	0.00005	0.00000	0.00004	2.53639
R7	2.70505	0.00001	-0.00012	0.00003	-0.00009	2.70496
R8	2.52987	0.00000	-0.00001	0.00000	-0.00001	2.52986
R9	2.03420	0.00000	0.00000	0.00000	0.00000	2.03420
R10	2.78606	0.00000	-0.00001	0.00001	0.00001	2.78607
R11	2.06237	0.00000	0.00000	0.00000	0.00000	2.06237
R12	2.05654	0.00000	-0.00002	0.00000	-0.00002	2.05653
R13	2.90189	-0.00001	-0.00003	-0.00003	-0.00006	2.90183
R14	4.42076	0.00001	0.00005	0.00006	0.00011	4.42087
R15	2.50686	0.00000	0.00005	0.00000	0.00004	2.50691
R16	2.04655	0.00000	0.00001	-0.00001	0.00000	2.04655
R17	2.04619	0.00000	-0.00002	0.00000	-0.00002	2.04616
R18	2.06362	0.00000	-0.00001	-0.00002	-0.00003	2.06359
R19	2.77052	0.00000	0.00002	-0.00002	-0.00001	2.77052
R20	2.76639	0.00000	-0.00003	0.00002	-0.00001	2.76638
R21	2.05292	0.00000	0.00000	0.00000	0.00000	2.05292
R22	2.05383	0.00000	0.00000	0.00000	0.00000	2.05382
R23	2.74374	0.00000	-0.00014	0.00004	-0.00010	2.74363
R24	2.05518	0.00000	-0.00001	0.00001	0.00000	2.05518
R25	2.84186	0.00000	0.00007	-0.00003	0.00004	2.84190

R26	3.09480	0.00000	-0.00019	-0.00003	-0.00022	3.09458
R27	2.06714	0.00000	0.00000	-0.00001	-0.00001	2.06714
R28	2.06780	0.00000	0.00000	0.00000	0.00000	2.06780
R29	2.06375	0.00000	-0.00002	0.00001	-0.00001	2.06373
R30	2.06854	0.00000	0.00000	0.00000	0.00000	2.06853
R31	2.06085	0.00000	-0.00001	0.00001	0.00001	2.06085
R32	2.88059	0.00000	0.00005	0.00000	0.00005	2.88064
R33	2.28321	0.00001	0.00004	-0.00001	0.00003	2.28324
R34	2.51717	0.00000	-0.00011	0.00002	-0.00010	2.51707
R35	1.89914	0.00000	-0.00003	0.00003	0.00000	1.89914
A1	1.88389	0.00000	0.00001	-0.00001	0.00000	1.88389
A2	2.27327	0.00000	-0.00006	0.00000	-0.00006	2.27321
A3	2.12551	0.00000	0.00006	0.00000	0.00006	2.12557
A4	1.85658	0.00000	0.00000	0.00002	0.00002	1.85660
A5	2.27004	-0.00002	0.00010	0.00002	0.00012	2.27016
A6	2.15017	0.00001	-0.00013	-0.00002	-0.00015	2.15002
A7	1.90056	0.00000	0.00000	-0.00001	-0.00001	1.90055
A8	2.21716	0.00000	-0.00008	-0.00004	-0.00012	2.21704
A9	2.16534	0.00000	0.00008	0.00005	0.00013	2.16547
A10	1.89644	0.00000	-0.00002	0.00001	-0.00002	1.89642
A11	2.19052	0.00000	-0.00002	-0.00001	-0.00003	2.19049
A12	2.19617	0.00000	0.00004	0.00000	0.00005	2.19622
A13	1.88730	0.00000	0.00002	-0.00001	0.00001	1.88731
A14	2.19028	-0.00001	-0.00002	-0.00007	-0.00009	2.19019
A15	2.20080	0.00001	0.00001	0.00006	0.00007	2.20086
A16	1.88882	0.00001	0.00010	0.00000	0.00010	1.88893
A17	1.85786	0.00000	-0.00006	-0.00001	-0.00007	1.85779
A18	1.96181	-0.00002	-0.00009	-0.00005	-0.00014	1.96167
A19	1.88884	0.00000	0.00005	0.00000	0.00005	1.88889
A20	1.93204	0.00000	0.00004	0.00002	0.00006	1.93209
A21	1.93140	0.00001	-0.00004	0.00004	0.00000	1.93140
A22	2.73182	-0.00001	-0.00007	-0.00038	-0.00045	2.73137
A23	2.15296	0.00001	0.00002	0.00000	0.00002	2.15298
A24	1.96469	-0.00001	0.00009	-0.00002	0.00007	1.96476
A25	2.16549	0.00000	-0.00011	0.00002	-0.00009	2.16540
A26	2.06443	0.00000	-0.00004	0.00001	-0.00004	2.06440
A27	2.15827	0.00000	-0.00008	0.00003	-0.00005	2.15822
A28	2.06021	0.00000	0.00011	-0.00003	0.00008	2.06029
A29	2.05841	0.00002	-0.00010	0.00016	0.00006	2.05846
A30	2.12798	-0.00002	0.00012	-0.00016	-0.00005	2.12794
A31	1.97583	0.00001	0.00006	-0.00003	0.00002	1.97585
A32	2.00003	-0.00001	-0.00001	0.00006	0.00006	2.00009
A33	2.02673	0.00000	-0.00001	-0.00002	-0.00003	2.02670
A34	2.04029	0.00000	0.00013	-0.00007	0.00007	2.04036

A35	2.13909	0.00001	-0.00015	0.00009	-0.00007	2.13903
A36	1.94503	0.00000	0.00008	-0.00001	0.00006	1.94510
A37	2.03854	0.00000	-0.00001	0.00004	0.00004	2.03858
A38	2.02373	-0.00001	-0.00002	-0.00003	-0.00005	2.02368
A39	2.10082	0.00000	-0.00047	-0.00021	-0.00068	2.10014
A40	2.36075	0.00003	0.00040	0.00021	0.00061	2.36136
A41	1.93520	0.00000	0.00004	-0.00002	0.00002	1.93522
A42	1.91421	0.00000	0.00000	-0.00003	-0.00003	1.91418
A43	1.93649	0.00000	-0.00008	0.00004	-0.00004	1.93645
A44	1.88207	0.00000	-0.00001	0.00001	0.00000	1.88207
A45	1.90028	0.00000	0.00001	0.00001	0.00003	1.90031
A46	1.89430	0.00000	0.00005	-0.00001	0.00003	1.89433
A47	1.88242	0.00001	0.00016	-0.00004	0.00012	1.88254
A48	1.94523	0.00000	0.00002	-0.00001	0.00000	1.94523
A49	1.97080	-0.00002	0.00001	-0.00003	-0.00002	1.97078
A50	1.88263	0.00000	-0.00006	0.00000	-0.00006	1.88258
A51	1.90137	0.00001	-0.00006	0.00003	-0.00002	1.90135
A52	1.87924	0.00001	-0.00007	0.00004	-0.00003	1.87921
A53	2.14831	0.00000	-0.00002	-0.00003	-0.00005	2.14826
A54	1.94957	0.00000	-0.00005	0.00005	0.00001	1.94958
A55	2.18500	0.00000	0.00007	-0.00002	0.00005	2.18505
A56	1.93532	0.00003	0.00023	0.00004	0.00027	1.93559
A57	2.81281	0.00004	0.00037	0.00033	0.00069	2.81350
D1	0.00354	-0.00001	0.00007	-0.00004	0.00003	0.00357
D2	3.02445	0.00000	-0.00019	0.00011	-0.00009	3.02436
D3	-3.10302	0.00000	-0.00021	0.00010	-0.00011	-3.10314
D4	-0.08211	0.00000	-0.00048	0.00025	-0.00023	-0.08234
D5	-0.00270	0.00001	-0.00001	-0.00003	-0.00004	-0.00274
D6	-3.04410	0.00001	-0.00008	0.00018	0.00009	-3.04401
D7	3.10744	0.00000	0.00024	-0.00016	0.00009	3.10753
D8	0.06604	0.00000	0.00017	0.00005	0.00022	0.06626
D9	-0.00317	0.00001	-0.00011	0.00010	-0.00001	-0.00318
D10	3.12179	0.00001	-0.00021	0.00012	-0.00009	3.12170
D11	-3.03443	0.00001	0.00011	-0.00004	0.00007	-3.03436
D12	0.09052	0.00001	0.00001	-0.00001	0.00000	0.09052
D13	-1.48631	0.00002	0.00135	0.00069	0.00204	-1.48427
D14	1.51680	0.00002	0.00106	0.00086	0.00192	1.51873
D15	0.00153	0.00000	0.00011	-0.00012	-0.00001	0.00152
D16	3.13264	0.00000	-0.00052	0.00005	-0.00047	3.13217
D17	-3.12403	0.00000	0.00021	-0.00014	0.00007	-3.12396
D18	0.00708	0.00000	-0.00042	0.00002	-0.00039	0.00668
D19	-0.19457	0.00001	0.00036	0.00009	0.00044	-0.19413
D20	2.95671	0.00000	0.00042	0.00010	0.00052	2.95723
D21	2.92802	0.00001	0.00024	0.00011	0.00035	2.92837

D22	-0.20388	0.00001	0.00030	0.00013	0.00043	-0.20345
D23	0.00070	0.00000	-0.00006	0.00009	0.00003	0.00073
D24	3.04134	-0.00001	0.00001	-0.00013	-0.00011	3.04122
D25	-3.13037	0.00000	0.00057	-0.00007	0.00049	-3.12988
D26	-0.08973	-0.00001	0.00064	-0.00029	0.00035	-0.08938
D27	-2.47026	-0.00001	0.00081	0.00003	0.00084	-2.46942
D28	-0.44337	0.00000	0.00089	0.00002	0.00092	-0.44245
D29	1.67385	0.00000	0.00075	0.00004	0.00079	1.67464
D30	0.78924	0.00000	0.00072	0.00028	0.00100	0.79024
D31	2.81614	0.00000	0.00080	0.00027	0.00107	2.81721
D32	-1.34983	0.00000	0.00066	0.00029	0.00095	-1.34888
D33	-3.00067	0.00000	-0.00002	0.00006	0.00004	-3.00063
D34	1.21913	0.00000	-0.00005	0.00009	0.00004	1.21916
D35	-0.89884	0.00000	0.00002	0.00006	0.00008	-0.89876
D36	1.16801	0.00000	-0.00011	0.00008	-0.00003	1.16798
D37	-0.89538	0.00000	-0.00015	0.00011	-0.00004	-0.89541
D38	-3.01334	0.00000	-0.00007	0.00008	0.00001	-3.01333
D39	-0.92608	0.00000	-0.00018	0.00004	-0.00013	-0.92621
D40	-2.98946	0.00000	-0.00021	0.00007	-0.00014	-2.98960
D41	1.17576	0.00000	-0.00014	0.00005	-0.00009	1.17567
D42	-3.13975	0.00000	0.00014	-0.00006	0.00008	-3.13967
D43	-0.02373	0.00000	-0.00009	0.00002	-0.00007	-0.02380
D44	-0.00896	0.00000	0.00006	-0.00008	-0.00001	-0.00897
D45	3.10706	0.00000	-0.00016	0.00001	-0.00015	3.10690
D46	-2.75251	0.00000	0.00013	-0.00010	0.00004	-2.75247
D47	-0.04757	0.00000	0.00003	-0.00013	-0.00010	-0.04766
D48	-0.01969	0.00000	0.00013	-0.00015	-0.00002	-0.01971
D49	2.68526	-0.00001	0.00003	-0.00019	-0.00016	2.68510
D50	0.31539	0.00001	0.00077	0.00009	0.00087	0.31625
D51	-2.06367	0.00001	0.00074	0.00008	0.00082	-2.06285
D52	2.54461	0.00001	0.00065	0.00047	0.00112	2.54573
D53	0.16262	0.00002	0.00060	0.00048	0.00108	0.16370
D54	2.55437	0.00000	0.00083	0.00031	0.00114	2.55551
D55	-1.65221	0.00000	0.00084	0.00029	0.00114	-1.65107
D56	0.44037	0.00000	0.00085	0.00028	0.00113	0.44150
D57	1.32799	0.00000	0.00086	0.00026	0.00112	1.32912
D58	-2.87859	0.00000	0.00088	0.00024	0.00112	-2.87747
D59	-0.78600	0.00000	0.00088	0.00023	0.00111	-0.78489
D60	-1.02005	0.00000	0.00077	0.00027	0.00104	-1.01901
D61	1.05655	0.00000	0.00078	0.00025	0.00103	1.05758
D62	-3.13405	0.00000	0.00078	0.00024	0.00103	-3.13302
D63	1.47380	-0.00001	-0.00043	0.00026	-0.00017	1.47363
D64	2.81994	0.00000	-0.00064	0.00012	-0.00052	2.81942
D65	2.25781	0.00000	0.00027	-0.00006	0.00021	2.25802

D66	-0.85873	-0.00001	0.00014	-0.00013	0.00001	-0.85872
D67	-1.93441	0.00000	0.00043	-0.00010	0.00033	-1.93408
D68	1.23223	-0.00001	0.00030	-0.00017	0.00013	1.23236
D69	0.10290	0.00000	0.00029	-0.00006	0.00023	0.10314
D70	-3.01364	0.00000	0.00017	-0.00013	0.00004	-3.01361
D71	2.92312	0.00001	0.00037	0.00036	0.00073	2.92385
D72	-0.19280	0.00000	0.00024	0.00029	0.00053	-0.19227
D73	-1.88330	-0.00002	-0.00153	-0.00065	-0.00218	-1.88548

Item	Value	Threshold	Converged?
Maximum Force	0.000038	0.000450	YES
RMS Force	0.000008	0.000300	YES
Maximum Displacement	0.004863	0.001800	NO
RMS Displacement	0.001424	0.001200	NO

Predicted change in Energy=-1.310127D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.847467	1.644912	1.538202
2	6	0	-1.504104	0.455257	1.574487
3	7	0	-2.364728	0.449689	0.484611
4	6	0	-2.228852	1.606475	-0.182389
5	7	0	-1.309348	2.354307	0.440104
6	6	0	-0.775476	3.645237	-0.031180
7	1	0	-0.075779	2.032489	2.179328
8	1	0	-1.352806	-0.415251	2.224524
9	1	0	-1.613213	4.259214	-0.366280
10	1	0	-0.325329	4.126982	0.834622
11	35	0	-0.392426	-2.431568	2.920970
12	1	0	-2.763962	1.879729	-1.075550
13	6	0	-3.249831	-0.603999	0.090591
14	6	0	-3.209607	-1.823439	0.611368
15	1	0	-3.943884	-0.296833	-0.681935
16	1	0	-3.917796	-2.558885	0.250804
17	1	0	-2.486377	-2.134866	1.367954
18	6	0	2.554767	-0.688363	1.130840
19	6	0	3.975186	-0.375485	1.315091
20	8	0	2.975708	0.654780	1.533072
21	1	0	2.170325	-0.730453	0.115652
22	1	0	1.982859	-1.227058	1.881800
23	1	0	4.431334	-0.691236	2.250511

24	6	0	4.916009	-0.173841	0.159315
25	1	0	5.677265	0.573253	0.402047
26	1	0	5.428838	-1.113701	-0.066559
27	1	0	4.375167	0.149626	-0.732592
28	6	0	0.257208	3.476061	-1.154993
29	1	0	0.708160	4.454878	-1.346712
30	1	0	-0.211324	3.136734	-2.079464
31	6	0	1.359663	2.483674	-0.803630
32	8	0	1.682864	1.572843	-1.528729
33	8	0	1.883162	2.733194	0.395476
34	1	0	2.456865	1.967355	0.702634

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.359327	0.000000			
3	N	2.200157	1.388716	0.000000		
4	C	2.206838	2.221976	1.342201	0.000000	
5	N	1.386504	2.220619	2.177929	1.338745	0.000000
6	C	2.543510	3.644865	3.606007	2.508330	1.474323
7	H	1.075528	2.212150	3.258313	3.224115	2.156423
8	H	2.229502	1.096915	2.190754	3.263136	3.294919
9	H	3.323852	4.271835	3.975081	2.729442	2.090756
10	H	2.632170	3.926636	4.219494	3.318232	2.065505
11	Br	4.328603	3.373811	4.257635	5.413786	5.468093
12	H	3.249583	3.261757	2.153719	1.076451	2.153679
13	C	3.595070	2.524189	1.431404	2.450124	3.555166
14	C	4.297463	3.004795	2.428374	3.654619	4.592807
15	H	4.276351	3.407287	2.100443	2.610261	3.902345
16	H	5.362483	4.082046	3.393849	4.515575	5.565905
17	H	4.123316	2.777814	2.734048	4.058019	4.732756
18	C	4.145516	4.240179	5.090599	5.465698	4.966522
19	C	5.233523	5.547976	6.447102	6.682866	6.011961
20	O	3.949311	4.484445	5.446246	5.562012	4.737582
21	H	4.095494	4.127413	4.700592	4.990272	4.661452
22	H	4.046852	3.883753	4.864682	5.479807	5.073785
23	H	5.816417	6.082835	7.113830	7.453627	6.745987
24	C	6.198938	6.604265	7.314624	7.371249	6.724986
25	H	6.709055	7.277403	8.043366	7.994735	7.210157
26	H	7.041108	7.295228	7.967914	8.127299	7.595192
27	H	5.887978	6.323121	6.855495	6.785145	6.208828
28	C	3.438999	4.435938	4.326867	3.259111	2.501353
29	H	4.317246	5.424434	5.370095	4.253832	3.416935
30	H	3.964557	4.713063	4.293232	3.164017	2.857634

31	C	3.325525	4.239231	4.434833	3.746046	2.947411
32	O	3.976660	4.586470	4.658112	4.137062	3.666104
33	O	3.153809	4.248839	4.823578	4.302566	3.215224
34	H	3.423558	4.328492	5.059506	4.782201	3.795131

		6	7	8	9	10
6	C	0.000000				
7	H	2.824337	0.000000			
8	H	4.680713	2.761209	0.000000		
9	H	1.091358	3.715121	5.350766	0.000000	
10	H	1.088266	2.501481	4.859981	1.765870	0.000000
11	Br	6.766792	4.536310	2.339424	7.553999	6.882726
12	H	2.856887	4.224203	4.260138	2.736647	3.826988
13	C	4.918665	4.624769	2.861467	5.151513	5.611458
14	C	6.020322	5.210332	2.834250	6.364192	6.616374
15	H	5.099236	5.345540	3.895537	5.127303	5.913038
16	H	6.960232	6.289755	3.881998	7.223460	7.612324
17	H	6.188243	4.882229	2.230643	6.682383	6.645698
18	C	5.587566	3.927102	4.066923	6.640176	5.618740
19	C	6.367688	4.791197	5.405197	7.452359	6.244797
20	O	5.045900	3.409883	4.512107	6.136586	4.841577
21	H	5.276928	4.115530	4.118149	6.280461	5.508165
22	H	5.916685	3.866673	3.450095	6.934319	5.923686
23	H	7.149964	5.266670	5.790780	8.239606	6.917067
24	C	6.856722	5.819475	6.604650	7.909422	6.813570
25	H	7.159793	6.195612	7.329425	8.205347	6.989081
26	H	7.819351	6.726316	7.192190	8.862761	7.835006
27	H	6.264216	5.642284	6.470958	7.272111	6.353754
28	C	1.535582	3.648627	5.399592	2.175747	2.172929
29	H	2.141803	4.349194	6.381180	2.527510	2.435947
30	H	2.184562	4.401708	5.695954	2.481986	3.079852
31	C	2.550437	3.340973	4.993092	3.490246	2.867670
32	O	3.546957	4.129622	5.220605	4.408174	4.017697
33	O	2.842923	2.740540	4.871305	3.890199	2.648193
34	H	3.715078	2.932432	4.744108	4.791736	3.524488

		11	12	13	14	15
11	Br	0.000000				
12	H	6.339056	0.000000			
13	C	4.417671	2.786549	0.000000		
14	C	3.693317	4.093622	1.326598	0.000000	
15	H	5.490980	2.506905	1.082985	2.131272	0.000000
16	H	4.424277	4.774080	2.072059	1.082783	2.446949
17	H	2.623836	4.707944	2.134965	1.092004	3.115243
18	C	3.863842	6.304929	5.897676	5.897987	6.758099
19	C	5.087471	7.497818	7.331609	7.362951	8.167372

20	O	4.774529	6.422556	6.513264	6.726755	7.327522
21	H	4.163087	5.707819	5.421688	5.512170	6.181239
22	H	2.858793	6.397683	5.565759	5.378789	6.524135
23	H	5.171744	8.333357	7.979546	7.896370	8.882515
24	C	6.395588	8.045122	8.177450	8.303683	8.900591
25	H	7.225999	8.668592	9.009770	9.206760	9.721038
26	H	6.674520	8.780698	8.695044	8.694023	9.428355
27	H	6.537662	7.353778	7.706242	7.951604	8.331176
28	C	7.206634	3.417903	5.522471	6.574461	5.666365
29	H	8.176034	4.331345	6.582079	7.655079	6.682978
30	H	7.486196	3.017262	5.285333	6.390117	5.260654
31	C	6.411089	4.176479	5.619679	6.436744	5.989461
32	O	6.335768	4.480381	5.629592	6.328587	5.989410
33	O	6.183137	4.948543	6.130042	6.837090	6.655549
34	H	5.691221	5.516036	6.289104	6.818163	6.929153

		16	17	18	19	20
16	H	0.000000				
17	H	1.864612	0.000000			
18	C	6.794659	5.249926	0.000000		
19	C	8.258276	6.697015	1.466094	0.000000	
20	O	7.713123	6.135451	1.463904	1.451867	0.000000
21	H	6.358195	5.022500	1.086359	2.195947	2.139297
22	H	6.265113	4.589359	1.086836	2.239577	2.156078
23	H	8.786064	7.121636	2.185218	1.087557	2.108393
24	C	9.150569	7.752531	2.604622	1.503870	2.517655
25	H	10.094472	8.655168	3.445694	2.151935	2.929893
26	H	9.463026	8.108713	3.142445	2.137059	3.421139
27	H	8.779313	7.530736	2.736506	2.151449	2.710517
28	C	7.471781	6.736099	5.276953	5.895684	4.751375
29	H	8.552450	7.810199	6.000095	6.410231	5.279742
30	H	7.183883	6.697039	5.708649	6.433161	5.419197
31	C	7.375013	6.390517	3.902853	4.416416	3.378851
32	O	7.183684	6.286529	3.598135	4.139811	3.448030
33	O	7.853543	6.613364	3.563546	3.858257	2.609136
34	H	7.831175	6.458058	2.691799	2.858199	1.637583

		21	22	23	24	25
21	H	0.000000				
22	H	1.844191	0.000000			
23	H	3.109876	2.533394	0.000000		
24	C	2.801875	3.560841	2.208100	0.000000	
25	H	3.752373	4.368000	2.562829	1.093883	0.000000
26	H	3.286029	3.960268	2.557792	1.094235	1.768367
27	H	2.520989	3.801768	3.099856	1.092080	1.778293
28	C	4.792631	5.858269	6.810811	6.062475	6.342530

29	H	5.582480	6.658269	7.299625	6.434217	6.543484
30	H	5.044395	6.288778	7.413253	6.500891	6.885116
31	C	3.439892	4.622709	5.370567	4.542822	4.872889
32	O	2.871720	4.422799	5.192571	4.043961	4.547782
33	O	3.486777	4.231157	4.654144	4.207705	4.365846
34	H	2.775755	3.437933	3.655483	3.305646	3.522051

		26	27	28	29	30
26	H	0.000000				
27	H	1.774772	0.000000			
28	C	6.999740	5.310478	0.000000		
29	H	7.411657	5.688522	1.094621	0.000000	
30	H	7.343665	5.636735	1.090555	1.766318	0.000000
31	C	5.481109	3.813934	1.524368	2.145936	2.126556
32	O	4.836091	3.147678	2.407158	3.047836	2.517342
33	O	5.252037	3.762639	2.366333	2.716624	3.267268
34	H	4.349389	3.007307	3.250456	3.666819	4.028244

		31	32	33	34
31	C	0.000000			
32	O	1.208238	0.000000		
33	O	1.331978	2.255903	0.000000	
34	H	1.933719	2.394514	1.004983	0.000000

Stoichiometry C11H17BrN2O3
Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.075588	1.329354	1.239316
2	6	0	-1.154387	1.256940	0.665132
3	7	0	-1.214638	2.288408	-0.262756
4	6	0	-0.053537	2.961355	-0.240560
5	7	0	0.751354	2.396805	0.668105
6	6	0	2.158955	2.753736	0.922836
7	1	0	0.534801	0.699185	1.980107
8	1	0	-1.940357	0.499370	0.772655
9	1	0	2.233734	3.841872	0.960660
10	1	0	2.402798	2.361359	1.908181
11	35	0	-3.070117	-1.498860	0.321413
12	1	0	0.190706	3.807306	-0.859801

13	6	0	-2.306718	2.601950	-1.133371
14	6	0	-3.348061	1.800419	-1.315074
15	1	0	-2.181690	3.556183	-1.630023
16	1	0	-4.128137	2.118955	-1.995101
17	1	0	-3.452389	0.825367	-0.834595
18	6	0	0.611261	-2.462704	-0.347711
19	6	0	1.586893	-3.514066	-0.044043
20	8	0	1.629610	-2.258632	0.683954
21	1	0	0.774120	-1.858174	-1.235515
22	1	0	-0.408991	-2.500463	0.024943
23	1	0	1.249299	-4.330331	0.590402
24	6	0	2.754998	-3.817769	-0.941217
25	1	0	3.622812	-4.137008	-0.356780
26	1	0	2.493134	-4.631604	-1.624188
27	1	0	3.030391	-2.942539	-1.533474
28	6	0	3.109118	2.180927	-0.138811
29	1	0	4.135322	2.362927	0.195816
30	1	0	2.977977	2.677332	-1.100941
31	6	0	2.918955	0.684779	-0.360341
32	8	0	2.771528	0.193478	-1.454292
33	8	0	2.906685	0.014106	0.790403
34	1	0	2.582591	-0.927254	0.653304

Rotational constants (GHZ): 0.3287417 0.2548547 0.1596103

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 538 symmetry adapted cartesian basis functions of A symmetry.

There are 519 symmetry adapted basis functions of A symmetry.

519 basis functions, 823 primitive gaussians, 538 cartesian basis functions

78 alpha electrons 78 beta electrons

nuclear repulsion energy 1572.9077503193 Hartrees.

NAtoms= 34 NActive= 34 NUniq= 34 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 519 RedAO= T EigKep= 3.53D-06 NBF= 519

NBsUse= 519 1.00D-06 EigRej= -1.00D+00 NBFU= 519

Initial guess from the checkpoint file: "./coohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000005 0.000017 -0.000167 Ang= 0.02 deg.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3338.90388346 A.U. after 9 cycles

NFock= 9 Conv=0.40D-08 -V/T= 2.0019

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000007084	0.000006334	0.000022093
2	6	0.000016564	-0.000002373	0.000000201
3	7	0.000021992	0.000031106	-0.000008496
4	6	0.000002175	-0.000018146	-0.000003853
5	7	-0.000016478	0.000003464	0.000001998
6	6	0.000020784	-0.000011963	-0.000009463
7	1	0.000000698	0.000000972	-0.000006954
8	1	-0.000015668	-0.000000028	-0.000017222
9	1	0.000002927	0.000001059	-0.000004795
10	1	-0.000002900	0.000004470	0.000002464
11	35	0.000002347	0.000001826	0.000009902
12	1	-0.000008574	0.000007564	0.000002505
13	6	-0.000025302	-0.000031408	-0.000008415
14	6	0.000003337	0.000025114	-0.000004620
15	1	0.000004034	0.000007096	-0.000004629
16	1	-0.000002809	-0.000002390	-0.000000278
17	1	-0.000005252	-0.000004550	-0.000000383
18	6	0.000000100	-0.000005871	-0.000004702
19	6	0.000008487	-0.000016079	-0.000028303
20	8	0.000014609	0.000036567	0.000010289
21	1	-0.000003297	-0.000006034	0.000006878
22	1	-0.000002317	0.000002475	0.000000828
23	1	-0.000010384	-0.000000618	0.000010906
24	6	0.000005564	-0.000001840	0.000025552
25	1	-0.000001258	-0.000003415	0.000004744
26	1	-0.000002485	-0.000003626	0.000004200
27	1	0.000001403	-0.000003919	0.000000306
28	6	0.000019359	-0.000001767	-0.000014308
29	1	-0.000002906	-0.000001736	0.000003940
30	1	0.000000706	-0.000000169	0.000001324
31	6	-0.000003200	0.000008505	-0.000025696
32	8	0.000000697	-0.000010045	0.000008698
33	8	0.000014327	0.000013129	0.000017943
34	1	-0.000030195	-0.000023702	0.000007346

Cartesian Forces: Max 0.000036567 RMS 0.000012050

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000032753 RMS 0.000006733

Search for a local minimum.

Step number 39 out of a maximum of 175

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 21 22 23 24 25
26 27 28 29 30
31 32 33 34 35
36 37 38 39

DE= 1.05D-07 DEPred=-1.31D-07 R=-8.01D-01

Trust test=-8.01D-01 RLast= 6.13D-03 DXMaxT set to 1.95D-01

ITU= -1 1 1 1 1 1 1 1 -1 1 1 1 1 1 -1 0 1 1 1 1

ITU= 1 1 1 1 1 1 0 0 -1 1 1 1 0 1 0 -1 0 1 0

Eigenvalues ---	0.00176	0.00258	0.00375	0.00404	0.00452
Eigenvalues ---	0.00554	0.00833	0.00952	0.01189	0.01240
Eigenvalues ---	0.01403	0.02015	0.02044	0.02209	0.02287
Eigenvalues ---	0.02377	0.02469	0.02632	0.03028	0.03146
Eigenvalues ---	0.03406	0.03613	0.03851	0.04333	0.04567
Eigenvalues ---	0.04865	0.05026	0.05281	0.05480	0.05732
Eigenvalues ---	0.05796	0.05964	0.06207	0.07490	0.09389
Eigenvalues ---	0.09634	0.11733	0.12580	0.12878	0.13114
Eigenvalues ---	0.13611	0.13981	0.15123	0.15665	0.15984
Eigenvalues ---	0.16005	0.16008	0.16043	0.16064	0.16203
Eigenvalues ---	0.16525	0.17660	0.19455	0.21238	0.22188
Eigenvalues ---	0.23307	0.23662	0.24042	0.25363	0.26513
Eigenvalues ---	0.28196	0.29098	0.29850	0.31538	0.32095
Eigenvalues ---	0.33359	0.34369	0.34507	0.34607	0.34747
Eigenvalues ---	0.34892	0.34902	0.34967	0.35088	0.35292
Eigenvalues ---	0.35332	0.35659	0.35794	0.35923	0.36619
Eigenvalues ---	0.37047	0.37263	0.38018	0.38585	0.39614
Eigenvalues ---	0.40808	0.45412	0.49307	0.50349	0.51037
Eigenvalues ---	0.54576	0.56036	0.56825	0.61442	0.90899
Eigenvalues ---	0.97604				

En-DIIS/RFO-DIIS IScMMF= 0 using points: 39 38 37 36 35

RFO step: Lambda=-1.70639101D-08.

DidBck=F Rises=F RFO-DIIS coefs: 1.34594 -0.24565 -0.34324 0.28410 -

0.04115

Iteration 1 RMS(Cart)= 0.00079446 RMS(Int)= 0.00000022

Iteration 2 RMS(Cart)= 0.00000033 RMS(Int)= 0.00000008

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56876	0.00000	-0.00001	0.00000	-0.00001	2.56874
R2	2.62011	0.00000	0.00000	0.00002	0.00002	2.62013
R3	2.03245	0.00000	0.00000	0.00000	0.00000	2.03246
R4	2.62429	0.00001	-0.00002	0.00000	-0.00001	2.62428
R5	2.07287	0.00000	-0.00003	0.00002	0.00000	2.07287
R6	2.53639	-0.00001	0.00001	-0.00002	-0.00001	2.53638
R7	2.70496	0.00003	0.00000	0.00003	0.00002	2.70499
R8	2.52986	0.00000	0.00000	0.00000	0.00000	2.52986
R9	2.03420	0.00000	0.00000	0.00000	0.00000	2.03420
R10	2.78607	0.00001	0.00001	0.00000	0.00001	2.78608
R11	2.06237	0.00000	0.00000	0.00000	0.00000	2.06237
R12	2.05653	0.00000	0.00000	0.00000	0.00000	2.05653
R13	2.90183	0.00001	-0.00002	0.00002	0.00000	2.90183
R14	4.42087	0.00001	0.00000	-0.00010	-0.00010	4.42077
R15	2.50691	-0.00001	0.00001	-0.00002	0.00000	2.50690
R16	2.04655	0.00000	0.00000	0.00000	0.00000	2.04654
R17	2.04616	0.00000	-0.00001	0.00001	0.00000	2.04616
R18	2.06359	0.00000	-0.00001	0.00000	0.00000	2.06358
R19	2.77052	0.00000	-0.00002	0.00000	-0.00002	2.77050
R20	2.76638	0.00001	0.00002	0.00001	0.00003	2.76641
R21	2.05292	0.00000	0.00000	0.00000	0.00000	2.05292
R22	2.05382	0.00000	0.00001	0.00000	0.00001	2.05383
R23	2.74363	0.00002	-0.00002	0.00002	-0.00001	2.74362
R24	2.05518	0.00000	0.00000	0.00000	0.00000	2.05519
R25	2.84190	-0.00001	0.00000	-0.00001	-0.00001	2.84189
R26	3.09458	-0.00001	0.00005	-0.00003	0.00002	3.09461
R27	2.06714	0.00000	-0.00001	0.00000	-0.00001	2.06713
R28	2.06780	0.00000	0.00000	0.00000	0.00000	2.06781
R29	2.06373	0.00000	0.00000	0.00000	0.00000	2.06373
R30	2.06853	0.00000	0.00000	-0.00001	-0.00001	2.06852
R31	2.06085	0.00000	0.00000	-0.00001	-0.00001	2.06085
R32	2.88064	-0.00001	0.00000	-0.00003	-0.00003	2.88061
R33	2.28324	0.00000	0.00000	0.00000	0.00000	2.28324
R34	2.51707	0.00002	0.00000	0.00002	0.00001	2.51709
R35	1.89914	0.00000	-0.00002	-0.00002	-0.00004	1.89910
A1	1.88389	0.00000	0.00000	-0.00001	-0.00001	1.88387
A2	2.27321	0.00001	-0.00002	0.00001	-0.00001	2.27320
A3	2.12557	0.00000	0.00002	0.00000	0.00002	2.12558
A4	1.85660	0.00000	0.00001	-0.00001	0.00000	1.85660

A5	2.27016	-0.00001	-0.00005	0.00007	0.00002	2.27018
A6	2.15002	0.00001	0.00004	-0.00006	-0.00001	2.15001
A7	1.90055	0.00000	-0.00001	0.00003	0.00002	1.90057
A8	2.21704	0.00001	-0.00001	-0.00005	-0.00006	2.21698
A9	2.16547	-0.00001	0.00002	0.00002	0.00004	2.16551
A10	1.89642	0.00000	0.00000	-0.00002	-0.00002	1.89640
A11	2.19049	0.00000	-0.00002	0.00002	0.00000	2.19049
A12	2.19622	0.00000	0.00002	0.00000	0.00002	2.19624
A13	1.88731	0.00000	-0.00001	0.00002	0.00001	1.88732
A14	2.19019	0.00000	-0.00006	0.00000	-0.00006	2.19013
A15	2.20086	0.00000	0.00004	-0.00002	0.00003	2.20089
A16	1.88893	-0.00001	0.00001	0.00001	0.00002	1.88895
A17	1.85779	-0.00001	-0.00001	-0.00002	-0.00004	1.85776
A18	1.96167	0.00002	-0.00004	0.00006	0.00001	1.96169
A19	1.88889	0.00000	0.00000	-0.00001	-0.00001	1.88888
A20	1.93209	-0.00001	-0.00001	-0.00001	-0.00002	1.93207
A21	1.93140	0.00000	0.00005	-0.00002	0.00003	1.93143
A22	2.73137	0.00001	0.00026	0.00022	0.00048	2.73185
A23	2.15298	0.00000	0.00003	-0.00006	-0.00003	2.15295
A24	1.96476	-0.00001	-0.00001	0.00001	0.00000	1.96476
A25	2.16540	0.00001	-0.00002	0.00005	0.00003	2.16543
A26	2.06440	0.00000	-0.00003	0.00002	0.00000	2.06439
A27	2.15822	0.00001	0.00001	0.00000	0.00001	2.15823
A28	2.06029	-0.00001	0.00002	-0.00003	-0.00001	2.06029
A29	2.05846	0.00001	0.00008	-0.00002	0.00006	2.05852
A30	2.12794	-0.00001	-0.00012	0.00005	-0.00007	2.12787
A31	1.97585	0.00001	0.00001	0.00003	0.00004	1.97589
A32	2.00009	-0.00001	0.00002	-0.00007	-0.00005	2.00004
A33	2.02670	0.00000	0.00002	0.00000	0.00002	2.02672
A34	2.04036	-0.00001	-0.00002	-0.00003	-0.00006	2.04030
A35	2.13903	0.00001	0.00003	0.00005	0.00008	2.13910
A36	1.94510	-0.00001	0.00001	-0.00007	-0.00006	1.94503
A37	2.03858	0.00001	0.00003	0.00004	0.00007	2.03865
A38	2.02368	0.00000	-0.00003	0.00000	-0.00003	2.02365
A39	2.10014	0.00000	-0.00021	-0.00013	-0.00034	2.09980
A40	2.36136	0.00001	0.00052	0.00023	0.00075	2.36211
A41	1.93522	0.00000	0.00000	0.00002	0.00002	1.93524
A42	1.91418	0.00000	-0.00002	0.00000	-0.00002	1.91416
A43	1.93645	0.00000	0.00000	0.00000	0.00000	1.93645
A44	1.88207	0.00000	0.00001	0.00001	0.00001	1.88208
A45	1.90031	0.00000	0.00001	0.00000	0.00001	1.90032
A46	1.89433	0.00000	-0.00001	-0.00002	-0.00003	1.89430
A47	1.88254	-0.00001	0.00003	-0.00004	-0.00001	1.88253
A48	1.94523	0.00000	-0.00002	-0.00002	-0.00004	1.94519

A49	1.97078	0.00000	0.00001	-0.00006	-0.00005	1.97072
A50	1.88258	0.00000	-0.00002	0.00005	0.00004	1.88261
A51	1.90135	0.00000	0.00000	0.00005	0.00005	1.90140
A52	1.87921	0.00000	0.00000	0.00002	0.00002	1.87923
A53	2.14826	0.00001	-0.00001	0.00004	0.00003	2.14829
A54	1.94958	0.00000	0.00001	-0.00005	-0.00004	1.94954
A55	2.18505	-0.00001	0.00000	0.00001	0.00000	2.18505
A56	1.93559	-0.00001	0.00006	-0.00006	0.00000	1.93558
A57	2.81350	0.00003	0.00007	0.00016	0.00023	2.81373
D1	0.00357	0.00000	-0.00003	-0.00001	-0.00004	0.00353
D2	3.02436	0.00000	0.00002	0.00002	0.00004	3.02440
D3	-3.10314	0.00000	0.00003	0.00003	0.00006	-3.10308
D4	-0.08234	0.00001	0.00008	0.00005	0.00014	-0.08221
D5	-0.00274	0.00000	0.00001	0.00008	0.00009	-0.00265
D6	-3.04401	0.00000	0.00022	0.00010	0.00032	-3.04369
D7	3.10753	0.00000	-0.00005	0.00005	0.00000	3.10753
D8	0.06626	0.00000	0.00016	0.00007	0.00023	0.06649
D9	-0.00318	0.00000	0.00005	-0.00007	-0.00002	-0.00320
D10	3.12170	0.00001	0.00012	0.00000	0.00011	3.12181
D11	-3.03436	0.00000	0.00001	-0.00011	-0.00009	-3.03445
D12	0.09052	0.00000	0.00008	-0.00004	0.00004	0.09056
D13	-1.48427	0.00000	-0.00030	0.00064	0.00035	-1.48392
D14	1.51873	0.00001	-0.00024	0.00068	0.00044	1.51916
D15	0.00152	0.00000	-0.00005	0.00012	0.00008	0.00159
D16	3.13217	0.00001	-0.00006	0.00010	0.00004	3.13221
D17	-3.12396	0.00000	-0.00011	0.00006	-0.00005	-3.12402
D18	0.00668	0.00000	-0.00013	0.00004	-0.00009	0.00659
D19	-0.19413	0.00000	0.00025	-0.00003	0.00023	-0.19391
D20	2.95723	0.00000	0.00028	-0.00003	0.00025	2.95748
D21	2.92837	0.00001	0.00033	0.00005	0.00038	2.92875
D22	-0.20345	0.00000	0.00036	0.00004	0.00040	-0.20305
D23	0.00073	0.00000	0.00003	-0.00012	-0.00010	0.00063
D24	3.04122	0.00000	-0.00020	-0.00015	-0.00034	3.04088
D25	-3.12988	-0.00001	0.00004	-0.00010	-0.00006	-3.12994
D26	-0.08938	-0.00001	-0.00018	-0.00013	-0.00031	-0.08969
D27	-2.46942	0.00000	-0.00029	0.00008	-0.00021	-2.46963
D28	-0.44245	-0.00001	-0.00028	0.00006	-0.00022	-0.44267
D29	1.67464	0.00000	-0.00026	0.00005	-0.00021	1.67443
D30	0.79024	0.00000	-0.00003	0.00010	0.00007	0.79031
D31	2.81721	-0.00001	-0.00003	0.00009	0.00006	2.81727
D32	-1.34888	0.00000	0.00000	0.00008	0.00007	-1.34881
D33	-3.00063	0.00000	0.00002	0.00006	0.00008	-3.00055
D34	1.21916	0.00000	0.00004	0.00003	0.00007	1.21923
D35	-0.89876	-0.00001	0.00005	0.00006	0.00011	-0.89865

D36	1.16798	0.00000	0.00004	0.00002	0.00006	1.16804
D37	-0.89541	0.00000	0.00005	-0.00001	0.00004	-0.89537
D38	-3.01333	0.00000	0.00007	0.00002	0.00009	-3.01324
D39	-0.92621	0.00000	0.00001	0.00005	0.00006	-0.92614
D40	-2.98960	0.00000	0.00003	0.00002	0.00005	-2.98955
D41	1.17567	0.00000	0.00004	0.00005	0.00009	1.17576
D42	-3.13967	0.00000	0.00003	0.00000	0.00003	-3.13964
D43	-0.02380	0.00000	0.00001	-0.00001	0.00001	-0.02379
D44	-0.00897	0.00000	0.00000	0.00001	0.00000	-0.00897
D45	3.10690	0.00000	-0.00002	0.00000	-0.00002	3.10688
D46	-2.75247	0.00000	0.00000	-0.00002	-0.00003	-2.75250
D47	-0.04766	0.00000	-0.00007	0.00002	-0.00005	-0.04771
D48	-0.01971	0.00000	-0.00005	0.00004	-0.00001	-0.01972
D49	2.68510	0.00000	-0.00011	0.00008	-0.00003	2.68507
D50	0.31625	0.00000	0.00058	0.00035	0.00093	0.31718
D51	-2.06285	0.00001	0.00052	0.00039	0.00091	-2.06193
D52	2.54573	0.00001	0.00051	0.00028	0.00078	2.54651
D53	0.16370	0.00001	0.00051	0.00031	0.00082	0.16452
D54	2.55551	0.00000	0.00044	0.00007	0.00051	2.55603
D55	-1.65107	0.00000	0.00044	0.00009	0.00053	-1.65054
D56	0.44150	0.00000	0.00043	0.00006	0.00049	0.44199
D57	1.32912	0.00000	0.00039	0.00003	0.00043	1.32955
D58	-2.87747	0.00000	0.00040	0.00005	0.00045	-2.87702
D59	-0.78489	0.00000	0.00038	0.00002	0.00040	-0.78449
D60	-1.01901	0.00000	0.00038	0.00010	0.00048	-1.01853
D61	1.05758	0.00000	0.00038	0.00012	0.00050	1.05809
D62	-3.13302	0.00000	0.00037	0.00009	0.00046	-3.13257
D63	1.47363	0.00001	0.00054	0.00049	0.00103	1.47466
D64	2.81942	0.00001	0.00054	0.00044	0.00098	2.82039
D65	2.25802	0.00000	-0.00015	-0.00045	-0.00061	2.25742
D66	-0.85872	0.00000	-0.00019	-0.00030	-0.00049	-0.85921
D67	-1.93408	-0.00001	-0.00011	-0.00051	-0.00062	-1.93469
D68	1.23236	0.00000	-0.00014	-0.00035	-0.00050	1.23187
D69	0.10314	0.00000	-0.00013	-0.00041	-0.00054	0.10260
D70	-3.01361	0.00000	-0.00016	-0.00025	-0.00042	-3.01402
D71	2.92385	0.00001	0.00011	-0.00009	0.00002	2.92387
D72	-0.19227	0.00001	0.00008	0.00006	0.00014	-0.19213
D73	-1.88548	0.00001	-0.00037	-0.00020	-0.00058	-1.88605

Item	Value	Threshold	Converged?
Maximum Force	0.000033	0.000450	YES
RMS Force	0.000007	0.000300	YES
Maximum Displacement	0.003845	0.001800	NO
RMS Displacement	0.000794	0.001200	YES

Predicted change in Energy=-3.839943D-08

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.847435	1.644891	1.538082
2	6	0	-1.503926	0.455158	1.574248
3	7	0	-2.364854	0.449770	0.484621
4	6	0	-2.229334	1.606740	-0.182123
5	7	0	-1.309682	2.354485	0.440256
6	6	0	-0.775771	3.645406	-0.031031
7	1	0	-0.075574	2.032365	2.179064
8	1	0	-1.352405	-0.415483	2.224052
9	1	0	-1.613501	4.259515	-0.365911
10	1	0	-0.325419	4.127008	0.834746
11	35	0	-0.392144	-2.431663	2.920885
12	1	0	-2.764768	1.880163	-1.075041
13	6	0	-3.250027	-0.603920	0.090717
14	6	0	-3.209710	-1.823350	0.611506
15	1	0	-3.944171	-0.296754	-0.681726
16	1	0	-3.917926	-2.558817	0.251037
17	1	0	-2.486374	-2.134763	1.367994
18	6	0	2.555029	-0.688123	1.130024
19	6	0	3.975382	-0.375563	1.315246
20	8	0	2.976018	0.654988	1.532373
21	1	0	2.171253	-0.730293	0.114589
22	1	0	1.982504	-1.226555	1.880711
23	1	0	4.430723	-0.691277	2.251073
24	6	0	4.917182	-0.174373	0.160196
25	1	0	5.678747	0.572195	0.403563
26	1	0	5.429549	-1.114548	-0.065425
27	1	0	4.377202	0.149531	-0.732075
28	6	0	0.256665	3.476238	-1.155076
29	1	0	0.707722	4.455013	-1.346730
30	1	0	-0.212135	3.137108	-2.079480
31	6	0	1.358971	2.483595	-0.804025
32	8	0	1.681497	1.572426	-1.529002
33	8	0	1.883081	2.733253	0.394792
34	1	0	2.456702	1.967345	0.701861

Distance matrix (angstroms):

	1	2	3	4	5

1	C	0.000000				
2	C	1.359321	0.000000			
3	N	2.200149	1.388710	0.000000		
4	C	2.206854	2.221981	1.342197	0.000000	
5	N	1.386513	2.220611	2.177911	1.338745	0.000000
6	C	2.543484	3.644834	3.605991	2.508353	1.474330
7	H	1.075529	2.212142	3.258304	3.224134	2.156440
8	H	2.229504	1.096913	2.190739	3.263138	3.294917
9	H	3.323899	4.271926	3.975184	2.729513	2.090777
10	H	2.632126	3.926605	4.219474	3.318232	2.065486
11	Br	4.328709	3.373903	4.257890	5.414114	5.468328
12	H	3.249604	3.261763	2.153718	1.076453	2.153690
13	C	3.595061	2.524160	1.431417	2.450158	3.555177
14	C	4.297392	3.004691	2.428365	3.654655	4.592792
15	H	4.276366	3.407285	2.100454	2.610279	3.902364
16	H	5.362421	4.081951	3.393846	4.515621	5.565903
17	H	4.123206	2.777667	2.734031	4.058051	4.732721
18	C	4.145627	4.240229	5.090835	5.466101	4.966813
19	C	5.233685	5.547972	6.447458	6.683573	6.012543
20	O	3.949523	4.484594	5.446541	5.562465	4.737957
21	H	4.096377	4.128297	4.701674	4.991485	4.662491
22	H	4.046128	3.882946	4.864017	5.479272	5.073189
23	H	5.815926	6.082143	7.113523	7.453703	6.745960
24	C	6.199927	6.605034	7.315931	7.373075	6.726618
25	H	6.710354	7.278392	8.044941	7.996940	7.212214
26	H	7.041751	7.295586	7.968837	8.128808	7.596521
27	H	5.889528	6.324571	6.857537	6.787653	6.211025
28	C	3.438891	4.435744	4.326717	3.259119	2.501371
29	H	4.317110	5.424237	5.369967	4.253854	3.416937
30	H	3.964476	4.712888	4.293087	3.164030	2.857652
31	C	3.325225	4.238741	4.434403	3.745874	2.947306
32	O	3.975896	4.585343	4.657036	4.136407	3.665616
33	O	3.153944	4.248841	4.823621	4.302769	3.215473
34	H	3.423531	4.328319	5.059410	4.782300	3.795255

		6	7	8	9	10
6	C	0.000000				
7	H	2.824304	0.000000			
8	H	4.680676	2.761210	0.000000		
9	H	1.091359	3.715146	5.350858	0.000000	
10	H	1.088268	2.501428	4.859948	1.765868	0.000000
11	Br	6.766960	4.536305	2.339372	7.554244	6.882775
12	H	2.856947	4.224230	4.260138	2.736712	3.827012
13	C	4.918693	4.624753	2.861398	5.151672	5.611470
14	C	6.020316	5.210238	2.834074	6.364312	6.616323

15	H	5.099293	5.345554	3.895497	5.127509	5.913097
16	H	6.960250	6.289666	3.881825	7.223617	7.612297
17	H	6.188197	4.882083	2.230391	6.682448	6.645588
18	C	5.587643	3.927036	4.066850	6.640300	5.618688
19	C	6.368211	4.791090	5.404890	7.452909	6.245071
20	O	5.046063	3.409926	4.512158	6.136756	4.841600
21	H	5.277584	4.116135	4.118871	6.281196	5.508663
22	H	5.915982	3.865910	3.449252	6.933651	5.922937
23	H	7.149994	5.265941	5.789763	8.239636	6.916845
24	C	6.858352	5.820063	6.604949	7.911129	6.814819
25	H	7.162004	6.196508	7.329855	8.207636	6.990896
26	H	7.820764	6.726602	7.192030	8.864276	7.836062
27	H	6.266238	5.643316	6.471964	7.274240	6.355305
28	C	1.535585	3.648512	5.399362	2.175735	2.172951
29	H	2.141794	4.349023	6.380936	2.527510	2.435941
30	H	2.184536	4.401625	5.695744	2.481924	3.079846
31	C	2.550382	3.340711	4.992541	3.490190	2.867673
32	O	3.546735	4.128994	5.219363	4.407974	4.017575
33	O	2.843035	2.740657	4.871252	3.890274	2.648318
34	H	3.715091	2.932367	4.743862	4.791736	3.524486

		11	12	13	14	15
11	Br	0.000000				
12	H	6.339449	0.000000			
13	C	4.417917	2.786600	0.000000		
14	C	3.693501	4.093706	1.326596	0.000000	
15	H	5.491224	2.506922	1.082985	2.131286	0.000000
16	H	4.424409	4.774180	2.072055	1.082783	2.446971
17	H	2.624008	4.708031	2.134966	1.092001	3.115254
18	C	3.864317	6.305446	5.897960	5.898289	6.758344
19	C	5.087328	7.498760	7.331996	7.363212	8.167829
20	O	4.774924	6.423106	6.513591	6.727064	7.327828
21	H	4.164248	5.709115	5.422805	5.513298	6.182272
22	H	2.858881	6.397246	5.565172	5.378302	6.523503
23	H	5.170845	8.333693	7.979267	7.895947	8.882332
24	C	6.395757	8.047315	8.178792	8.304768	8.902100
25	H	7.226049	8.671216	9.011333	9.207960	9.722833
26	H	6.674200	8.782622	8.695986	8.694678	9.429488
27	H	6.538604	7.356660	7.708392	7.953534	8.333484
28	C	7.206782	3.418028	5.522371	6.574360	5.666265
29	H	8.176096	4.331496	6.582009	7.654986	6.682936
30	H	7.486472	3.017407	5.285247	6.390071	5.260534
31	C	6.411016	4.176458	5.619269	6.436331	5.989042
32	O	6.335156	4.479961	5.628490	6.327478	5.988310
33	O	6.183377	4.948805	6.130089	6.837113	6.655577

34	H	5.691332	5.516224	6.289011	6.818046	6.929043
		16	17	18	19	20
16	H	0.000000				
17	H	1.864607	0.000000			
18	C	6.794944	5.250251	0.000000		
19	C	8.258538	6.697153	1.466085	0.000000	
20	O	7.713419	6.135752	1.463920	1.451863	0.000000
21	H	6.359262	5.023648	1.086357	2.195973	2.139337
22	H	6.264650	4.588964	1.086841	2.239531	2.156064
23	H	8.785658	7.121075	2.185175	1.087559	2.108347
24	C	9.151664	7.753356	2.604663	1.503863	2.517702
25	H	10.095673	8.656034	3.445832	2.151943	2.930155
26	H	9.463686	8.109091	3.142260	2.137043	3.421115
27	H	8.781276	7.532394	2.736675	2.151443	2.710448
28	C	7.471697	6.735984	5.276937	5.896416	4.751496
29	H	8.552385	7.810065	5.999892	6.410786	5.279639
30	H	7.183854	6.697004	5.708809	6.434153	5.419476
31	C	7.374600	6.390116	3.902678	4.417205	3.378965
32	O	7.182565	6.285458	3.597716	4.140811	3.448114
33	O	7.853557	6.613383	3.563410	3.858716	2.609173
34	H	7.831045	6.457942	2.691561	2.858644	1.637596
		21	22	23	24	25
21	H	0.000000				
22	H	1.844204	0.000000			
23	H	3.109871	2.533272	0.000000		
24	C	2.802009	3.560841	2.208076	0.000000	
25	H	3.752665	4.368028	2.562659	1.093879	0.000000
26	H	3.285811	3.960064	2.557924	1.094236	1.768375
27	H	2.521337	3.801952	3.099838	1.092080	1.778296
28	C	4.792974	5.857541	6.811227	6.064431	6.345218
29	H	5.582542	6.657451	7.299947	6.435961	6.546059
30	H	5.044924	6.288172	7.413930	6.503226	6.888161
31	C	3.439874	4.621884	5.371136	4.544819	4.875672
32	O	2.871196	4.421656	5.193416	4.046524	4.551184
33	O	3.486790	4.230593	4.654424	4.208930	4.367759
34	H	2.775539	3.437375	3.655830	3.306708	3.523776
		26	27	28	29	30
26	H	0.000000				
27	H	1.774754	0.000000			
28	C	7.001528	5.312696	0.000000		
29	H	7.413326	5.690348	1.094616	0.000000	
30	H	7.345855	5.639426	1.090553	1.766334	0.000000
31	C	5.482861	3.816117	1.524354	2.145959	2.126555
32	O	4.838366	3.150643	2.407170	3.048076	2.517359

33	O	5.253075	3.763786	2.366295	2.716400	3.267270
34	H	4.350242	3.008146	3.250406	3.666626	4.028262

		31	32	33	34
31	C	0.000000			
32	O	1.208240	0.000000		
33	O	1.331985	2.255912	0.000000	
34	H	1.933706	2.394504	1.004961	0.000000

Stoichiometry C11H17BrN2O3
Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.075624	1.329366	1.239226
2	6	0	-1.154275	1.256795	0.664913
3	7	0	-1.214702	2.288485	-0.262707
4	6	0	-0.053794	2.961746	-0.240230
5	7	0	0.751185	2.397113	0.668305
6	6	0	2.158802	2.754035	0.923001
7	1	0	0.534941	0.699085	1.979859
8	1	0	-1.940101	0.499045	0.772204
9	1	0	2.233576	3.842165	0.961038
10	1	0	2.402691	2.361470	1.908262
11	35	0	-3.069978	-1.499170	0.321456
12	1	0	0.190262	3.807946	-0.859208
13	6	0	-2.306885	2.601999	-1.133224
14	6	0	-3.348164	1.800376	-1.314869
15	1	0	-2.181959	3.556263	-1.629842
16	1	0	-4.128318	2.118858	-1.994831
17	1	0	-3.452363	0.825293	-0.834429
18	6	0	0.611928	-2.462591	-0.348121
19	6	0	1.586915	-3.514334	-0.043751
20	8	0	1.630243	-2.258557	0.683610
21	1	0	0.775208	-1.858597	-1.236210
22	1	0	-0.408386	-2.499630	0.024453
23	1	0	1.248719	-4.330032	0.591107
24	6	0	2.754972	-3.819303	-0.940546
25	1	0	3.622347	-4.139217	-0.355835
26	1	0	2.492515	-4.633029	-1.623422

27	1	0	3.031310	-2.944460	-1.532936
28	6	0	3.108917	2.181471	-0.138825
29	1	0	4.135129	2.363369	0.195818
30	1	0	2.977714	2.678131	-1.100812
31	6	0	2.918632	0.685402	-0.360691
32	8	0	2.770517	0.194395	-1.454683
33	8	0	2.906954	0.014437	0.789897
34	1	0	2.582809	-0.926872	0.652727

Rotational constants (GHZ): 0.3286683 0.2548718 0.1595970

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 538 symmetry adapted cartesian basis functions of A symmetry.

There are 519 symmetry adapted basis functions of A symmetry.

519 basis functions, 823 primitive gaussians, 538 cartesian basis functions

78 alpha electrons 78 beta electrons

nuclear repulsion energy 1572.8728623223 Hartrees.

NAtoms= 34 NActive= 34 NUniq= 34 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 519 RedAO= T EigKep= 3.52D-06 NBF= 519

NBsUse= 519 1.00D-06 EigRej= -1.00D+00 NBFU= 519

Initial guess from the checkpoint file: "./coohpo.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000003 -0.000019 -0.000031 Ang= 0.00 deg.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3338.90388354 A.U. after 9 cycles

NFock= 9 Conv=0.22D-08 -V/T= 2.0019

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000002622	0.000002624	0.000010627
2	6	0.000014421	-0.000000353	-0.000000040
3	7	0.000003686	0.000022572	-0.000003190
4	6	0.000011353	-0.000023526	-0.000008326

5	7	-0.000010067	0.000013105	0.000003983
6	6	0.000010577	-0.000008852	-0.000001749
7	1	-0.000000192	0.000002556	-0.000007345
8	1	-0.000013304	-0.000002095	-0.000009936
9	1	0.000001833	-0.000000242	-0.000003771
10	1	-0.000000856	0.000006553	-0.000000601
11	35	0.000002190	0.000005105	0.000006279
12	1	-0.000005515	0.000007279	0.000002645
13	6	-0.000017056	-0.000021328	-0.000008021
14	6	0.000001764	0.000022431	-0.000007987
15	1	0.000003176	0.000005764	-0.000003717
16	1	-0.000002810	-0.000002768	0.000000531
17	1	-0.000005512	-0.000005792	0.000000310
18	6	-0.000004156	-0.000007713	0.000005305
19	6	0.000012239	-0.000014378	-0.000014815
20	8	0.000002967	0.000031663	-0.000000199
21	1	-0.000002685	-0.000000332	0.000004142
22	1	0.000000367	-0.000003450	0.000000143
23	1	-0.000008007	-0.000003263	0.000008051
24	6	-0.000000234	-0.000002264	0.000020268
25	1	-0.000002885	-0.000001968	0.000004601
26	1	-0.000000874	-0.000002599	0.000005146
27	1	0.000001554	-0.000004753	-0.000000335
28	6	0.000015251	-0.000003927	-0.000017886
29	1	-0.000001665	-0.000000370	0.000003648
30	1	0.000001360	-0.000000285	-0.000000900
31	6	-0.000005613	0.000000075	-0.000019404
32	8	0.000001268	-0.000001347	0.000010126
33	8	0.000010075	0.000012768	0.000013588
34	1	-0.000010030	-0.000020894	0.000008833

Cartesian Forces: Max 0.000031663 RMS 0.000009248

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000019535 RMS 0.000005168

Search for a local minimum.

Step number 40 out of a maximum of 175

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 21 22 23 24 25

26 27 28 29 30
31 32 33 34 35
36 37 38 39 40

DE= -7.27D-08 DEPred=-3.84D-08 R= 1.89D+00

Trust test= 1.89D+00 RLast= 3.39D-03 DXMaxT set to 1.95D-01

ITU= 0 -1 1 1 1 1 1 1 1 -1 1 1 1 1 1 -1 0 1 1 1

ITU= 1 1 1 1 1 1 1 0 0 -1 1 1 1 0 1 0 -1 0 1 0

Eigenvalues --- 0.00162 0.00266 0.00356 0.00413 0.00471

Eigenvalues --- 0.00562 0.00892 0.00918 0.01068 0.01201

Eigenvalues --- 0.01402 0.01760 0.02053 0.02212 0.02289

Eigenvalues --- 0.02364 0.02401 0.02643 0.03010 0.03144

Eigenvalues --- 0.03390 0.03661 0.03813 0.04309 0.04456

Eigenvalues --- 0.04923 0.05029 0.05272 0.05503 0.05696

Eigenvalues --- 0.05789 0.05957 0.06188 0.07310 0.09350

Eigenvalues --- 0.09605 0.11776 0.12499 0.12756 0.12901

Eigenvalues --- 0.13578 0.14340 0.15001 0.15672 0.15881

Eigenvalues --- 0.16000 0.16007 0.16040 0.16050 0.16107

Eigenvalues --- 0.16356 0.17722 0.19454 0.21173 0.21991

Eigenvalues --- 0.23298 0.23725 0.24151 0.25358 0.26305

Eigenvalues --- 0.28409 0.28991 0.29975 0.31406 0.32016

Eigenvalues --- 0.33396 0.34386 0.34506 0.34608 0.34749

Eigenvalues --- 0.34879 0.34909 0.34969 0.35096 0.35333

Eigenvalues --- 0.35464 0.35682 0.35815 0.35920 0.36643

Eigenvalues --- 0.36995 0.37265 0.37835 0.38408 0.39664

Eigenvalues --- 0.40393 0.45352 0.49188 0.50482 0.50976

Eigenvalues --- 0.54751 0.55914 0.56886 0.61366 0.91079

Eigenvalues --- 0.97009

En-DIIS/RFO-DIIS IScMMF= 0 using points: 40 39 38 37 36

RFO step: Lambda=-1.04322298D-08.

DidBck=F Rises=F RFO-DIIS coefs: 1.56704 -0.32960 -0.40320 0.10966 0.05611

Iteration 1 RMS(Cart)= 0.00069128 RMS(Int)= 0.00000016

Iteration 2 RMS(Cart)= 0.00000027 RMS(Int)= 0.00000002

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56874	0.00000	-0.00001	0.00000	-0.00001	2.56874
R2	2.62013	0.00000	0.00001	0.00000	0.00001	2.62014
R3	2.03246	0.00000	0.00000	0.00000	0.00000	2.03245
R4	2.62428	0.00001	-0.00002	0.00001	0.00000	2.62428
R5	2.07287	0.00000	-0.00003	0.00002	-0.00001	2.07286
R6	2.53638	-0.00001	-0.00001	-0.00001	-0.00002	2.53637
R7	2.70499	0.00002	0.00004	0.00001	0.00005	2.70504
R8	2.52986	0.00000	0.00000	0.00001	0.00001	2.52987
R9	2.03420	0.00000	0.00000	0.00000	0.00000	2.03420

R10	2.78608	0.00000	0.00002	-0.00001	0.00000	2.78608
R11	2.06237	0.00000	0.00000	0.00000	0.00000	2.06237
R12	2.05653	0.00000	0.00000	0.00000	0.00001	2.05654
R13	2.90183	0.00001	-0.00001	0.00004	0.00003	2.90187
R14	4.42077	0.00000	0.00003	-0.00036	-0.00033	4.42044
R15	2.50690	-0.00001	-0.00001	0.00000	-0.00001	2.50689
R16	2.04654	0.00000	0.00000	0.00000	0.00000	2.04654
R17	2.04616	0.00000	0.00000	0.00000	0.00000	2.04617
R18	2.06358	0.00000	0.00000	-0.00001	-0.00001	2.06357
R19	2.77050	0.00000	-0.00002	0.00000	-0.00002	2.77047
R20	2.76641	0.00001	0.00003	0.00002	0.00005	2.76646
R21	2.05292	0.00000	-0.00001	0.00000	0.00000	2.05292
R22	2.05383	0.00000	0.00001	0.00000	0.00001	2.05384
R23	2.74362	0.00002	0.00002	0.00002	0.00004	2.74367
R24	2.05519	0.00000	0.00001	0.00000	0.00001	2.05519
R25	2.84189	-0.00001	-0.00002	-0.00002	-0.00004	2.84185
R26	3.09461	-0.00001	0.00001	-0.00003	-0.00003	3.09458
R27	2.06713	0.00000	-0.00001	0.00000	-0.00001	2.06712
R28	2.06781	0.00000	0.00000	0.00000	0.00000	2.06781
R29	2.06373	0.00000	0.00000	0.00001	0.00001	2.06374
R30	2.06852	0.00000	-0.00001	-0.00001	-0.00001	2.06851
R31	2.06085	0.00000	0.00000	0.00000	0.00000	2.06084
R32	2.88061	0.00000	-0.00002	-0.00001	-0.00003	2.88058
R33	2.28324	-0.00001	0.00000	0.00000	0.00000	2.28324
R34	2.51709	0.00002	0.00002	0.00002	0.00004	2.51713
R35	1.89910	0.00001	-0.00001	0.00001	-0.00001	1.89909
A1	1.88387	0.00000	-0.00001	0.00001	0.00000	1.88387
A2	2.27320	0.00000	0.00000	0.00002	0.00002	2.27322
A3	2.12558	0.00000	0.00001	-0.00003	-0.00002	2.12556
A4	1.85660	0.00000	0.00001	0.00000	0.00001	1.85660
A5	2.27018	-0.00001	-0.00001	0.00002	0.00001	2.27018
A6	2.15001	0.00001	0.00002	-0.00001	0.00000	2.15002
A7	1.90057	0.00000	0.00001	-0.00001	0.00000	1.90057
A8	2.21698	0.00002	-0.00004	0.00002	-0.00002	2.21696
A9	2.16551	-0.00001	0.00003	-0.00001	0.00002	2.16553
A10	1.89640	0.00000	-0.00001	0.00002	0.00001	1.89641
A11	2.19049	0.00000	0.00000	0.00001	0.00001	2.19050
A12	2.19624	0.00000	0.00001	-0.00002	-0.00001	2.19622
A13	1.88732	0.00000	0.00001	-0.00002	-0.00001	1.88731
A14	2.19013	0.00000	-0.00006	0.00000	-0.00005	2.19007
A15	2.20089	0.00000	0.00003	0.00001	0.00003	2.20092
A16	1.88895	0.00000	0.00000	-0.00001	0.00000	1.88894
A17	1.85776	0.00000	-0.00003	0.00003	0.00000	1.85776
A18	1.96169	0.00001	0.00001	0.00001	0.00001	1.96170

A19	1.88888	0.00000	-0.00001	-0.00001	-0.00003	1.88886
A20	1.93207	0.00000	-0.00002	0.00000	-0.00002	1.93205
A21	1.93143	0.00000	0.00005	-0.00001	0.00003	1.93146
A22	2.73185	0.00000	0.00016	0.00030	0.00046	2.73230
A23	2.15295	0.00001	-0.00002	0.00003	0.00000	2.15296
A24	1.96476	-0.00001	-0.00001	-0.00003	-0.00004	1.96472
A25	2.16543	0.00000	0.00004	0.00000	0.00003	2.16546
A26	2.06439	0.00000	-0.00001	0.00002	0.00001	2.06441
A27	2.15823	0.00001	0.00002	0.00004	0.00006	2.15829
A28	2.06029	-0.00001	-0.00001	-0.00006	-0.00007	2.06022
A29	2.05852	0.00001	0.00010	-0.00001	0.00009	2.05861
A30	2.12787	-0.00001	-0.00010	-0.00003	-0.00013	2.12774
A31	1.97589	0.00000	0.00003	-0.00003	-0.00001	1.97589
A32	2.00004	0.00000	-0.00003	0.00006	0.00003	2.00006
A33	2.02672	0.00000	0.00000	0.00002	0.00002	2.02673
A34	2.04030	-0.00001	-0.00007	-0.00003	-0.00010	2.04020
A35	2.13910	0.00001	0.00010	0.00001	0.00012	2.13922
A36	1.94503	0.00000	-0.00006	0.00000	-0.00007	1.94497
A37	2.03865	0.00000	0.00006	-0.00001	0.00006	2.03871
A38	2.02365	0.00000	-0.00003	0.00002	-0.00002	2.02363
A39	2.09980	0.00001	-0.00024	0.00003	-0.00021	2.09959
A40	2.36211	0.00001	0.00043	0.00012	0.00056	2.36267
A41	1.93524	0.00000	0.00001	0.00000	0.00000	1.93524
A42	1.91416	0.00000	-0.00002	0.00000	-0.00002	1.91414
A43	1.93645	0.00000	0.00002	0.00001	0.00004	1.93648
A44	1.88208	0.00000	0.00001	0.00001	0.00002	1.88210
A45	1.90032	0.00000	0.00001	-0.00001	0.00000	1.90032
A46	1.89430	0.00000	-0.00003	-0.00001	-0.00004	1.89426
A47	1.88253	-0.00001	-0.00003	-0.00002	-0.00005	1.88248
A48	1.94519	0.00000	-0.00004	0.00000	-0.00003	1.94516
A49	1.97072	0.00000	-0.00003	-0.00005	-0.00007	1.97065
A50	1.88261	0.00000	0.00002	0.00003	0.00005	1.88266
A51	1.90140	0.00000	0.00004	0.00004	0.00008	1.90149
A52	1.87923	0.00000	0.00002	0.00001	0.00003	1.87926
A53	2.14829	0.00000	0.00002	0.00001	0.00002	2.14832
A54	1.94954	0.00001	-0.00001	0.00003	0.00002	1.94956
A55	2.18505	-0.00001	-0.00001	-0.00004	-0.00004	2.18501
A56	1.93558	-0.00001	-0.00001	-0.00008	-0.00008	1.93550
A57	2.81373	0.00002	0.00020	0.00001	0.00021	2.81394
D1	0.00353	0.00000	-0.00004	0.00000	-0.00004	0.00348
D2	3.02440	0.00000	0.00008	0.00003	0.00011	3.02451
D3	-3.10308	0.00000	0.00012	-0.00002	0.00010	-3.10298
D4	-0.08221	0.00000	0.00024	0.00001	0.00025	-0.08196
D5	-0.00265	0.00000	0.00006	-0.00007	-0.00001	-0.00266

D6	-3.04369	0.00000	0.00029	0.00003	0.00033	-3.04336
D7	3.10753	0.00000	-0.00008	-0.00005	-0.00013	3.10739
D8	0.06649	0.00000	0.00015	0.00005	0.00020	0.06669
D9	-0.00320	0.00000	0.00001	0.00007	0.00008	-0.00312
D10	3.12181	0.00000	0.00014	0.00001	0.00015	3.12197
D11	-3.03445	0.00000	-0.00010	0.00004	-0.00006	-3.03451
D12	0.09056	0.00000	0.00004	-0.00002	0.00001	0.09058
D13	-1.48392	0.00001	0.00005	0.00042	0.00047	-1.48345
D14	1.51916	0.00001	0.00018	0.00046	0.00065	1.51981
D15	0.00159	0.00000	0.00003	-0.00011	-0.00008	0.00151
D16	3.13221	0.00000	0.00012	0.00006	0.00018	3.13239
D17	-3.12402	0.00000	-0.00010	-0.00005	-0.00016	-3.12417
D18	0.00659	0.00000	-0.00001	0.00012	0.00011	0.00670
D19	-0.19391	0.00000	0.00001	0.00033	0.00034	-0.19357
D20	2.95748	0.00000	0.00002	0.00035	0.00037	2.95785
D21	2.92875	0.00000	0.00016	0.00026	0.00043	2.92917
D22	-0.20305	0.00000	0.00017	0.00028	0.00046	-0.20259
D23	0.00063	0.00000	-0.00006	0.00011	0.00006	0.00068
D24	3.04088	0.00000	-0.00030	0.00001	-0.00029	3.04060
D25	-3.12994	-0.00001	-0.00015	-0.00006	-0.00021	-3.13015
D26	-0.08969	-0.00001	-0.00039	-0.00016	-0.00055	-0.09024
D27	-2.46963	0.00000	-0.00029	-0.00014	-0.00042	-2.47005
D28	-0.44267	0.00000	-0.00031	-0.00014	-0.00045	-0.44313
D29	1.67443	0.00000	-0.00027	-0.00013	-0.00040	1.67403
D30	0.79031	0.00000	-0.00001	-0.00002	-0.00003	0.79028
D31	2.81727	0.00000	-0.00004	-0.00002	-0.00006	2.81721
D32	-1.34881	0.00000	0.00001	-0.00001	0.00000	-1.34882
D33	-3.00055	0.00000	0.00002	0.00018	0.00020	-3.00035
D34	1.21923	0.00000	0.00003	0.00016	0.00018	1.21941
D35	-0.89865	0.00000	0.00004	0.00018	0.00022	-0.89843
D36	1.16804	0.00000	0.00002	0.00018	0.00021	1.16825
D37	-0.89537	0.00000	0.00003	0.00016	0.00019	-0.89518
D38	-3.01324	0.00000	0.00004	0.00019	0.00023	-3.01301
D39	-0.92614	0.00000	0.00002	0.00021	0.00023	-0.92591
D40	-2.98955	0.00000	0.00003	0.00019	0.00022	-2.98934
D41	1.17576	0.00000	0.00004	0.00021	0.00026	1.17601
D42	-3.13964	0.00000	0.00000	0.00001	0.00001	-3.13963
D43	-0.02379	0.00000	0.00003	0.00000	0.00003	-0.02376
D44	-0.00897	0.00000	-0.00001	-0.00001	-0.00002	-0.00899
D45	3.10688	0.00000	0.00002	-0.00002	0.00000	3.10688
D46	-2.75250	0.00000	-0.00005	-0.00002	-0.00007	-2.75257
D47	-0.04771	0.00000	-0.00006	-0.00002	-0.00008	-0.04779
D48	-0.01972	0.00000	-0.00005	-0.00008	-0.00013	-0.01984
D49	2.68507	0.00000	-0.00005	-0.00008	-0.00013	2.68493

D50	0.31718	0.00000	0.00046	0.00013	0.00059	0.31777
D51	-2.06193	0.00000	0.00047	0.00007	0.00054	-2.06139
D52	2.54651	0.00001	0.00056	0.00003	0.00059	2.54710
D53	0.16452	0.00001	0.00061	0.00002	0.00063	0.16515
D54	2.55603	0.00000	0.00030	-0.00012	0.00018	2.55621
D55	-1.65054	0.00000	0.00031	-0.00012	0.00019	-1.65035
D56	0.44199	0.00000	0.00027	-0.00012	0.00015	0.44214
D57	1.32955	0.00000	0.00022	-0.00013	0.00009	1.32964
D58	-2.87702	0.00000	0.00023	-0.00012	0.00010	-2.87691
D59	-0.78449	0.00000	0.00019	-0.00013	0.00007	-0.78442
D60	-1.01853	0.00000	0.00028	-0.00013	0.00015	-1.01838
D61	1.05809	0.00000	0.00029	-0.00013	0.00016	1.05825
D62	-3.13257	0.00000	0.00026	-0.00013	0.00013	-3.13244
D63	1.47466	0.00000	0.00079	0.00031	0.00110	1.47576
D64	2.82039	0.00000	0.00071	0.00037	0.00107	2.82147
D65	2.25742	0.00000	-0.00048	-0.00027	-0.00075	2.25667
D66	-0.85921	0.00000	-0.00040	-0.00026	-0.00066	-0.85987
D67	-1.93469	0.00000	-0.00050	-0.00030	-0.00080	-1.93549
D68	1.23187	0.00000	-0.00042	-0.00029	-0.00071	1.23116
D69	0.10260	0.00000	-0.00043	-0.00025	-0.00068	0.10192
D70	-3.01402	0.00000	-0.00036	-0.00023	-0.00059	-3.01461
D71	2.92387	0.00000	0.00005	-0.00002	0.00003	2.92390
D72	-0.19213	0.00000	0.00013	0.00000	0.00012	-0.19200
D73	-1.88605	0.00000	-0.00031	-0.00011	-0.00042	-1.88647

Item	Value	Threshold	Converged?
Maximum Force	0.000020	0.000450	YES
RMS Force	0.000005	0.000300	YES
Maximum Displacement	0.003299	0.001800	NO
RMS Displacement	0.000691	0.001200	YES

Predicted change in Energy=-2.757522D-08

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.847311	1.644847	1.537863
2	6	0	-1.503640	0.455026	1.573935
3	7	0	-2.364941	0.449815	0.484602
4	6	0	-2.229725	1.606930	-0.181933
5	7	0	-1.309982	2.354655	0.440346
6	6	0	-0.776068	3.645572	-0.030957
7	1	0	-0.075226	2.032228	2.178627

8	1	0	-1.351877	-0.415720	2.223533
9	1	0	-1.613808	4.259710	-0.365764
10	1	0	-0.325664	4.127161	0.834805
11	35	0	-0.391631	-2.431555	2.920803
12	1	0	-2.765592	1.880580	-1.074522
13	6	0	-3.250249	-0.603851	0.090839
14	6	0	-3.209977	-1.823252	0.611687
15	1	0	-3.944407	-0.296646	-0.681573
16	1	0	-3.918275	-2.558696	0.251328
17	1	0	-2.486639	-2.134726	1.368139
18	6	0	2.555257	-0.688038	1.129286
19	6	0	3.975532	-0.375671	1.315338
20	8	0	2.976189	0.655074	1.531789
21	1	0	2.171988	-0.730212	0.113660
22	1	0	1.982337	-1.226418	1.879716
23	1	0	4.430165	-0.691398	2.251510
24	6	0	4.918183	-0.174725	0.160967
25	1	0	5.679788	0.571616	0.404884
26	1	0	5.430421	-1.115052	-0.064313
27	1	0	4.378948	0.149334	-0.731703
28	6	0	0.256271	3.476417	-1.155117
29	1	0	0.707448	4.455163	-1.346598
30	1	0	-0.212681	3.137511	-2.079523
31	6	0	1.358357	2.483494	-0.804229
32	8	0	1.680184	1.571908	-1.528987
33	8	0	1.883111	2.733341	0.394292
34	1	0	2.456588	1.967290	0.701260

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.359317	0.000000			
3	N	2.200150	1.388708	0.000000		
4	C	2.206853	2.221971	1.342188	0.000000	
5	N	1.386519	2.220612	2.177915	1.338750	0.000000
6	C	2.543456	3.644807	3.605992	2.508380	1.474332
7	H	1.075528	2.212146	3.258305	3.224126	2.156433
8	H	2.229500	1.096909	2.190737	3.263127	3.294919
9	H	3.323976	4.272024	3.975252	2.729540	2.090779
10	H	2.632164	3.926642	4.219498	3.318248	2.065492
11	Br	4.328651	3.373866	4.258088	5.414325	5.468441
12	H	3.249604	3.261756	2.153713	1.076454	2.153688
13	C	3.595085	2.524171	1.431445	2.450190	3.555215
14	C	4.297406	3.004672	2.428388	3.654706	4.592847

15	H	4.276365	3.407297	2.100449	2.610245	3.902345
16	H	5.362440	4.081945	3.393877	4.515679	5.565963
17	H	4.123272	2.777671	2.734099	4.058167	4.732850
18	C	4.145692	4.240160	5.091038	5.466464	4.967162
19	C	5.233720	5.547815	6.447723	6.684140	6.013065
20	O	3.949537	4.484492	5.446687	5.562770	4.738258
21	H	4.097002	4.128854	4.702529	4.992462	4.663394
22	H	4.045730	3.882369	4.863632	5.479025	5.072991
23	H	5.815418	6.081401	7.113212	7.453729	6.745965
24	C	6.200613	6.605519	7.317013	7.374582	6.727991
25	H	6.711072	7.278868	8.046046	7.998539	7.213694
26	H	7.042296	7.295903	7.969804	8.130243	7.597801
27	H	5.890779	6.325682	6.859280	6.789800	6.212976
28	C	3.438704	4.435518	4.326633	3.259179	2.501400
29	H	4.316858	5.423976	5.369887	4.253923	3.416918
30	H	3.964377	4.712755	4.293096	3.164173	2.857739
31	C	3.324710	4.238086	4.433947	3.745657	2.947135
32	O	3.974811	4.583917	4.655821	4.135598	3.664978
33	O	3.154010	4.248807	4.823752	4.303051	3.215800
34	H	3.423394	4.328038	5.059329	4.782407	3.795416

		6	7	8	9	10
6	C	0.000000				
7	H	2.824238	0.000000			
8	H	4.680638	2.761215	0.000000		
9	H	1.091361	3.715217	5.350955	0.000000	
10	H	1.088272	2.501464	4.859985	1.765856	0.000000
11	Br	6.766989	4.536110	2.339198	7.554354	6.882768
12	H	2.856996	4.224222	4.260135	2.736641	3.826997
13	C	4.918740	4.624776	2.861397	5.151762	5.611521
14	C	6.020376	5.210249	2.834030	6.364400	6.616378
15	H	5.099290	5.345556	3.895514	5.127554	5.913102
16	H	6.960322	6.289682	3.881796	7.223713	7.612358
17	H	6.188325	4.882143	2.230328	6.682594	6.645712
18	C	5.587850	3.926883	4.066600	6.640519	5.618947
19	C	6.368721	4.790812	5.404415	7.453427	6.245534
20	O	5.046255	3.409705	4.511903	6.136952	4.841839
21	H	5.278203	4.116447	4.119234	6.281832	5.509300
22	H	5.915720	3.865448	3.448539	6.933400	5.922796
23	H	7.150092	5.265168	5.788678	8.239733	6.916897
24	C	6.859737	5.820286	6.604991	7.912557	6.816026
25	H	7.163605	6.196752	7.329845	8.209292	6.992295
26	H	7.822094	6.726686	7.191862	8.865669	7.837201
27	H	6.268087	5.644021	6.472639	7.276141	6.356920
28	C	1.535602	3.648208	5.399088	2.175735	2.172994

29	H	2.141768	4.348609	6.380608	2.527541	2.435861
30	H	2.184526	4.401408	5.695570	2.481825	3.079851
31	C	2.550322	3.340095	4.991809	3.490123	2.867752
32	O	3.546457	4.127925	5.217803	4.407693	4.017494
33	O	2.843279	2.740528	4.871125	3.890492	2.648674
34	H	3.715217	2.932049	4.743465	4.791853	3.524742

		11	12	13	14	15
11	Br	0.000000				
12	H	6.339781	0.000000			
13	C	4.418246	2.786640	0.000000		
14	C	3.693931	4.093794	1.326590	0.000000	
15	H	5.491555	2.506857	1.082982	2.131299	0.000000
16	H	4.424871	4.774278	2.072060	1.082785	2.447010
17	H	2.624487	4.708194	2.134988	1.091995	3.115276
18	C	3.864393	6.306029	5.898251	5.898691	6.758553
19	C	5.086873	7.499657	7.332351	7.363569	8.168190
20	O	4.774814	6.423611	6.513814	6.727358	7.327988
21	H	4.164944	5.710316	5.423757	5.514374	6.183095
22	H	2.858660	6.397170	5.564856	5.378125	6.523110
23	H	5.169701	8.334055	7.979031	7.895688	8.882132
24	C	6.395631	8.049292	8.179997	8.305888	8.903384
25	H	7.225718	8.673320	9.012542	9.209022	9.724166
26	H	6.673858	8.784587	8.697094	8.695689	9.430705
27	H	6.539129	7.359293	7.710286	7.955349	8.335445
28	C	7.206736	3.418311	5.522380	6.574418	5.666211
29	H	8.175914	4.331802	6.582038	7.655037	6.682941
30	H	7.486640	3.017823	5.285365	6.390271	5.260559
31	C	6.410619	4.176544	5.618906	6.436036	5.988617
32	O	6.334096	4.479592	5.627339	6.326395	5.987122
33	O	6.183353	4.949247	6.130279	6.837349	6.655695
34	H	5.691095	5.516529	6.288989	6.818079	6.928952

		16	17	18	19	20
16	H	0.000000				
17	H	1.864564	0.000000			
18	C	6.795351	5.250779	0.000000		
19	C	8.258929	6.697515	1.466072	0.000000	
20	O	7.713724	6.136144	1.463948	1.451886	0.000000
21	H	6.360315	5.024856	1.086356	2.196019	2.139357
22	H	6.264490	4.588952	1.086847	2.239446	2.156110
23	H	8.785442	7.120795	2.185103	1.087562	2.108324
24	C	9.152840	7.754370	2.604717	1.503843	2.517749
25	H	10.096794	8.656944	3.445893	2.151922	2.930243
26	H	9.464769	8.109963	3.142226	2.137013	3.421132
27	H	8.783148	7.534093	2.736844	2.151453	2.710517

28	C	7.471782	6.736120	5.276980	5.897002	4.751568
29	H	8.552479	7.810162	5.999743	6.411181	5.279486
30	H	7.184085	6.697294	5.709007	6.434956	5.419683
31	C	7.374329	6.389925	3.902521	4.417805	3.378977
32	O	7.181515	6.284496	3.597155	4.141482	3.447980
33	O	7.853800	6.613711	3.563402	3.859081	2.609198
34	H	7.831084	6.458077	2.691414	2.858977	1.637582

		21	22	23	24	25
21	H	0.000000				
22	H	1.844218	0.000000			
23	H	3.109867	2.533050	0.000000		
24	C	2.802212	3.560808	2.208049	0.000000	
25	H	3.752896	4.367975	2.562574	1.093875	0.000000
26	H	3.285904	3.959916	2.557935	1.094237	1.768382
27	H	2.521688	3.802098	3.099840	1.092084	1.778296
28	C	4.793276	5.857147	6.811547	6.065998	6.347126
29	H	5.582593	6.656937	7.300143	6.437306	6.547809
30	H	5.045392	6.287889	7.414473	6.505111	6.890376
31	C	3.439829	4.621294	5.371544	4.546437	4.877705
32	O	2.870526	4.420541	5.193949	4.048618	4.553819
33	O	3.486890	4.230369	4.654630	4.209863	4.368973
34	H	2.775390	3.437069	3.656077	3.307506	3.524878

		26	27	28	29	30
26	H	0.000000				
27	H	1.774732	0.000000			
28	C	7.003090	5.314624	0.000000		
29	H	7.414717	5.691940	1.094609	0.000000	
30	H	7.347786	5.641709	1.090550	1.766359	0.000000
31	C	5.484407	3.818054	1.524340	2.146002	2.126563
32	O	4.840382	3.153205	2.407170	3.048384	2.517368
33	O	5.253937	3.764859	2.366313	2.716165	3.267331
34	H	4.350933	3.008956	3.250384	3.666432	4.028296

		31	32	33	34
31	C	0.000000			
32	O	1.208237	0.000000		
33	O	1.332007	2.255905	0.000000	
34	H	1.933670	2.394397	1.004958	0.000000

Stoichiometry C11H17BrN2O3
Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.075655	1.329339	1.239033
2	6	0	-1.154178	1.256553	0.664615
3	7	0	-1.214886	2.288519	-0.262678
4	6	0	-0.054172	2.962089	-0.239978
5	7	0	0.750929	2.397461	0.668459
6	6	0	2.158539	2.754454	0.923108
7	1	0	0.535170	0.698934	1.979436
8	1	0	-1.939814	0.498584	0.771700
9	1	0	2.233246	3.842589	0.961199
10	1	0	2.402491	2.361877	1.908352
11	35	0	-3.069551	-1.499646	0.321566
12	1	0	0.189603	3.808651	-0.858574
13	6	0	-2.307219	2.602042	-1.133049
14	6	0	-3.348493	1.800399	-1.314594
15	1	0	-2.182340	3.556322	-1.629643
16	1	0	-4.128752	2.118873	-1.994443
17	1	0	-3.452665	0.825300	-0.834195
18	6	0	0.612475	-2.462485	-0.348624
19	6	0	1.586994	-3.514465	-0.043636
20	8	0	1.630702	-2.258382	0.683219
21	1	0	0.776084	-1.858855	-1.236900
22	1	0	-0.407921	-2.499139	0.023778
23	1	0	1.248283	-4.329705	0.591541
24	6	0	2.755101	-3.820419	-0.939996
25	1	0	3.622140	-4.140596	-0.354939
26	1	0	2.492349	-4.634248	-1.622637
27	1	0	3.032096	-2.945978	-1.532680
28	6	0	3.108663	2.182034	-0.138812
29	1	0	4.134850	2.363823	0.195942
30	1	0	2.977488	2.678903	-1.100693
31	6	0	2.918187	0.686041	-0.360927
32	8	0	2.769286	0.195294	-1.454926
33	8	0	2.907191	0.014763	0.789511
34	1	0	2.582946	-0.926487	0.652209

Rotational constants (GHZ): 0.3286020 0.2549077 0.1595917

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 538 symmetry adapted cartesian basis functions of A symmetry.

There are 519 symmetry adapted basis functions of A symmetry.

519 basis functions, 823 primitive gaussians, 538 cartesian basis functions

78 alpha electrons 78 beta electrons
nuclear repulsion energy 1572.8597848832 Hartrees.
NAtoms= 34 NActive= 34 NUniq= 34 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 519 RedAO= T EigKep= 3.52D-06 NBF= 519
NBsUse= 519 1.00D-06 EigRej= -1.00D+00 NBFU= 519
Initial guess from the checkpoint file: "./coohpo.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 -0.000003 -0.000026 -0.000052 Ang= -0.01 deg.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3338.90388354 A.U. after 9 cycles
NFock= 9 Conv=0.22D-08 -V/T= 2.0019
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000001324	-0.000000794	0.000002563
2	6	0.000005746	0.000007636	0.000003043
3	7	-0.000001579	0.000006476	-0.000002238
4	6	0.000000759	-0.000007814	-0.000008230
5	7	0.000000394	0.000004321	-0.000001015
6	6	-0.000000507	-0.000006011	-0.000001827
7	1	-0.000001494	0.000002529	-0.000003194
8	1	-0.000010095	-0.000007157	-0.000003149
9	1	0.000001986	-0.000000921	-0.000003327
10	1	0.000001534	0.000003986	-0.000002631
11	35	-0.000001182	0.000002628	0.000003883
12	1	-0.000001120	0.000004560	-0.000000631
13	6	-0.000000123	-0.000001317	-0.000005779
14	6	-0.000001130	0.000011790	-0.000004471
15	1	0.000000031	0.000002139	-0.000003487
16	1	-0.000003094	0.000000028	-0.000001589
17	1	-0.000000989	-0.000000037	-0.000000342
18	6	-0.000003292	-0.000008579	0.000009121

19	6	0.000006218	-0.000005482	-0.000001871
20	8	-0.000003137	0.000010569	-0.000003377
21	1	0.000000794	0.000001949	0.000002111
22	1	-0.000003912	0.000001710	0.000000960
23	1	-0.000004134	-0.000002681	0.000004625
24	6	-0.000002529	-0.000002348	0.000009197
25	1	-0.000001392	-0.000000644	0.000004020
26	1	0.000001109	-0.000002005	0.000005953
27	1	0.000000817	-0.000004839	0.000002520
28	6	0.000007518	-0.000002690	-0.000009212
29	1	0.000002543	-0.000000057	0.000001213
30	1	0.000002673	-0.000001533	-0.000001363
31	6	0.000004249	-0.000000923	-0.000004639
32	8	-0.000000175	-0.000000046	0.000003197
33	8	0.000000683	0.000007061	-0.000001828
34	1	0.000001505	-0.000011504	0.000011794

Cartesian Forces: Max 0.000011794 RMS 0.000004451

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000008992 RMS 0.000002344
Search for a local minimum.
Step number 41 out of a maximum of 175
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 21 22 23 24 25
26 27 28 29 30
31 32 33 34 35
36 37 38 39 40
41
DE= -7.99D-09 DEPred=-2.76D-08 R= 2.90D-01
Trust test= 2.90D-01 RLast= 3.31D-03 DXMaxT set to 1.95D-01
ITU= 0 0 -1 1 1 1 1 1 1 1 -1 1 1 1 1 1 -1 0 1 1
ITU= 1 1 1 1 1 1 1 1 0 0 -1 1 1 1 0 1 0 -1 0 1
ITU= 0
Eigenvalues --- 0.00156 0.00274 0.00338 0.00412 0.00489
Eigenvalues --- 0.00566 0.00784 0.00926 0.01034 0.01219
Eigenvalues --- 0.01399 0.01682 0.02024 0.02215 0.02289
Eigenvalues --- 0.02337 0.02389 0.02634 0.03008 0.03151
Eigenvalues --- 0.03404 0.03710 0.03820 0.04301 0.04441

Eigenvalues --- 0.04927 0.05031 0.05270 0.05444 0.05726
Eigenvalues --- 0.05849 0.05958 0.06210 0.07361 0.09233
Eigenvalues --- 0.09602 0.11778 0.12588 0.12871 0.13030
Eigenvalues --- 0.13572 0.14283 0.14890 0.15566 0.15694
Eigenvalues --- 0.16004 0.16009 0.16025 0.16048 0.16118
Eigenvalues --- 0.16352 0.17490 0.19450 0.20702 0.21870
Eigenvalues --- 0.23309 0.23733 0.24324 0.25300 0.26452
Eigenvalues --- 0.28237 0.28899 0.29927 0.31314 0.32045
Eigenvalues --- 0.33346 0.34380 0.34506 0.34610 0.34737
Eigenvalues --- 0.34856 0.34900 0.34972 0.35093 0.35317
Eigenvalues --- 0.35352 0.35681 0.35749 0.35930 0.36604
Eigenvalues --- 0.36976 0.37264 0.37377 0.38576 0.39750
Eigenvalues --- 0.40517 0.45477 0.49117 0.50481 0.50848
Eigenvalues --- 0.54392 0.55778 0.56416 0.61037 0.90613
Eigenvalues --- 0.96982
En-DIIS/RFO-DIIS IScMMF= 0 using points: 41 40 39 38 37
RFO step: Lambda=-2.18813497D-09.
DidBck=F Rises=F RFO-DIIS coefs: 1.02048 0.11420 -0.08235 -0.17323 0.12090
Iteration 1 RMS(Cart)= 0.00016723 RMS(Int)= 0.00000003
Iteration 2 RMS(Cart)= 0.00000002 RMS(Int)= 0.00000002

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.56874	0.00000	0.00000	0.00000	0.00000	2.56874
R2	2.62014	0.00000	0.00000	0.00001	0.00001	2.62015
R3	2.03245	0.00000	0.00000	0.00000	0.00000	2.03245
R4	2.62428	0.00001	0.00000	0.00001	0.00000	2.62428
R5	2.07286	0.00001	-0.00001	0.00002	0.00001	2.07286
R6	2.53637	-0.00001	-0.00001	-0.00001	-0.00002	2.53635
R7	2.70504	0.00000	0.00003	-0.00001	0.00002	2.70505
R8	2.52987	0.00000	0.00000	0.00000	0.00000	2.52987
R9	2.03420	0.00000	0.00000	0.00000	0.00000	2.03420
R10	2.78608	0.00000	0.00001	-0.00001	-0.00001	2.78608
R11	2.06237	0.00000	0.00000	0.00000	0.00000	2.06237
R12	2.05654	0.00000	0.00000	0.00000	0.00000	2.05654
R13	2.90187	0.00000	0.00000	0.00002	0.00002	2.90188
R14	4.42044	0.00000	0.00003	-0.00004	-0.00001	4.42043
R15	2.50689	-0.00001	-0.00001	0.00000	-0.00001	2.50688
R16	2.04654	0.00000	0.00000	0.00000	0.00000	2.04654
R17	2.04617	0.00000	0.00000	0.00000	0.00001	2.04617
R18	2.06357	0.00000	0.00000	0.00000	0.00000	2.06358
R19	2.77047	0.00000	-0.00001	0.00001	0.00000	2.77047
R20	2.76646	0.00000	0.00001	0.00000	0.00001	2.76647
R21	2.05292	0.00000	0.00000	0.00000	0.00000	2.05291

R22	2.05384	0.00000	0.00000	0.00000	0.00000	2.05384
R23	2.74367	0.00000	0.00003	0.00000	0.00003	2.74370
R24	2.05519	0.00000	0.00000	0.00000	0.00000	2.05520
R25	2.84185	0.00000	-0.00001	0.00000	-0.00002	2.84183
R26	3.09458	-0.00001	0.00000	-0.00005	-0.00005	3.09453
R27	2.06712	0.00000	0.00000	0.00000	0.00000	2.06712
R28	2.06781	0.00000	0.00000	0.00000	0.00000	2.06781
R29	2.06374	0.00000	0.00000	0.00000	0.00000	2.06374
R30	2.06851	0.00000	0.00000	0.00000	0.00000	2.06851
R31	2.06084	0.00000	0.00000	0.00000	0.00000	2.06084
R32	2.88058	0.00000	-0.00001	0.00000	-0.00001	2.88057
R33	2.28324	0.00000	0.00000	0.00000	0.00000	2.28323
R34	2.51713	0.00000	0.00002	0.00000	0.00001	2.51714
R35	1.89909	0.00001	0.00001	0.00001	0.00001	1.89911
A1	1.88387	0.00000	-0.00001	0.00000	-0.00001	1.88386
A2	2.27322	0.00000	0.00001	0.00001	0.00002	2.27324
A3	2.12556	0.00000	0.00000	-0.00001	-0.00001	2.12555
A4	1.85660	0.00000	0.00000	-0.00001	0.00000	1.85660
A5	2.27018	0.00000	-0.00001	0.00005	0.00004	2.27023
A6	2.15002	0.00000	0.00001	-0.00004	-0.00003	2.14998
A7	1.90057	0.00000	0.00000	0.00001	0.00002	1.90059
A8	2.21696	0.00000	0.00000	-0.00002	-0.00002	2.21694
A9	2.16553	-0.00001	0.00000	0.00000	0.00001	2.16554
A10	1.89641	0.00000	0.00000	-0.00001	-0.00001	1.89640
A11	2.19050	0.00000	0.00000	0.00002	0.00002	2.19052
A12	2.19622	0.00000	0.00000	-0.00001	-0.00001	2.19622
A13	1.88731	0.00000	0.00000	0.00001	0.00001	1.88732
A14	2.19007	0.00001	-0.00001	0.00002	0.00001	2.19008
A15	2.20092	-0.00001	0.00000	-0.00002	-0.00002	2.20090
A16	1.88894	0.00000	-0.00001	-0.00001	-0.00002	1.88892
A17	1.85776	0.00000	0.00000	0.00002	0.00001	1.85777
A18	1.96170	0.00001	0.00001	0.00002	0.00003	1.96173
A19	1.88886	0.00000	-0.00001	0.00000	-0.00001	1.88884
A20	1.93205	0.00000	-0.00001	0.00000	-0.00001	1.93204
A21	1.93146	0.00000	0.00002	-0.00002	0.00000	1.93146
A22	2.73230	0.00000	-0.00002	0.00003	0.00000	2.73231
A23	2.15296	0.00000	-0.00001	-0.00002	-0.00003	2.15293
A24	1.96472	0.00000	-0.00001	0.00001	0.00000	1.96472
A25	2.16546	0.00000	0.00002	0.00000	0.00003	2.16549
A26	2.06441	0.00000	0.00000	0.00001	0.00002	2.06442
A27	2.15829	0.00000	0.00001	-0.00001	0.00001	2.15829
A28	2.06022	0.00000	-0.00002	-0.00001	-0.00002	2.06020
A29	2.05861	0.00000	0.00004	-0.00003	0.00001	2.05862
A30	2.12774	0.00000	-0.00003	0.00003	0.00001	2.12774

A31	1.97589	0.00000	0.00000	-0.00003	-0.00002	1.97587
A32	2.00006	0.00000	-0.00001	0.00000	-0.00002	2.00005
A33	2.02673	0.00000	-0.00001	0.00001	0.00000	2.02673
A34	2.04020	0.00000	-0.00003	0.00000	-0.00003	2.04017
A35	2.13922	0.00000	0.00005	-0.00001	0.00004	2.13926
A36	1.94497	0.00000	-0.00003	0.00000	-0.00003	1.94494
A37	2.03871	0.00000	0.00002	-0.00001	0.00001	2.03872
A38	2.02363	0.00000	-0.00001	0.00001	0.00000	2.02364
A39	2.09959	0.00000	-0.00001	0.00001	0.00000	2.09960
A40	2.36267	0.00000	0.00000	0.00001	0.00001	2.36268
A41	1.93524	0.00000	0.00000	0.00000	0.00000	1.93524
A42	1.91414	0.00000	-0.00001	0.00001	0.00000	1.91415
A43	1.93648	0.00000	0.00002	0.00000	0.00001	1.93650
A44	1.88210	0.00000	0.00000	0.00000	0.00000	1.88210
A45	1.90032	0.00000	0.00000	0.00000	0.00000	1.90032
A46	1.89426	0.00000	-0.00001	0.00000	-0.00001	1.89425
A47	1.88248	0.00000	-0.00003	-0.00002	-0.00005	1.88243
A48	1.94516	0.00000	-0.00001	0.00000	-0.00001	1.94515
A49	1.97065	0.00000	-0.00001	-0.00003	-0.00003	1.97062
A50	1.88266	0.00000	0.00001	0.00002	0.00004	1.88270
A51	1.90149	0.00000	0.00002	0.00001	0.00003	1.90152
A52	1.87926	0.00000	0.00002	0.00001	0.00002	1.87928
A53	2.14832	0.00000	0.00001	0.00000	0.00000	2.14832
A54	1.94956	0.00000	0.00000	0.00000	0.00000	1.94955
A55	2.18501	0.00000	-0.00001	0.00001	0.00000	2.18501
A56	1.93550	0.00000	-0.00003	0.00001	-0.00002	1.93548
A57	2.81394	0.00001	0.00004	0.00008	0.00011	2.81405
D1	0.00348	0.00000	-0.00001	0.00001	0.00000	0.00348
D2	3.02451	0.00000	0.00005	0.00001	0.00006	3.02457
D3	-3.10298	0.00000	0.00006	-0.00003	0.00003	-3.10295
D4	-0.08196	0.00000	0.00012	-0.00003	0.00009	-0.08187
D5	-0.00266	0.00000	0.00002	-0.00001	0.00001	-0.00265
D6	-3.04336	0.00000	0.00008	-0.00003	0.00004	-3.04332
D7	3.10739	0.00000	-0.00005	0.00003	-0.00002	3.10738
D8	0.06669	0.00000	0.00001	0.00001	0.00002	0.06670
D9	-0.00312	0.00000	0.00001	-0.00001	-0.00001	-0.00313
D10	3.12197	0.00000	0.00005	-0.00005	0.00000	3.12197
D11	-3.03451	0.00000	-0.00005	-0.00002	-0.00007	-3.03458
D12	0.09058	0.00000	0.00000	-0.00006	-0.00006	0.09051
D13	-1.48345	0.00000	-0.00005	0.00046	0.00041	-1.48304
D14	1.51981	0.00000	0.00002	0.00046	0.00048	1.52029
D15	0.00151	0.00000	0.00001	0.00001	0.00001	0.00152
D16	3.13239	0.00000	0.00010	0.00004	0.00014	3.13252
D17	-3.12417	0.00000	-0.00004	0.00004	0.00001	-3.12417

D18	0.00670	0.00000	0.00006	0.00008	0.00013	0.00684
D19	-0.19357	0.00000	-0.00009	0.00000	-0.00009	-0.19366
D20	2.95785	0.00000	-0.00010	-0.00001	-0.00011	2.95774
D21	2.92917	0.00000	-0.00004	-0.00004	-0.00009	2.92909
D22	-0.20259	0.00000	-0.00005	-0.00006	-0.00011	-0.20270
D23	0.00068	0.00000	-0.00002	0.00000	-0.00001	0.00067
D24	3.04060	0.00000	-0.00007	0.00003	-0.00005	3.04055
D25	-3.13015	0.00000	-0.00011	-0.00003	-0.00014	-3.13029
D26	-0.09024	0.00000	-0.00017	0.00000	-0.00017	-0.09041
D27	-2.47005	0.00000	-0.00012	0.00000	-0.00011	-2.47016
D28	-0.44313	0.00000	-0.00013	0.00000	-0.00013	-0.44326
D29	1.67403	0.00000	-0.00011	0.00000	-0.00011	1.67392
D30	0.79028	0.00000	-0.00005	-0.00003	-0.00008	0.79021
D31	2.81721	0.00000	-0.00007	-0.00003	-0.00009	2.81712
D32	-1.34882	0.00000	-0.00004	-0.00003	-0.00007	-1.34889
D33	-3.00035	0.00000	0.00000	0.00005	0.00005	-3.00030
D34	1.21941	0.00000	0.00000	0.00004	0.00004	1.21945
D35	-0.89843	0.00000	0.00000	0.00004	0.00004	-0.89839
D36	1.16825	0.00000	0.00000	0.00006	0.00006	1.16831
D37	-0.89518	0.00000	0.00001	0.00004	0.00005	-0.89513
D38	-3.01301	0.00000	0.00000	0.00004	0.00005	-3.01297
D39	-0.92591	0.00000	0.00001	0.00007	0.00008	-0.92583
D40	-2.98934	0.00000	0.00002	0.00005	0.00007	-2.98926
D41	1.17601	0.00000	0.00001	0.00006	0.00007	1.17608
D42	-3.13963	0.00000	-0.00002	-0.00002	-0.00004	-3.13967
D43	-0.02376	0.00000	0.00002	-0.00001	0.00001	-0.02375
D44	-0.00899	0.00000	-0.00001	0.00000	-0.00001	-0.00901
D45	3.10688	0.00000	0.00002	0.00001	0.00003	3.10691
D46	-2.75257	0.00000	-0.00003	-0.00002	-0.00005	-2.75262
D47	-0.04779	0.00000	-0.00001	-0.00001	-0.00002	-0.04781
D48	-0.01984	0.00000	-0.00002	0.00002	-0.00001	-0.01985
D49	2.68493	0.00000	0.00000	0.00003	0.00003	2.68496
D50	0.31777	0.00000	-0.00005	0.00003	-0.00001	0.31776
D51	-2.06139	0.00000	-0.00003	0.00006	0.00003	-2.06136
D52	2.54710	0.00000	0.00005	-0.00002	0.00003	2.54713
D53	0.16515	0.00000	0.00007	-0.00002	0.00006	0.16521
D54	2.55621	0.00000	-0.00005	-0.00017	-0.00022	2.55599
D55	-1.65035	0.00000	-0.00005	-0.00016	-0.00021	-1.65056
D56	0.44214	0.00000	-0.00006	-0.00016	-0.00022	0.44193
D57	1.32964	0.00000	-0.00007	-0.00016	-0.00023	1.32941
D58	-2.87691	0.00000	-0.00007	-0.00015	-0.00023	-2.87714
D59	-0.78442	0.00000	-0.00008	-0.00015	-0.00023	-0.78465
D60	-1.01838	0.00000	-0.00004	-0.00015	-0.00019	-1.01857
D61	1.05825	0.00000	-0.00004	-0.00015	-0.00019	1.05807

D62	-3.13244	0.00000	-0.00005	-0.00015	-0.00019	-3.13263
D63	1.47576	0.00000	0.00020	-0.00002	0.00018	1.47594
D64	2.82147	0.00000	0.00017	0.00000	0.00017	2.82164
D65	2.25667	0.00000	-0.00016	-0.00012	-0.00028	2.25639
D66	-0.85987	0.00000	-0.00012	-0.00009	-0.00021	-0.86008
D67	-1.93549	0.00000	-0.00019	-0.00016	-0.00034	-1.93583
D68	1.23116	0.00000	-0.00015	-0.00012	-0.00027	1.23089
D69	0.10192	0.00000	-0.00015	-0.00012	-0.00027	0.10165
D70	-3.01461	0.00000	-0.00011	-0.00008	-0.00020	-3.01481
D71	2.92390	0.00000	-0.00002	-0.00003	-0.00005	2.92385
D72	-0.19200	0.00000	0.00002	0.00000	0.00002	-0.19199
D73	-1.88647	0.00000	0.00008	0.00004	0.00011	-1.88636

Item	Value	Threshold	Converged?
Maximum Force	0.000009	0.000450	YES
RMS Force	0.000002	0.000300	YES
Maximum Displacement	0.000747	0.001800	YES
RMS Displacement	0.000167	0.001200	YES

Predicted change in Energy=-6.089297D-09

Optimization completed.

-- Stationary point found.

```
                          ----------------------------
                          !     Optimized Parameters     !
                          ! (Angstroms and Degrees)    !
--------------------------                              --------------------------
! Name  Definition              Value          Derivative Info.                !
--------------------------------------------------------------------------------
! R1    R(1,2)                  1.3593         -DE/DX =    0.0                 !
! R2    R(1,5)                  1.3865         -DE/DX =    0.0                 !
! R3    R(1,7)                  1.0755         -DE/DX =    0.0                 !
! R4    R(2,3)                  1.3887         -DE/DX =    0.0                 !
! R5    R(2,8)                  1.0969         -DE/DX =    0.0                 !
! R6    R(3,4)                  1.3422         -DE/DX =    0.0                 !
! R7    R(3,13)                 1.4314         -DE/DX =    0.0                 !
! R8    R(4,5)                  1.3387         -DE/DX =    0.0                 !
! R9    R(4,12)                 1.0765         -DE/DX =    0.0                 !
! R10   R(5,6)                  1.4743         -DE/DX =    0.0                 !
! R11   R(6,9)                  1.0914         -DE/DX =    0.0                 !
! R12   R(6,10)                 1.0883         -DE/DX =    0.0                 !
! R13   R(6,28)                 1.5356         -DE/DX =    0.0                 !
! R14   R(8,11)                 2.3392         -DE/DX =    0.0                 !
! R15   R(13,14)                1.3266         -DE/DX =    0.0                 !
! R16   R(13,15)                1.083          -DE/DX =    0.0                 !
! R17   R(14,16)                1.0828         -DE/DX =    0.0                 !
! R18   R(14,17)                1.092          -DE/DX =    0.0                 !
```

! R19	R(18,19)	1.4661	-DE/DX =	0.0	!
! R20	R(18,20)	1.4639	-DE/DX =	0.0	!
! R21	R(18,21)	1.0864	-DE/DX =	0.0	!
! R22	R(18,22)	1.0868	-DE/DX =	0.0	!
! R23	R(19,20)	1.4519	-DE/DX =	0.0	!
! R24	R(19,23)	1.0876	-DE/DX =	0.0	!
! R25	R(19,24)	1.5038	-DE/DX =	0.0	!
! R26	R(20,34)	1.6376	-DE/DX =	0.0	!
! R27	R(24,25)	1.0939	-DE/DX =	0.0	!
! R28	R(24,26)	1.0942	-DE/DX =	0.0	!
! R29	R(24,27)	1.0921	-DE/DX =	0.0	!
! R30	R(28,29)	1.0946	-DE/DX =	0.0	!
! R31	R(28,30)	1.0906	-DE/DX =	0.0	!
! R32	R(28,31)	1.5243	-DE/DX =	0.0	!
! R33	R(31,32)	1.2082	-DE/DX =	0.0	!
! R34	R(31,33)	1.332	-DE/DX =	0.0	!
! R35	R(33,34)	1.005	-DE/DX =	0.0	!
! A1	A(2,1,5)	107.938	-DE/DX =	0.0	!
! A2	A(2,1,7)	130.2459	-DE/DX =	0.0	!
! A3	A(5,1,7)	121.7859	-DE/DX =	0.0	!
! A4	A(1,2,3)	106.3756	-DE/DX =	0.0	!
! A5	A(1,2,8)	130.0719	-DE/DX =	0.0	!
! A6	A(3,2,8)	123.1869	-DE/DX =	0.0	!
! A7	A(2,3,4)	108.8946	-DE/DX =	0.0	!
! A8	A(2,3,13)	127.0225	-DE/DX =	0.0	!
! A9	A(4,3,13)	124.0757	-DE/DX =	0.0	!
! A10	A(3,4,5)	108.6563	-DE/DX =	0.0	!
! A11	A(3,4,12)	125.5062	-DE/DX =	0.0	!
! A12	A(5,4,12)	125.8343	-DE/DX =	0.0	!
! A13	A(1,5,4)	108.1351	-DE/DX =	0.0	!
! A14	A(1,5,6)	125.4818	-DE/DX =	0.0	!
! A15	A(4,5,6)	126.1036	-DE/DX =	0.0	!
! A16	A(5,6,9)	108.2285	-DE/DX =	0.0	!
! A17	A(5,6,10)	106.4418	-DE/DX =	0.0	!
! A18	A(5,6,28)	112.3972	-DE/DX =	0.0	!
! A19	A(9,6,10)	108.2235	-DE/DX =	0.0	!
! A20	A(9,6,28)	110.6982	-DE/DX =	0.0	!
! A21	A(10,6,28)	110.6647	-DE/DX =	0.0	!
! A22	A(2,8,11)	156.5495	-DE/DX =	0.0	!
! A23	A(3,13,14)	123.3554	-DE/DX =	0.0	!
! A24	A(3,13,15)	112.5702	-DE/DX =	0.0	!
! A25	A(14,13,15)	124.0719	-DE/DX =	0.0	!
! A26	A(13,14,16)	118.2818	-DE/DX =	0.0	!
! A27	A(13,14,17)	123.6608	-DE/DX =	0.0	!

! A28	A(16,14,17)	118.0417	-DE/DX =	0.0	!
! A29	A(19,18,21)	117.9497	-DE/DX =	0.0	!
! A30	A(19,18,22)	121.9104	-DE/DX =	0.0	!
! A31	A(20,18,21)	113.21	-DE/DX =	0.0	!
! A32	A(20,18,22)	114.5951	-DE/DX =	0.0	!
! A33	A(21,18,22)	116.1232	-DE/DX =	0.0	!
! A34	A(18,19,23)	116.895	-DE/DX =	0.0	!
! A35	A(18,19,24)	122.5682	-DE/DX =	0.0	!
! A36	A(20,19,23)	111.4384	-DE/DX =	0.0	!
! A37	A(20,19,24)	116.8094	-DE/DX =	0.0	!
! A38	A(23,19,24)	115.9457	-DE/DX =	0.0	!
! A39	A(18,20,34)	120.2979	-DE/DX =	0.0	!
! A40	A(19,20,34)	135.3709	-DE/DX =	0.0	!
! A41	A(19,24,25)	110.8811	-DE/DX =	0.0	!
! A42	A(19,24,26)	109.6724	-DE/DX =	0.0	!
! A43	A(19,24,27)	110.9523	-DE/DX =	0.0	!
! A44	A(25,24,26)	107.8365	-DE/DX =	0.0	!
! A45	A(25,24,27)	108.8803	-DE/DX =	0.0	!
! A46	A(26,24,27)	108.5333	-DE/DX =	0.0	!
! A47	A(6,28,29)	107.8582	-DE/DX =	0.0	!
! A48	A(6,28,30)	111.4496	-DE/DX =	0.0	!
! A49	A(6,28,31)	112.91	-DE/DX =	0.0	!
! A50	A(29,28,30)	107.8686	-DE/DX =	0.0	!
! A51	A(29,28,31)	108.9471	-DE/DX =	0.0	!
! A52	A(30,28,31)	107.6734	-DE/DX =	0.0	!
! A53	A(28,31,32)	123.0895	-DE/DX =	0.0	!
! A54	A(28,31,33)	111.7014	-DE/DX =	0.0	!
! A55	A(32,31,33)	125.192	-DE/DX =	0.0	!
! A56	A(31,33,34)	110.8961	-DE/DX =	0.0	!
! A57	A(20,34,33)	161.2269	-DE/DX =	0.0	!
! D1	D(5,1,2,3)	0.1996	-DE/DX =	0.0	!
! D2	D(5,1,2,8)	173.2915	-DE/DX =	0.0	!
! D3	D(7,1,2,3)	-177.7876	-DE/DX =	0.0	!
! D4	D(7,1,2,8)	-4.6957	-DE/DX =	0.0	!
! D5	D(2,1,5,4)	-0.1521	-DE/DX =	0.0	!
! D6	D(2,1,5,6)	-174.3718	-DE/DX =	0.0	!
! D7	D(7,1,5,4)	178.0406	-DE/DX =	0.0	!
! D8	D(7,1,5,6)	3.8209	-DE/DX =	0.0	!
! D9	D(1,2,3,4)	-0.1789	-DE/DX =	0.0	!
! D10	D(1,2,3,13)	178.8755	-DE/DX =	0.0	!
! D11	D(8,2,3,4)	-173.8647	-DE/DX =	0.0	!
! D12	D(8,2,3,13)	5.1897	-DE/DX =	0.0	!
! D13	D(1,2,8,11)	-84.9956	-DE/DX =	0.0	!
! D14	D(3,2,8,11)	87.0787	-DE/DX =	0.0	!

! D15	D(2,3,4,5)	0.0865	-DE/DX =	0.0	!
! D16	D(2,3,4,12)	179.4725	-DE/DX =	0.0	!
! D17	D(13,3,4,5)	-179.002	-DE/DX =	0.0	!
! D18	D(13,3,4,12)	0.384	-DE/DX =	0.0	!
! D19	D(2,3,13,14)	-11.0906	-DE/DX =	0.0	!
! D20	D(2,3,13,15)	169.4725	-DE/DX =	0.0	!
! D21	D(4,3,13,14)	167.8293	-DE/DX =	0.0	!
! D22	D(4,3,13,15)	-11.6076	-DE/DX =	0.0	!
! D23	D(3,4,5,1)	0.0392	-DE/DX =	0.0	!
! D24	D(3,4,5,6)	174.2133	-DE/DX =	0.0	!
! D25	D(12,4,5,1)	-179.3442	-DE/DX =	0.0	!
! D26	D(12,4,5,6)	-5.1702	-DE/DX =	0.0	!
! D27	D(1,5,6,9)	-141.5234	-DE/DX =	0.0	!
! D28	D(1,5,6,10)	-25.3892	-DE/DX =	0.0	!
! D29	D(1,5,6,28)	95.9151	-DE/DX =	0.0	!
! D30	D(4,5,6,9)	45.28	-DE/DX =	0.0	!
! D31	D(4,5,6,10)	161.4141	-DE/DX =	0.0	!
! D32	D(4,5,6,28)	-77.2815	-DE/DX =	0.0	!
! D33	D(5,6,28,29)	-171.9076	-DE/DX =	0.0	!
! D34	D(5,6,28,30)	69.867	-DE/DX =	0.0	!
! D35	D(5,6,28,31)	-51.4761	-DE/DX =	0.0	!
! D36	D(9,6,28,29)	66.9355	-DE/DX =	0.0	!
! D37	D(9,6,28,30)	-51.2899	-DE/DX =	0.0	!
! D38	D(9,6,28,31)	-172.633	-DE/DX =	0.0	!
! D39	D(10,6,28,29)	-53.0509	-DE/DX =	0.0	!
! D40	D(10,6,28,30)	-171.2763	-DE/DX =	0.0	!
! D41	D(10,6,28,31)	67.3806	-DE/DX =	0.0	!
! D42	D(3,13,14,16)	-179.8876	-DE/DX =	0.0	!
! D43	D(3,13,14,17)	-1.3612	-DE/DX =	0.0	!
! D44	D(15,13,14,16)	-0.5153	-DE/DX =	0.0	!
! D45	D(15,13,14,17)	178.0111	-DE/DX =	0.0	!
! D46	D(21,18,19,23)	-157.7106	-DE/DX =	0.0	!
! D47	D(21,18,19,24)	-2.7383	-DE/DX =	0.0	!
! D48	D(22,18,19,23)	-1.137	-DE/DX =	0.0	!
! D49	D(22,18,19,24)	153.8353	-DE/DX =	0.0	!
! D50	D(21,18,20,34)	18.2071	-DE/DX =	0.0	!
! D51	D(22,18,20,34)	-118.1087	-DE/DX =	0.0	!
! D52	D(23,19,20,34)	145.9381	-DE/DX =	0.0	!
! D53	D(24,19,20,34)	9.4624	-DE/DX =	0.0	!
! D54	D(18,19,24,25)	146.4598	-DE/DX =	0.0	!
! D55	D(18,19,24,26)	-94.558	-DE/DX =	0.0	!
! D56	D(18,19,24,27)	25.333	-DE/DX =	0.0	!
! D57	D(20,19,24,25)	76.1828	-DE/DX =	0.0	!
! D58	D(20,19,24,26)	-164.835	-DE/DX =	0.0	!

! D59	D(20,19,24,27)	-44.944	-DE/DX =	0.0	!
! D60	D(23,19,24,25)	-58.3488	-DE/DX =	0.0	!
! D61	D(23,19,24,26)	60.6334	-DE/DX =	0.0	!
! D62	D(23,19,24,27)	-179.4756	-DE/DX =	0.0	!
! D63	D(18,20,34,33)	84.555	-DE/DX =	0.0	!
! D64	D(19,20,34,33)	161.6582	-DE/DX =	0.0	!
! D65	D(6,28,31,32)	129.2976	-DE/DX =	0.0	!
! D66	D(6,28,31,33)	-49.2667	-DE/DX =	0.0	!
! D67	D(29,28,31,32)	-110.8954	-DE/DX =	0.0	!
! D68	D(29,28,31,33)	70.5403	-DE/DX =	0.0	!
! D69	D(30,28,31,32)	5.8397	-DE/DX =	0.0	!
! D70	D(30,28,31,33)	-172.7246	-DE/DX =	0.0	!
! D71	D(28,31,33,34)	167.5271	-DE/DX =	0.0	!
! D72	D(32,31,33,34)	-11.001	-DE/DX =	0.0	!
! D73	D(31,33,34,20)	-108.087	-DE/DX =	0.0	!

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.847311	1.644847	1.537863
2	6	0	-1.503640	0.455026	1.573935
3	7	0	-2.364941	0.449815	0.484602
4	6	0	-2.229725	1.606930	-0.181933
5	7	0	-1.309982	2.354655	0.440346
6	6	0	-0.776068	3.645572	-0.030957
7	1	0	-0.075226	2.032228	2.178627
8	1	0	-1.351877	-0.415720	2.223533
9	1	0	-1.613808	4.259710	-0.365764
10	1	0	-0.325664	4.127161	0.834805
11	35	0	-0.391631	-2.431555	2.920803
12	1	0	-2.765592	1.880580	-1.074522
13	6	0	-3.250249	-0.603851	0.090839
14	6	0	-3.209977	-1.823252	0.611687
15	1	0	-3.944407	-0.296646	-0.681573
16	1	0	-3.918275	-2.558696	0.251328
17	1	0	-2.486639	-2.134726	1.368139
18	6	0	2.555257	-0.688038	1.129286
19	6	0	3.975532	-0.375671	1.315338
20	8	0	2.976189	0.655074	1.531789
21	1	0	2.171988	-0.730212	0.113660

22	1	0	1.982337	-1.226418	1.879716
23	1	0	4.430165	-0.691398	2.251510
24	6	0	4.918183	-0.174725	0.160967
25	1	0	5.679788	0.571616	0.404884
26	1	0	5.430421	-1.115052	-0.064313
27	1	0	4.378948	0.149334	-0.731703
28	6	0	0.256271	3.476417	-1.155117
29	1	0	0.707448	4.455163	-1.346598
30	1	0	-0.212681	3.137511	-2.079523
31	6	0	1.358357	2.483494	-0.804229
32	8	0	1.680184	1.571908	-1.528987
33	8	0	1.883111	2.733341	0.394292
34	1	0	2.456588	1.967290	0.701260

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.359317	0.000000			
3	N	2.200150	1.388708	0.000000		
4	C	2.206853	2.221971	1.342188	0.000000	
5	N	1.386519	2.220612	2.177915	1.338750	0.000000
6	C	2.543456	3.644807	3.605992	2.508380	1.474332
7	H	1.075528	2.212146	3.258305	3.224126	2.156433
8	H	2.229500	1.096909	2.190737	3.263127	3.294919
9	H	3.323976	4.272024	3.975252	2.729540	2.090779
10	H	2.632164	3.926642	4.219498	3.318248	2.065492
11	Br	4.328651	3.373866	4.258088	5.414325	5.468441
12	H	3.249604	3.261756	2.153713	1.076454	2.153688
13	C	3.595085	2.524171	1.431445	2.450190	3.555215
14	C	4.297406	3.004672	2.428388	3.654706	4.592847
15	H	4.276365	3.407297	2.100449	2.610245	3.902345
16	H	5.362440	4.081945	3.393877	4.515679	5.565963
17	H	4.123272	2.777671	2.734099	4.058167	4.732850
18	C	4.145692	4.240160	5.091038	5.466464	4.967162
19	C	5.233720	5.547815	6.447723	6.684140	6.013065
20	O	3.949537	4.484492	5.446687	5.562770	4.738258
21	H	4.097002	4.128854	4.702529	4.992462	4.663394
22	H	4.045730	3.882369	4.863632	5.479025	5.072991
23	H	5.815418	6.081401	7.113212	7.453729	6.745965
24	C	6.200613	6.605519	7.317013	7.374582	6.727991
25	H	6.711072	7.278868	8.046046	7.998539	7.213694
26	H	7.042296	7.295903	7.969804	8.130243	7.597801
27	H	5.890779	6.325682	6.859280	6.789800	6.212976
28	C	3.438704	4.435518	4.326633	3.259179	2.501400

29	H	4.316858	5.423976	5.369887	4.253923	3.416918
30	H	3.964377	4.712755	4.293096	3.164173	2.857739
31	C	3.324710	4.238086	4.433947	3.745657	2.947135
32	O	3.974811	4.583917	4.655821	4.135598	3.664978
33	O	3.154010	4.248807	4.823752	4.303051	3.215800
34	H	3.423394	4.328038	5.059329	4.782407	3.795416

		6	7	8	9	10
6	C	0.000000				
7	H	2.824238	0.000000			
8	H	4.680638	2.761215	0.000000		
9	H	1.091361	3.715217	5.350955	0.000000	
10	H	1.088272	2.501464	4.859985	1.765856	0.000000
11	Br	6.766989	4.536110	2.339198	7.554354	6.882768
12	H	2.856996	4.224222	4.260135	2.736641	3.826997
13	C	4.918740	4.624776	2.861397	5.151762	5.611521
14	C	6.020376	5.210249	2.834030	6.364400	6.616378
15	H	5.099290	5.345556	3.895514	5.127554	5.913102
16	H	6.960322	6.289682	3.881796	7.223713	7.612358
17	H	6.188325	4.882143	2.230328	6.682594	6.645712
18	C	5.587850	3.926883	4.066600	6.640519	5.618947
19	C	6.368721	4.790812	5.404415	7.453427	6.245534
20	O	5.046255	3.409705	4.511903	6.136952	4.841839
21	H	5.278203	4.116447	4.119234	6.281832	5.509300
22	H	5.915720	3.865448	3.448539	6.933400	5.922796
23	H	7.150092	5.265168	5.788678	8.239733	6.916897
24	C	6.859737	5.820286	6.604991	7.912557	6.816026
25	H	7.163605	6.196752	7.329845	8.209292	6.992295
26	H	7.822094	6.726686	7.191862	8.865669	7.837201
27	H	6.268087	5.644021	6.472639	7.276141	6.356920
28	C	1.535602	3.648208	5.399088	2.175735	2.172994
29	H	2.141768	4.348609	6.380608	2.527541	2.435861
30	H	2.184526	4.401408	5.695570	2.481825	3.079851
31	C	2.550322	3.340095	4.991809	3.490123	2.867752
32	O	3.546457	4.127925	5.217803	4.407693	4.017494
33	O	2.843279	2.740528	4.871125	3.890492	2.648674
34	H	3.715217	2.932049	4.743465	4.791853	3.524742

		11	12	13	14	15
11	Br	0.000000				
12	H	6.339781	0.000000			
13	C	4.418246	2.786640	0.000000		
14	C	3.693931	4.093794	1.326590	0.000000	
15	H	5.491555	2.506857	1.082982	2.131299	0.000000
16	H	4.424871	4.774278	2.072060	1.082785	2.447010
17	H	2.624487	4.708194	2.134988	1.091995	3.115276

18	C	3.864393	6.306029	5.898251	5.898691	6.758553
19	C	5.086873	7.499657	7.332351	7.363569	8.168190
20	O	4.774814	6.423611	6.513814	6.727358	7.327988
21	H	4.164944	5.710316	5.423757	5.514374	6.183095
22	H	2.858660	6.397170	5.564856	5.378125	6.523110
23	H	5.169701	8.334055	7.979031	7.895688	8.882132
24	C	6.395631	8.049292	8.179997	8.305888	8.903384
25	H	7.225718	8.673320	9.012542	9.209022	9.724166
26	H	6.673858	8.784587	8.697094	8.695689	9.430705
27	H	6.539129	7.359293	7.710286	7.955349	8.335445
28	C	7.206736	3.418311	5.522380	6.574418	5.666211
29	H	8.175914	4.331802	6.582038	7.655037	6.682941
30	H	7.486640	3.017823	5.285365	6.390271	5.260559
31	C	6.410619	4.176544	5.618906	6.436036	5.988617
32	O	6.334096	4.479592	5.627339	6.326395	5.987122
33	O	6.183353	4.949247	6.130279	6.837349	6.655695
34	H	5.691095	5.516529	6.288989	6.818079	6.928952

		16	17	18	19	20
16	H	0.000000				
17	H	1.864564	0.000000			
18	C	6.795351	5.250779	0.000000		
19	C	8.258929	6.697515	1.466072	0.000000	
20	O	7.713724	6.136144	1.463948	1.451886	0.000000
21	H	6.360315	5.024856	1.086356	2.196019	2.139357
22	H	6.264490	4.588952	1.086847	2.239446	2.156110
23	H	8.785442	7.120795	2.185103	1.087562	2.108324
24	C	9.152840	7.754370	2.604717	1.503843	2.517749
25	H	10.096794	8.656944	3.445893	2.151922	2.930243
26	H	9.464769	8.109963	3.142226	2.137013	3.421132
27	H	8.783148	7.534093	2.736844	2.151453	2.710517
28	C	7.471782	6.736120	5.276980	5.897002	4.751568
29	H	8.552479	7.810162	5.999743	6.411181	5.279486
30	H	7.184085	6.697294	5.709007	6.434956	5.419683
31	C	7.374329	6.389925	3.902521	4.417805	3.378977
32	O	7.181515	6.284496	3.597155	4.141482	3.447980
33	O	7.853800	6.613711	3.563402	3.859081	2.609198
34	H	7.831084	6.458077	2.691414	2.858977	1.637582

		21	22	23	24	25
21	H	0.000000				
22	H	1.844218	0.000000			
23	H	3.109867	2.533050	0.000000		
24	C	2.802212	3.560808	2.208049	0.000000	
25	H	3.752896	4.367975	2.562574	1.093875	0.000000
26	H	3.285904	3.959916	2.557935	1.094237	1.768382

27	H	2.521688	3.802098	3.099840	1.092084	1.778296
28	C	4.793276	5.857147	6.811547	6.065998	6.347126
29	H	5.582593	6.656937	7.300143	6.437306	6.547809
30	H	5.045392	6.287889	7.414473	6.505111	6.890376
31	C	3.439829	4.621294	5.371544	4.546437	4.877705
32	O	2.870526	4.420541	5.193949	4.048618	4.553819
33	O	3.486890	4.230369	4.654630	4.209863	4.368973
34	H	2.775390	3.437069	3.656077	3.307506	3.524878

		26	27	28	29	30
26	H	0.000000				
27	H	1.774732	0.000000			
28	C	7.003090	5.314624	0.000000		
29	H	7.414717	5.691940	1.094609	0.000000	
30	H	7.347786	5.641709	1.090550	1.766359	0.000000
31	C	5.484407	3.818054	1.524340	2.146002	2.126563
32	O	4.840382	3.153205	2.407170	3.048384	2.517368
33	O	5.253937	3.764859	2.366313	2.716165	3.267331
34	H	4.350933	3.008956	3.250384	3.666432	4.028296

		31	32	33	34
31	C	0.000000			
32	O	1.208237	0.000000		
33	O	1.332007	2.255905	0.000000	
34	H	1.933670	2.394397	1.004958	0.000000

Stoichiometry C11H17BrN2O3
Framework group C1[X(C11H17BrN2O3)]
Deg. of freedom 96
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.075655	1.329339	1.239033
2	6	0	-1.154178	1.256553	0.664615
3	7	0	-1.214886	2.288519	-0.262678
4	6	0	-0.054172	2.962089	-0.239978
5	7	0	0.750929	2.397461	0.668459
6	6	0	2.158539	2.754454	0.923108
7	1	0	0.535170	0.698934	1.979436
8	1	0	-1.939814	0.498584	0.771700
9	1	0	2.233246	3.842589	0.961199
10	1	0	2.402491	2.361877	1.908352

11	35	0	-3.069551	-1.499646	0.321566
12	1	0	0.189603	3.808651	-0.858574
13	6	0	-2.307219	2.602042	-1.133049
14	6	0	-3.348493	1.800399	-1.314594
15	1	0	-2.182340	3.556322	-1.629643
16	1	0	-4.128752	2.118873	-1.994443
17	1	0	-3.452665	0.825300	-0.834195
18	6	0	0.612475	-2.462485	-0.348624
19	6	0	1.586994	-3.514465	-0.043636
20	8	0	1.630702	-2.258382	0.683219
21	1	0	0.776084	-1.858855	-1.236900
22	1	0	-0.407921	-2.499139	0.023778
23	1	0	1.248283	-4.329705	0.591541
24	6	0	2.755101	-3.820419	-0.939996
25	1	0	3.622140	-4.140596	-0.354939
26	1	0	2.492349	-4.634248	-1.622637
27	1	0	3.032096	-2.945978	-1.532680
28	6	0	3.108663	2.182034	-0.138812
29	1	0	4.134850	2.363823	0.195942
30	1	0	2.977488	2.678903	-1.100693
31	6	0	2.918187	0.686041	-0.360927
32	8	0	2.769286	0.195294	-1.454926
33	8	0	2.907191	0.014763	0.789511
34	1	0	2.582946	-0.926487	0.652209

Rotational constants (GHZ): 0.3286020 0.2549077 0.1595917

****

Population analysis using the SCF density.

****

Orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A)

The electronic state is 1-A.

Alpha occ. eigenvalues -- -482.68095 -62.33430 -56.15208 -56.15199 -56.15196
Alpha occ. eigenvalues -- -19.17558 -19.15065 -19.13455 -14.45345 -14.45336
Alpha occ. eigenvalues -- -10.33000 -10.31687 -10.28446 -10.25804 -10.25395
Alpha occ. eigenvalues -- -10.24548 -10.23619 -10.23359 -10.21555 -10.19837
Alpha occ. eigenvalues -- -10.17330 -8.54337 -6.36657 -6.36609 -6.36594
Alpha occ. eigenvalues -- -2.47897 -2.47885 -2.47871 -2.47833 -2.47833
Alpha occ. eigenvalues -- -1.12649 -1.11851 -1.07752 -1.03940 -1.00697
Alpha occ. eigenvalues -- -0.86455 -0.82638 -0.81020 -0.75725 -0.74330
Alpha occ. eigenvalues -- -0.70288 -0.67712 -0.66573 -0.64181 -0.63293

Alpha occ. eigenvalues -- -0.62043 -0.60176 -0.58595 -0.55391 -0.54000
Alpha occ. eigenvalues -- -0.52917 -0.51323 -0.51104 -0.50580 -0.49963
Alpha occ. eigenvalues -- -0.49451 -0.48914 -0.47691 -0.46811 -0.46479
Alpha occ. eigenvalues -- -0.44128 -0.43415 -0.42329 -0.41303 -0.41231
Alpha occ. eigenvalues -- -0.40422 -0.39412 -0.38207 -0.37151 -0.34399
Alpha occ. eigenvalues -- -0.32048 -0.30845 -0.30223 -0.29364 -0.29321
Alpha occ. eigenvalues -- -0.18407 -0.18030 -0.17848
Alpha virt. eigenvalues -- -0.08562 -0.04544 -0.03785 -0.03177 -0.01806
Alpha virt. eigenvalues -- -0.00767 -0.00685 0.00109 0.00361 0.01142
Alpha virt. eigenvalues -- 0.01376 0.02098 0.02755 0.02929 0.03567
Alpha virt. eigenvalues -- 0.03760 0.04206 0.04652 0.05114 0.05486
Alpha virt. eigenvalues -- 0.05888 0.06322 0.06586 0.07150 0.07322
Alpha virt. eigenvalues -- 0.07568 0.07971 0.08135 0.08394 0.09014
Alpha virt. eigenvalues -- 0.09176 0.09759 0.10034 0.10185 0.10628
Alpha virt. eigenvalues -- 0.10798 0.10917 0.11064 0.11389 0.11760
Alpha virt. eigenvalues -- 0.11826 0.12144 0.12654 0.12695 0.12822
Alpha virt. eigenvalues -- 0.13097 0.13655 0.14113 0.14373 0.14492
Alpha virt. eigenvalues -- 0.14850 0.14910 0.15331 0.15568 0.15816
Alpha virt. eigenvalues -- 0.16445 0.16588 0.16985 0.17116 0.17581
Alpha virt. eigenvalues -- 0.17685 0.17767 0.18070 0.18366 0.18869
Alpha virt. eigenvalues -- 0.19365 0.19526 0.19796 0.20217 0.20303
Alpha virt. eigenvalues -- 0.20843 0.21305 0.21896 0.22227 0.22427
Alpha virt. eigenvalues -- 0.22528 0.23110 0.23433 0.23849 0.24392
Alpha virt. eigenvalues -- 0.24664 0.24879 0.25160 0.25706 0.25999
Alpha virt. eigenvalues -- 0.26372 0.26745 0.27101 0.27491 0.27833
Alpha virt. eigenvalues -- 0.28099 0.28625 0.28972 0.29223 0.29639
Alpha virt. eigenvalues -- 0.30187 0.30911 0.31190 0.31892 0.32639
Alpha virt. eigenvalues -- 0.32932 0.33427 0.33814 0.34250 0.34905
Alpha virt. eigenvalues -- 0.35086 0.35253 0.35501 0.35985 0.36570
Alpha virt. eigenvalues -- 0.37529 0.38132 0.38960 0.39707 0.40529
Alpha virt. eigenvalues -- 0.40761 0.41776 0.42778 0.43564 0.44086
Alpha virt. eigenvalues -- 0.46143 0.47362 0.47787 0.49569 0.50470
Alpha virt. eigenvalues -- 0.50830 0.51428 0.52471 0.53083 0.53536
Alpha virt. eigenvalues -- 0.53942 0.54720 0.54988 0.55980 0.56266
Alpha virt. eigenvalues -- 0.57633 0.58740 0.58915 0.59240 0.59887
Alpha virt. eigenvalues -- 0.60329 0.61752 0.62046 0.62660 0.62778
Alpha virt. eigenvalues -- 0.63603 0.64083 0.64800 0.64965 0.65560
Alpha virt. eigenvalues -- 0.66571 0.66683 0.66838 0.67818 0.68236
Alpha virt. eigenvalues -- 0.68314 0.69099 0.69765 0.70123 0.70282
Alpha virt. eigenvalues -- 0.71238 0.71970 0.72404 0.72622 0.73626
Alpha virt. eigenvalues -- 0.74253 0.74777 0.75636 0.76450 0.76561
Alpha virt. eigenvalues -- 0.77644 0.78025 0.78474 0.78682 0.79973
Alpha virt. eigenvalues -- 0.81550 0.83035 0.84060 0.85035 0.86574
Alpha virt. eigenvalues -- 0.88010 0.89270 0.89701 0.90545 0.92145

Alpha virt. eigenvalues --	0.93215	0.94245	0.95700	0.96415	0.97496
Alpha virt. eigenvalues --	0.98133	0.99725	1.00647	1.00795	1.03894
Alpha virt. eigenvalues --	1.03921	1.05331	1.05380	1.06934	1.07341
Alpha virt. eigenvalues --	1.08352	1.10203	1.11368	1.12081	1.13312
Alpha virt. eigenvalues --	1.15056	1.15757	1.16748	1.18224	1.18894
Alpha virt. eigenvalues --	1.20300	1.21988	1.22258	1.24610	1.25449
Alpha virt. eigenvalues --	1.27504	1.28485	1.29753	1.31105	1.32582
Alpha virt. eigenvalues --	1.34093	1.34691	1.36344	1.37755	1.42976
Alpha virt. eigenvalues --	1.43551	1.45521	1.47183	1.47973	1.48256
Alpha virt. eigenvalues --	1.49595	1.50845	1.51203	1.52914	1.53192
Alpha virt. eigenvalues --	1.54108	1.55345	1.56375	1.56577	1.57913
Alpha virt. eigenvalues --	1.58589	1.59227	1.59613	1.60064	1.60613
Alpha virt. eigenvalues --	1.61787	1.62597	1.62992	1.63393	1.64185
Alpha virt. eigenvalues --	1.65713	1.66473	1.67085	1.68543	1.69808
Alpha virt. eigenvalues --	1.70920	1.71324	1.72693	1.73039	1.73609
Alpha virt. eigenvalues --	1.75107	1.75978	1.77057	1.78592	1.79415
Alpha virt. eigenvalues --	1.80191	1.82083	1.83155	1.83939	1.85380
Alpha virt. eigenvalues --	1.86443	1.87961	1.89105	1.90939	1.91067
Alpha virt. eigenvalues --	1.92421	1.94473	1.96340	1.97896	1.98701
Alpha virt. eigenvalues --	2.03252	2.04509	2.05842	2.07973	2.08274
Alpha virt. eigenvalues --	2.09305	2.11208	2.12256	2.12983	2.14624
Alpha virt. eigenvalues --	2.15966	2.16741	2.17192	2.17812	2.18686
Alpha virt. eigenvalues --	2.19607	2.21804	2.23408	2.24220	2.26300
Alpha virt. eigenvalues --	2.26742	2.29335	2.31157	2.34008	2.36606
Alpha virt. eigenvalues --	2.37600	2.39876	2.41976	2.44913	2.47212
Alpha virt. eigenvalues --	2.47883	2.48376	2.49187	2.51255	2.51883
Alpha virt. eigenvalues --	2.52676	2.54422	2.54840	2.55412	2.57450
Alpha virt. eigenvalues --	2.57724	2.59244	2.60506	2.61327	2.62444
Alpha virt. eigenvalues --	2.64552	2.65928	2.67364	2.69059	2.69853
Alpha virt. eigenvalues --	2.71468	2.72497	2.74159	2.74994	2.76634
Alpha virt. eigenvalues --	2.77036	2.77267	2.77791	2.80026	2.80556
Alpha virt. eigenvalues --	2.81748	2.82530	2.83689	2.84118	2.84841
Alpha virt. eigenvalues --	2.85451	2.87434	2.88321	2.88645	2.89674
Alpha virt. eigenvalues --	2.92299	2.94439	2.95147	2.96340	2.99109
Alpha virt. eigenvalues --	3.01637	3.06577	3.07331	3.11255	3.12355
Alpha virt. eigenvalues --	3.13052	3.15219	3.19678	3.21000	3.23583
Alpha virt. eigenvalues --	3.26855	3.27791	3.30728	3.36008	3.37206
Alpha virt. eigenvalues --	3.40888	3.50028	3.54626	3.56473	3.58987
Alpha virt. eigenvalues --	3.62655	3.64570	3.70328	3.70518	3.74674
Alpha virt. eigenvalues --	3.75058	3.77446	3.78396	3.79569	3.81060
Alpha virt. eigenvalues --	3.83529	3.84209	3.85606	3.86102	3.90509
Alpha virt. eigenvalues --	3.93505	4.05739	4.06383	4.09535	4.10310
Alpha virt. eigenvalues --	4.11057	4.22376	4.29164	4.30653	4.32742
Alpha virt. eigenvalues --	4.37239	4.42110	4.50654	4.68346	4.89285

Alpha virt. eigenvalues -- 5.01806 5.07276 5.09263 5.10528 5.21312
Alpha virt. eigenvalues -- 5.22343 5.41177 5.47325 5.56146 5.67401
Alpha virt. eigenvalues -- 5.88666 6.77704 7.70331 7.74064 7.75100
Alpha virt. eigenvalues -- 23.71502 23.75831 23.78153 23.83740 23.85063
Alpha virt. eigenvalues -- 23.86846 23.88806 23.90427 23.97661 24.14618
Alpha virt. eigenvalues -- 24.23889 35.42752 35.56722 48.06289 49.88984
Alpha virt. eigenvalues -- 49.92609 49.99768 289.91119 289.95143 289.95930
Alpha virt. eigenvalues -- 1020.84877

Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	12.829203	-6.404773	0.675441	0.078430	-1.052887	-0.084375
2	C	-6.404773	12.524082	-0.452972	-0.454945	1.124762	-0.184628
3	N	0.675441	-0.452972	6.713383	0.470953	-0.373304	-0.069058
4	C	0.078430	-0.454945	0.470953	5.718018	0.343425	-0.193752
5	N	-1.052887	1.124762	-0.373304	0.343425	7.106674	0.119434
6	C	-0.084375	-0.184628	-0.069058	-0.193752	0.119434	6.358964
7	H	0.662921	-0.201748	0.058758	0.021398	-0.132944	-0.025577
8	H	-0.431142	0.255726	-0.155312	-0.099075	0.057061	0.041509
9	H	-0.023570	0.024328	-0.000536	-0.011170	-0.053527	0.395222
10	H	0.052359	-0.031097	-0.007314	-0.010988	-0.064715	0.512260
11	Br	-0.213679	0.063617	-0.010778	-0.040682	0.002829	-0.001828
12	H	0.107703	-0.093483	-0.036937	0.446076	-0.061901	-0.001009
13	C	0.641864	-0.739580	0.120192	0.037809	-0.125923	-0.029992
14	C	-0.550350	0.558936	-0.044884	-0.147994	0.015060	-0.047003
15	H	-0.005322	0.007116	-0.107104	0.044623	0.005181	0.005184
16	H	-0.012472	0.004283	0.028701	0.004420	-0.001099	-0.000760
17	H	0.055226	-0.028900	-0.024885	-0.032974	0.019330	0.003054
18	C	-0.018127	-0.008585	-0.010861	-0.021233	-0.002254	-0.001165
19	C	0.075772	-0.074338	0.012592	0.018594	0.006736	-0.006073
20	O	-0.018860	0.024188	-0.000163	-0.007617	-0.000765	0.009554
21	H	0.025343	-0.029929	0.005051	0.007491	0.002746	-0.003685
22	H	-0.074893	0.081684	-0.001051	0.005735	-0.001969	0.004215
23	H	-0.002001	-0.000018	0.000197	0.000316	0.000688	-0.000502
24	C	-0.000449	0.009763	-0.000899	-0.002863	-0.002799	-0.005003
25	H	0.000922	-0.001208	0.000055	0.000127	-0.000005	0.000837
26	H	-0.000687	0.000900	-0.000064	-0.000140	-0.000074	-0.000257
27	H	0.000556	-0.000289	-0.000192	-0.000077	-0.001069	0.001921
28	C	-0.231197	0.318382	-0.038841	-0.110532	0.056452	-0.429429
29	H	0.002882	0.009388	-0.004176	-0.018572	0.012741	-0.057851
30	H	0.012767	-0.007796	0.000104	-0.001784	-0.009546	0.021877
31	C	0.001771	-0.084243	0.034890	0.131195	-0.089905	-0.079966
32	O	-0.067680	0.042152	-0.000061	-0.001849	0.007990	-0.007161
33	O	-0.072625	0.087171	-0.005479	-0.050272	-0.033015	0.036949
34	H	-0.007687	0.018932	-0.000774	-0.000092	0.007141	-0.030955

		7	8	9	10	11	12
1	C	0.662921	-0.431142	-0.023570	0.052359	-0.213679	0.107703
2	C	-0.201748	0.255726	0.024328	-0.031097	0.063617	-0.093483
3	N	0.058758	-0.155312	-0.000536	-0.007314	-0.010778	-0.036937
4	C	0.021398	-0.099075	-0.011170	-0.010988	-0.040682	0.446076
5	N	-0.132944	0.057061	-0.053527	-0.064715	0.002829	-0.061901
6	C	-0.025577	0.041509	0.395222	0.512260	-0.001828	-0.001009
7	H	0.477346	-0.073971	0.002938	-0.006077	-0.009154	-0.000582
8	H	-0.073971	1.378669	0.001662	0.002247	0.283658	-0.002410
9	H	0.002938	0.001662	0.547154	-0.028658	0.000351	-0.012923
10	H	-0.006077	0.002247	-0.028658	0.487741	-0.000907	0.004964
11	Br	-0.009154	0.283658	0.000351	-0.000907	35.656404	-0.002734
12	H	-0.000582	-0.002410	-0.012923	0.004964	-0.002734	0.492175
13	C	0.026269	-0.192723	0.002487	-0.002993	-0.080994	-0.000523
14	C	-0.010724	-0.023086	0.000300	-0.001987	-0.054847	-0.007434
15	H	0.000685	-0.001722	0.000370	0.000084	-0.000203	0.000027
16	H	-0.000118	0.002635	-0.000105	0.000067	-0.011732	0.001067
17	H	-0.001951	0.018347	0.000319	-0.000496	0.149139	-0.004740
18	C	-0.015333	0.057429	-0.000082	0.000022	-0.046608	-0.001164
19	C	0.002997	-0.037467	-0.001057	0.001465	-0.017229	0.000998
20	O	0.002892	-0.002086	0.000847	-0.000819	0.003109	-0.000510
21	H	-0.000050	-0.008563	-0.000328	0.000038	-0.000456	0.000982
22	H	-0.000138	-0.010864	0.000046	0.001097	0.055488	0.000525
23	H	-0.001272	0.000927	-0.000048	-0.000096	0.000074	0.000001
24	C	0.000846	0.000673	0.000238	-0.001201	0.001638	-0.000135
25	H	0.000363	-0.000249	0.000004	0.000164	-0.000374	0.000010
26	H	-0.000192	0.000285	-0.000002	-0.000013	0.000181	0.000000
27	H	0.000621	0.000736	0.000026	-0.000430	0.000300	-0.000026
28	C	0.013427	0.010656	-0.008761	-0.048396	0.003436	-0.022730
29	H	-0.003940	0.001912	-0.014410	-0.000033	0.000032	0.003521
30	H	0.001907	-0.001813	-0.009016	0.007679	-0.000105	-0.003329
31	C	-0.013387	-0.017638	-0.025026	-0.063417	-0.007929	0.018065
32	O	-0.000118	-0.001210	0.001927	-0.001436	0.000772	0.000379
33	O	-0.001251	0.009745	0.010855	-0.025131	0.001729	-0.002961
34	H	-0.006108	0.002568	0.000301	0.000528	0.001963	-0.000503
		13	14	15	16	17	18
1	C	0.641864	-0.550350	-0.005322	-0.012472	0.055226	-0.018127
2	C	-0.739580	0.558936	0.007116	0.004283	-0.028900	-0.008585
3	N	0.120192	-0.044884	-0.107104	0.028701	-0.024885	-0.010861
4	C	0.037809	-0.147994	0.044623	0.004420	-0.032974	-0.021233
5	N	-0.125923	0.015060	0.005181	-0.001099	0.019330	-0.002254
6	C	-0.029992	-0.047003	0.005184	-0.000760	0.003054	-0.001165
7	H	0.026269	-0.010724	0.000685	-0.000118	-0.001951	-0.015333
8	H	-0.192723	-0.023086	-0.001722	0.002635	0.018347	0.057429

9	H	0.002487	0.000300	0.000370	-0.000105	0.000319	-0.000082
10	H	-0.002993	-0.001987	0.000084	0.000067	-0.000496	0.000022
11	Br	-0.080994	-0.054847	-0.000203	-0.011732	0.149139	-0.046608
12	H	-0.000523	-0.007434	0.000027	0.001067	-0.004740	-0.001164
13	C	6.043201	-0.006226	0.443410	-0.102370	-0.126170	-0.002596
14	C	-0.006226	5.999497	-0.078499	0.448966	0.225410	-0.010618
15	H	0.443410	-0.078499	0.545414	-0.011636	0.006185	0.000296
16	H	-0.102370	0.448966	-0.011636	0.490976	-0.037470	-0.000924
17	H	-0.126170	0.225410	0.006185	-0.037470	0.707290	0.016107
18	C	-0.002596	-0.010618	0.000296	-0.000924	0.016107	7.801773
19	C	-0.001390	0.002553	-0.000246	-0.000046	0.001494	-2.513045
20	O	-0.000015	0.000029	-0.000013	-0.000033	0.000585	0.219445
21	H	-0.004395	0.006012	-0.000370	0.000224	0.000271	0.217302
22	H	0.008612	0.009270	-0.000103	0.001407	-0.028010	0.312367
23	H	-0.000292	0.000158	-0.000001	-0.000002	0.000178	-0.023722
24	C	0.000529	-0.000618	0.000028	-0.000059	0.001078	0.443995
25	H	0.000041	-0.000026	0.000001	0.000001	-0.000026	0.012846
26	H	-0.000033	0.000025	-0.000002	0.000001	-0.000029	0.022596
27	H	-0.000109	-0.000114	0.000004	-0.000012	0.000136	-0.073898
28	C	-0.021384	-0.009090	0.001285	0.000622	-0.006426	0.016939
29	H	-0.002497	-0.000536	-0.000123	-0.000003	0.000013	0.002583
30	H	0.000389	-0.001383	0.000761	0.000072	-0.000229	-0.002045
31	C	0.018471	0.020366	-0.002461	-0.000513	0.007228	-0.111964
32	O	-0.001529	0.001545	-0.000175	0.000032	-0.000278	0.005332
33	O	0.000113	0.000425	-0.000039	-0.000034	0.000498	0.100181
34	H	-0.000511	0.001238	0.000009	-0.000010	0.000307	0.010872

		19	20	21	22	23	24
1	C	0.075772	-0.018860	0.025343	-0.074893	-0.002001	-0.000449
2	C	-0.074338	0.024188	-0.029929	0.081684	-0.000018	0.009763
3	N	0.012592	-0.000163	0.005051	-0.001051	0.000197	-0.000899
4	C	0.018594	-0.007617	0.007491	0.005735	0.000316	-0.002863
5	N	0.006736	-0.000765	0.002746	-0.001969	0.000688	-0.002799
6	C	-0.006073	0.009554	-0.003685	0.004215	-0.000502	-0.005003
7	H	0.002997	0.002892	-0.000050	-0.000138	-0.001272	0.000846
8	H	-0.037467	-0.002086	-0.008563	-0.010864	0.000927	0.000673
9	H	-0.001057	0.000847	-0.000328	0.000046	-0.000048	0.000238
10	H	0.001465	-0.000819	0.000038	0.001097	-0.000096	-0.001201
11	Br	-0.017229	0.003109	-0.000456	0.055488	0.000074	0.001638
12	H	0.000998	-0.000510	0.000982	0.000525	0.000001	-0.000135
13	C	-0.001390	-0.000015	-0.004395	0.008612	-0.000292	0.000529
14	C	0.002553	0.000029	0.006012	0.009270	0.000158	-0.000618
15	H	-0.000246	-0.000013	-0.000370	-0.000103	-0.000001	0.000028
16	H	-0.000046	-0.000033	0.000224	0.001407	-0.000002	-0.000059
17	H	0.001494	0.000585	0.000271	-0.028010	0.000178	0.001078

18	C	-2.513045	0.219445	0.217302	0.312367	-0.023722	0.443995
19	C	8.614836	-0.134918	0.222681	-0.015070	0.380821	-0.627295
20	O	-0.134918	8.322064	-0.091672	-0.013651	-0.006089	-0.049654
21	H	0.222681	-0.091672	0.576024	-0.044402	0.006862	-0.059862
22	H	-0.015070	-0.013651	-0.044402	0.562333	-0.003479	-0.032196
23	H	0.380821	-0.006089	0.006862	-0.003479	0.488878	-0.052584
24	C	-0.627295	-0.049654	-0.059862	-0.032196	-0.052584	5.762484
25	H	-0.008075	-0.015229	-0.005350	0.005312	-0.004044	0.353573
26	H	-0.105632	0.017198	-0.004625	0.002952	-0.005767	0.440959
27	H	0.038047	-0.005711	0.006770	-0.000409	0.006719	0.380815
28	C	-0.022924	0.042325	-0.012883	0.018586	-0.001660	-0.024889
29	H	-0.002842	-0.000093	-0.000650	-0.000296	0.000012	0.002011
30	H	0.001145	0.000979	0.000651	0.000513	0.000027	-0.001675
31	C	0.185565	-0.078193	0.025030	-0.017315	0.004798	-0.061956
32	O	0.005634	0.012618	-0.003724	0.005497	-0.001226	-0.032833
33	O	-0.134609	0.055549	-0.020585	-0.001065	-0.002558	0.056092
34	H	0.009710	-0.022646	0.007588	-0.005978	0.005934	0.007069

		25	26	27	28	29	30
1	C	0.000922	-0.000687	0.000556	-0.231197	0.002882	0.012767
2	C	-0.001208	0.000900	-0.000289	0.318382	0.009388	-0.007796
3	N	0.000055	-0.000064	-0.000192	-0.038841	-0.004176	0.000104
4	C	0.000127	-0.000140	-0.000077	-0.110532	-0.018572	-0.001784
5	N	-0.000005	-0.000074	-0.001069	0.056452	0.012741	-0.009546
6	C	0.000837	-0.000257	0.001921	-0.429429	-0.057851	0.021877
7	H	0.000363	-0.000192	0.000621	0.013427	-0.003940	0.001907
8	H	-0.000249	0.000285	0.000736	0.010656	0.001912	-0.001813
9	H	0.000004	-0.000002	0.000026	-0.008761	-0.014410	-0.009016
10	H	0.000164	-0.000013	-0.000430	-0.048396	-0.000033	0.007679
11	Br	-0.000374	0.000181	0.000300	0.003436	0.000032	-0.000105
12	H	0.000010	0.000000	-0.000026	-0.022730	0.003521	-0.003329
13	C	0.000041	-0.000033	-0.000109	-0.021384	-0.002497	0.000389
14	C	-0.000026	0.000025	-0.000114	-0.009090	-0.000536	-0.001383
15	H	0.000001	-0.000002	0.000004	0.001285	-0.000123	0.000761
16	H	0.000001	0.000001	-0.000012	0.000622	-0.000003	0.000072
17	H	-0.000026	-0.000029	0.000136	-0.006426	0.000013	-0.000229
18	C	0.012846	0.022596	-0.073898	0.016939	0.002583	-0.002045
19	C	-0.008075	-0.105632	0.038047	-0.022924	-0.002842	0.001145
20	O	-0.015229	0.017198	-0.005711	0.042325	-0.000093	0.000979
21	H	-0.005350	-0.004625	0.006770	-0.012883	-0.000650	0.000651
22	H	0.005312	0.002952	-0.000409	0.018586	-0.000296	0.000513
23	H	-0.004044	-0.005767	0.006719	-0.001660	0.000012	0.000027
24	C	0.353573	0.440959	0.380815	-0.024889	0.002011	-0.001675
25	H	0.574765	-0.032987	-0.032054	0.003686	-0.000189	0.000153
26	H	-0.032987	0.550359	-0.035789	-0.000317	0.000068	-0.000077

27	H	-0.032054	-0.035789	0.549710	-0.012615	0.000156	-0.000132
28	C	0.003686	-0.000317	-0.012615	8.039436	0.333392	0.465215
29	H	-0.000189	0.000068	0.000156	0.333392	0.526002	-0.019746
30	H	0.000153	-0.000077	-0.000132	0.465215	-0.019746	0.491838
31	C	0.003653	-0.000917	0.008797	-1.508485	0.012437	-0.164648
32	O	0.002673	-0.000814	0.007222	-0.098857	-0.005368	-0.005776
33	O	-0.004142	0.001648	-0.005099	-0.378508	0.021431	0.002030
34	H	-0.004187	-0.000226	-0.001316	-0.008435	0.000977	0.000939

		31	32	33	34
1	C	0.001771	-0.067680	-0.072625	-0.007687
2	C	-0.084243	0.042152	0.087171	0.018932
3	N	0.034890	-0.000061	-0.005479	-0.000774
4	C	0.131195	-0.001849	-0.050272	-0.000092
5	N	-0.089905	0.007990	-0.033015	0.007141
6	C	-0.079966	-0.007161	0.036949	-0.030955
7	H	-0.013387	-0.000118	-0.001251	-0.006108
8	H	-0.017638	-0.001210	0.009745	0.002568
9	H	-0.025026	0.001927	0.010855	0.000301
10	H	-0.063417	-0.001436	-0.025131	0.000528
11	Br	-0.007929	0.000772	0.001729	0.001963
12	H	0.018065	0.000379	-0.002961	-0.000503
13	C	0.018471	-0.001529	0.000113	-0.000511
14	C	0.020366	0.001545	0.000425	0.001238
15	H	-0.002461	-0.000175	-0.000039	0.000009
16	H	-0.000513	0.000032	-0.000034	-0.000010
17	H	0.007228	-0.000278	0.000498	0.000307
18	C	-0.111964	0.005332	0.100181	0.010872
19	C	0.185565	0.005634	-0.134609	0.009710
20	O	-0.078193	0.012618	0.055549	-0.022646
21	H	0.025030	-0.003724	-0.020585	0.007588
22	H	-0.017315	0.005497	-0.001065	-0.005978
23	H	0.004798	-0.001226	-0.002558	0.005934
24	C	-0.061956	-0.032833	0.056092	0.007069
25	H	0.003653	0.002673	-0.004142	-0.004187
26	H	-0.000917	-0.000814	0.001648	-0.000226
27	H	0.008797	0.007222	-0.005099	-0.001316
28	C	-1.508485	-0.098857	-0.378508	-0.008435
29	H	0.012437	-0.005368	0.021431	0.000977
30	H	-0.164648	-0.005776	0.002030	0.000939
31	C	7.152810	0.574116	0.258588	0.001260
32	O	0.574116	7.902070	-0.153458	-0.000176
33	O	0.258588	-0.153458	8.239421	0.227509
34	H	0.001260	-0.000176	0.227509	0.288956

Mulliken charges:

		1
1	C	0.049617
2	C	-0.356876
3	N	0.225325
4	C	-0.122000
5	N	0.119451
6	C	-0.250953
7	H	0.231267
8	H	-0.067113
9	H	0.199844
10	H	0.225492
11	Br	-0.724480
12	H	0.179542
13	C	0.098857
14	C	-0.294373
15	H	0.147356
16	H	0.195924
17	H	0.080387
18	C	-0.375860
19	C	0.120612
20	O	-0.262643
21	H	0.180465
22	H	0.175248
23	H	0.208770
24	C	-0.504821
25	H	0.148960
26	H	0.151469
27	H	0.166806
28	C	-0.327482
29	H	0.201767
30	H	0.220054
31	C	-0.131078
32	O	-0.186227
33	O	-0.219106
34	H	0.495802

Sum of Mulliken charges = 0.00000

Mulliken charges with hydrogens summed into heavy atoms:

		1
1	C	0.280883
2	C	-0.423989
3	N	0.225325
4	C	0.057542
5	N	0.119451
6	C	0.174383

11 Br -0.724480
13 C 0.246213
14 C -0.018062
18 C -0.020147
19 C 0.329382
20 O -0.262643
24 C -0.037586
28 C 0.094338
31 C -0.131078
32 O -0.186227
33 O 0.276696

Electronic spatial extent (au): <R**2>= 6544.9449

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= 9.0187 Y= 11.0861 Z= -0.8715 Tot= 14.3178

Quadrupole moment (field-independent basis, Debye-Ang):

XX= -136.3779 YY= -85.6770 ZZ= -118.6333

XY= -14.9106 XZ= 12.1220 YZ= 0.7080

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

XX= -22.8151 YY= 27.8857 ZZ= -5.0705

XY= -14.9106 XZ= 12.1220 YZ= 0.7080

Octapole moment (field-independent basis, Debye-Ang**2):

XXX= 51.1078 YYY= 11.8870 ZZZ= 16.8316 XYY= 52.9308

XXY= 75.3734 XXZ= -16.8366 XZZ= -26.9010 YZZ= 0.4681

YYZ= -22.6375 XYZ= 17.8614

Hexadecapole moment (field-independent basis, Debye-Ang**3):

XXXX= -4216.9963 YYYY= -3128.1183 ZZZZ= -606.5419 XXXY= -44.3205

XXXZ= 124.7661 YYYX= 37.5695 YYYZ= -67.1554 ZZZX= 21.3652

ZZZY= -12.5568 XXYY= -1216.1277 XXZZ= -797.6426 YYZZ= -666.9699

XXYZ= -10.5733 YYXZ= 37.6402 ZZXY= 17.3418

N-N= 1.572859784883D+03 E-N=-1.108474563616D+04 KE= 3.332709436656D+03

1\1\GINC-CN006\FOpt\RB3LYP\6-311++G(d,p)\C11H17Br1N2O3\SYWANG\22-Jul-2024\0\\# opt b3lyp/6-311++g(d,p)\\coohpo\\0,1\C,-0.8473113188,1.644847

0169,1.5378626721\C,-1.5036403253,0.4550261588,1.5739350025\N,-2.36494

05488,0.4498145661,0.4846024934\C,-2.2297245399,1.6069297005,-0.181933

1931\N,-1.309982433,2.3546552269,0.4403460422\C,-0.7760682968,3.645571

5354,-0.030957103\H,-0.0752256777,2.0322284323,2.1786274193\H,-1.35187

72295,-0.4157204074,2.2235330025\H,-1.6138078998,4.2597098857,-0.36576

39865\H,-0.3256640451,4.1271610513,0.8348046797\Br,-0.3916305249,-2.43
15546497,2.9208034678\H,-2.7655919679,1.8805803089,-1.0745221418\C,-3.
2502494446,-0.6038514381,0.0908387157\C,-3.2099773485,-1.8232517208,0.
6116873796\H,-3.9444071483,-0.2966464168,-0.6815733425\H,-3.9182751755
,-2.5586963258,0.2513279606\H,-2.4866390523,-2.1347261204,1.3681391868
\C,2.5552573383,-0.6880378458,1.1292860005\C,3.9755316084,-0.375671180
7,1.3153381403\O,2.976189347,0.6550744813,1.5317890526\H,2.1719878245,
-0.7302119131,0.1136602597\H,1.9823365025,-1.226417764,1.8797161452\H,
4.4301649847,-0.6913975604,2.2515096398\C,4.9181828609,-0.1747246447,0
.1609670646\H,5.679788022,0.5716156961,0.4048837379\H,5.43042095,-1.11
5051765,-0.0643130183\H,4.3789479432,0.1493336747,-0.7317027025\C,0.25
62710218,3.4764172818,-1.1551172158\H,0.7074476585,4.4551633018,-1.346
5976041\H,-0.2126809716,3.1375108963,-2.0795231411\C,1.3583568377,2.48
34942412,-0.8042294316\O,1.6801844203,1.5719076898,-1.5289874234\O,1.8
831105591,2.7333409892,0.394291525\H,2.4565881393,1.9672903276,0.70126
04057\\Version=EM64L-G09RevD.01\State=1-A\HF=-3338.9038835\RMSD=2.213e
-09\RMSF=4.451e-06\Dipole=-1.4467819,4.4728195,-3.1035413\Quadrupole=1
8.1851231,-5.0684789,-13.1166442,-9.8376761,11.8518119,8.2953664\PG=C0
1 [X(C11H17Br1N2O3)]\\@

ADAM SMITH SAID, "THE REAL PRICE OF ANYTHING IS THE TOIL AND TROUBLE
OF ACQUIRING IT." BUT IN ALL UNDERTAKINGS WITH NATURE WE SHOULD FIRST
READ CAREFULLY THE SMALL PRINT IN THE CONTRACT. THIS MIGHT DISCLOSE
THAT THE REAL PRICE IS TO BE PAID BY THOSE WHO INHERIT THE DEPLETION
AND DESPOILATION THAT FOLLOWS.
-- E. R. HARRISON IN "COSMOLOGY" (1980)
Job cpu time: 1 days 2 hours 5 minutes 20.9 seconds.
File lengths (MBytes): RWF= 160 Int= 0 D2E= 0 Chk= 19 Scr= 1
Normal termination of Gaussian 09 at Mon Jul 22 20:37:19 2024.

Entering Gaussian System, Link 0=g09
Input=cooh.gjf
Output=cooh.log
Initial command:
/apps/gaussian/09_D01/g09/l1.exe "/scr/tmp/sywang/91539/Gau-26321.inp" -
scrdir="/scr/tmp/sywang/91539/"
Entering Link 1 = /apps/gaussian/09_D01/g09/l1.exe PID= 26322.

This is part of the Gaussian(R) 09 program. It is based on
the Gaussian(R) 03 system (copyright 2003, Gaussian, Inc.),

Cite this work as:
Gaussian 09, Revision D.01,
M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria,
M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci,
G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian,
A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada,
M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima,
Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr.,
J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers,
K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand,
K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi,
M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross,
V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann,
O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski,
R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth,
P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels,
O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski,
and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

****
Gaussian 09: EM64L-G09RevD.01 24-Apr-2013
                22-Jul-2024
****
%chk=./cooh.chk
%mem=40000MB
%nprocl=1
Will use up to 1 processors via Linda.
%nprocs=28
Will use up to 28 processors via shared memory.
---
opt b3lyp/6-311++g(d,p)

1/14=-1,18=20,19=15,26=3,38=1/1,3;
2/9=110,12=2,17=6,18=5,40=1/2;
3/5=4,6=6,7=1111,11=2,16=1,25=1,30=1,71=1,74=-5/1,2,3;
4//1;
5/5=2,38=5/2;
6/7=2,8=2,9=2,10=2,28=1/1;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(2);
2/9=110/2;
99//99;
2/9=110/2;

3/5=4,6=6,7=1111,11=2,16=1,25=1,30=1,71=1,74=-5/1,2,3;
4/5=5,16=3,69=1/1;
5/5=2,38=5/2;
7//1,2,3,16;
1/14=-1,18=20,19=15,26=3/3(-5);
2/9=110/2;
6/7=2,8=2,9=2,10=2,19=2,28=1/1;
99/9=1/99;
---
cooh

Symbolic Z-matrix:
Charge = 0 Multiplicity = 1

C	-0.32729	-2.13805	-0.47352
C	-1.59791	-1.73421	-0.68918
N	-1.84847	-0.67052	0.17912
C	-0.70821	-0.38861	0.85177
N	0.2015	-1.33195	0.53049
C	1.57862	-1.31457	0.99766
H	0.25965	-2.89324	-0.96448
H	-2.33068	-2.07178	-1.39907
H	1.63228	-0.73878	1.919
H	1.89169	-2.33854	1.22037
Br	0.20275	1.98933	-0.13189
H	-0.65006	0.24824	1.71232
C	-3.01051	0.13624	0.24172
C	-4.23057	-0.30142	-0.04838
H	-2.78369	1.16128	0.51229
H	-5.0636	0.38746	-0.0239
H	-4.43907	-1.33019	-0.31681
C	2.61002	-0.70862	0.02779
H	2.65486	-1.30192	-0.86153
H	2.31928	0.28989	-0.22389
C	3.99533	-0.68589	0.70009
O	4.30568	-0.449	1.86677
O	4.99468	-0.97856	-0.16999
H	5.8557	-0.95739	0.27873

Add virtual bond connecting atoms C4 and Br11 Dist= 5.16D+00.
Add virtual bond connecting atoms H12 and Br11 Dist= 5.06D+00.
Add virtual bond connecting atoms H20 and Br11 Dist= 5.13D+00.

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.

Initialization pass.

Initial Parameters (Angstroms and Degrees)			
Name	Definition	Value	Derivative Info.
R1	R(1,2)	1.3506	estimate D2E/DX2
R2	R(1,5)	1.3919	estimate D2E/DX2
R3	R(1,7)	1.0751	estimate D2E/DX2
R4	R(2,3)	1.3958	estimate D2E/DX2
R5	R(2,8)	1.0746	estimate D2E/DX2
R6	R(3,4)	1.3536	estimate D2E/DX2
R7	R(3,13)	1.416	estimate D2E/DX2
R8	R(4,5)	1.3493	estimate D2E/DX2
R9	R(4,11)	2.7298	estimate D2E/DX2
R10	R(4,12)	1.0722	estimate D2E/DX2
R11	R(5,6)	1.4543	estimate D2E/DX2
R12	R(6,9)	1.0878	estimate D2E/DX2
R13	R(6,10)	1.0937	estimate D2E/DX2
R14	R(6,18)	1.54	estimate D2E/DX2
R15	R(11,12)	2.6758	estimate D2E/DX2
R16	R(11,20)	2.7159	estimate D2E/DX2
R17	R(13,14)	1.3282	estimate D2E/DX2
R18	R(13,15)	1.0841	estimate D2E/DX2
R19	R(14,16)	1.0813	estimate D2E/DX2
R20	R(14,17)	1.0835	estimate D2E/DX2
R21	R(18,19)	1.07	estimate D2E/DX2
R22	R(18,20)	1.07	estimate D2E/DX2
R23	R(18,21)	1.54	estimate D2E/DX2
R24	R(21,22)	1.2303	estimate D2E/DX2
R25	R(21,23)	1.357	estimate D2E/DX2
R26	R(23,24)	0.9712	estimate D2E/DX2
A1	A(2,1,5)	107.4226	estimate D2E/DX2
A2	A(2,1,7)	130.5964	estimate D2E/DX2
A3	A(5,1,7)	121.9243	estimate D2E/DX2
A4	A(1,2,3)	107.3029	estimate D2E/DX2
A5	A(1,2,8)	130.7724	estimate D2E/DX2
A6	A(3,2,8)	121.8658	estimate D2E/DX2
A7	A(2,3,4)	108.46	estimate D2E/DX2
A8	A(2,3,13)	127.5178	estimate D2E/DX2
A9	A(4,3,13)	123.4142	estimate D2E/DX2
A10	A(3,4,5)	107.6994	estimate D2E/DX2
A11	A(3,4,11)	106.4677	estimate D2E/DX2

! A12	A(3,4,12)	124.6299	estimate D2E/DX2	!
! A13	A(5,4,11)	107.3506	estimate D2E/DX2	!
! A14	A(5,4,12)	124.7372	estimate D2E/DX2	!
! A15	A(1,5,4)	108.6932	estimate D2E/DX2	!
! A16	A(1,5,6)	126.7524	estimate D2E/DX2	!
! A17	A(4,5,6)	123.6127	estimate D2E/DX2	!
! A18	A(5,6,9)	108.9722	estimate D2E/DX2	!
! A19	A(5,6,10)	108.9833	estimate D2E/DX2	!
! A20	A(5,6,18)	115.8866	estimate D2E/DX2	!
! A21	A(9,6,10)	107.9978	estimate D2E/DX2	!
! A22	A(9,6,18)	106.9843	estimate D2E/DX2	!
! A23	A(10,6,18)	107.7537	estimate D2E/DX2	!
! A24	A(4,11,20)	74.1685	estimate D2E/DX2	!
! A25	A(12,11,20)	82.2162	estimate D2E/DX2	!
! A26	A(3,13,14)	123.8076	estimate D2E/DX2	!
! A27	A(3,13,15)	112.2115	estimate D2E/DX2	!
! A28	A(14,13,15)	123.9327	estimate D2E/DX2	!
! A29	A(13,14,16)	119.5254	estimate D2E/DX2	!
! A30	A(13,14,17)	122.9387	estimate D2E/DX2	!
! A31	A(16,14,17)	117.5355	estimate D2E/DX2	!
! A32	A(6,18,19)	109.4712	estimate D2E/DX2	!
! A33	A(6,18,20)	109.4712	estimate D2E/DX2	!
! A34	A(6,18,21)	109.4712	estimate D2E/DX2	!
! A35	A(19,18,20)	109.4712	estimate D2E/DX2	!
! A36	A(19,18,21)	109.4713	estimate D2E/DX2	!
! A37	A(20,18,21)	109.4712	estimate D2E/DX2	!
! A38	A(11,20,18)	141.9723	estimate D2E/DX2	!
! A39	A(18,21,22)	130.0733	estimate D2E/DX2	!
! A40	A(18,21,23)	112.2947	estimate D2E/DX2	!
! A41	A(22,21,23)	117.632	estimate D2E/DX2	!
! A42	A(21,23,24)	110.6079	estimate D2E/DX2	!
! D1	D(5,1,2,3)	0.3774	estimate D2E/DX2	!
! D2	D(5,1,2,8)	177.5633	estimate D2E/DX2	!
! D3	D(7,1,2,3)	-176.8652	estimate D2E/DX2	!
! D4	D(7,1,2,8)	0.3208	estimate D2E/DX2	!
! D5	D(2,1,5,4)	-4.2823	estimate D2E/DX2	!
! D6	D(2,1,5,6)	-173.4144	estimate D2E/DX2	!
! D7	D(7,1,5,4)	173.251	estimate D2E/DX2	!
! D8	D(7,1,5,6)	4.1189	estimate D2E/DX2	!
! D9	D(1,2,3,4)	3.6377	estimate D2E/DX2	!
! D10	D(1,2,3,13)	174.8521	estimate D2E/DX2	!
! D11	D(8,2,3,4)	-173.8533	estimate D2E/DX2	!
! D12	D(8,2,3,13)	-2.6388	estimate D2E/DX2	!
! D13	D(2,3,4,5)	-6.2906	estimate D2E/DX2	!

! D14	D(2,3,4,11)	108.592	estimate D2E/DX2	!
! D15	D(2,3,4,12)	-167.6072	estimate D2E/DX2	!
! D16	D(13,3,4,5)	-177.9455	estimate D2E/DX2	!
! D17	D(13,3,4,11)	-63.0629	estimate D2E/DX2	!
! D18	D(13,3,4,12)	20.7378	estimate D2E/DX2	!
! D19	D(2,3,13,14)	31.6646	estimate D2E/DX2	!
! D20	D(2,3,13,15)	-145.8955	estimate D2E/DX2	!
! D21	D(4,3,13,14)	-158.3307	estimate D2E/DX2	!
! D22	D(4,3,13,15)	24.1093	estimate D2E/DX2	!
! D23	D(3,4,5,1)	6.5387	estimate D2E/DX2	!
! D24	D(3,4,5,6)	176.0875	estimate D2E/DX2	!
! D25	D(11,4,5,1)	-107.7574	estimate D2E/DX2	!
! D26	D(11,4,5,6)	61.7914	estimate D2E/DX2	!
! D27	D(12,4,5,1)	167.8302	estimate D2E/DX2	!
! D28	D(12,4,5,6)	-22.621	estimate D2E/DX2	!
! D29	D(3,4,11,20)	-129.4861	estimate D2E/DX2	!
! D30	D(5,4,11,20)	-14.3674	estimate D2E/DX2	!
! D31	D(1,5,6,9)	-168.2008	estimate D2E/DX2	!
! D32	D(1,5,6,10)	-50.5692	estimate D2E/DX2	!
! D33	D(1,5,6,18)	71.1238	estimate D2E/DX2	!
! D34	D(4,5,6,9)	24.183	estimate D2E/DX2	!
! D35	D(4,5,6,10)	141.8145	estimate D2E/DX2	!
! D36	D(4,5,6,18)	-96.4925	estimate D2E/DX2	!
! D37	D(5,6,18,19)	-63.4253	estimate D2E/DX2	!
! D38	D(5,6,18,20)	56.5747	estimate D2E/DX2	!
! D39	D(5,6,18,21)	176.5747	estimate D2E/DX2	!
! D40	D(9,6,18,19)	174.8344	estimate D2E/DX2	!
! D41	D(9,6,18,20)	-65.1656	estimate D2E/DX2	!
! D42	D(9,6,18,21)	54.8344	estimate D2E/DX2	!
! D43	D(10,6,18,19)	58.9206	estimate D2E/DX2	!
! D44	D(10,6,18,20)	178.9206	estimate D2E/DX2	!
! D45	D(10,6,18,21)	-61.0794	estimate D2E/DX2	!
! D46	D(4,11,20,18)	-2.569	estimate D2E/DX2	!
! D47	D(12,11,20,18)	19.307	estimate D2E/DX2	!
! D48	D(3,13,14,16)	-177.0315	estimate D2E/DX2	!
! D49	D(3,13,14,17)	2.7322	estimate D2E/DX2	!
! D50	D(15,13,14,16)	0.2458	estimate D2E/DX2	!
! D51	D(15,13,14,17)	-179.9906	estimate D2E/DX2	!
! D52	D(6,18,20,11)	-15.523	estimate D2E/DX2	!
! D53	D(19,18,20,11)	104.4769	estimate D2E/DX2	!
! D54	D(21,18,20,11)	-135.523	estimate D2E/DX2	!
! D55	D(6,18,21,22)	-38.1824	estimate D2E/DX2	!
! D56	D(6,18,21,23)	141.8207	estimate D2E/DX2	!
! D57	D(19,18,21,22)	-158.1824	estimate D2E/DX2	!

! D58 D(19,18,21,23) 21.8207 estimate D2E/DX2 !
! D59 D(20,18,21,22) 81.8176 estimate D2E/DX2 !
! D60 D(20,18,21,23) -98.1793 estimate D2E/DX2 !
! D61 D(18,21,23,24) 179.9996 estimate D2E/DX2 !
! D62 D(22,21,23,24) 0.0023 estimate D2E/DX2 !

Trust Radius=3.00D-01 FncErr=1.00D-07 GrdErr=1.00D-06
Number of steps in this run= 140 maximum allowed number of steps= 144.
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.327286	-2.138046	-0.473515
2	6	0	-1.597914	-1.734205	-0.689175
3	7	0	-1.848474	-0.670522	0.179118
4	6	0	-0.708208	-0.388612	0.851768
5	7	0	0.201498	-1.331948	0.530492
6	6	0	1.578618	-1.314572	0.997655
7	1	0	0.259653	-2.893236	-0.964483
8	1	0	-2.330681	-2.071776	-1.399070
9	1	0	1.632276	-0.738780	1.919003
10	1	0	1.891689	-2.338537	1.220372
11	35	0	0.202751	1.989331	-0.131890
12	1	0	-0.650055	0.248241	1.712324
13	6	0	-3.010509	0.136241	0.241716
14	6	0	-4.230567	-0.301418	-0.048384
15	1	0	-2.783692	1.161283	0.512286
16	1	0	-5.063604	0.387460	-0.023902
17	1	0	-4.439067	-1.330186	-0.316808
18	6	0	2.610017	-0.708624	0.027787
19	1	0	2.654857	-1.301919	-0.861533
20	1	0	2.319276	0.289890	-0.223886
21	6	0	3.995327	-0.685890	0.700095
22	8	0	4.305684	-0.448999	1.866767
23	8	0	4.994679	-0.978562	-0.169991
24	1	0	5.855704	-0.957388	0.278727

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.350590	0.000000			

3	N	2.212141	1.395756	0.000000		
4	C	2.227554	2.230852	1.353565	0.000000	
5	N	1.391918	2.210720	2.182506	1.349321	0.000000
6	C	2.544587	3.621028	3.581866	2.471489	1.454305
7	H	1.075109	2.206740	3.269936	3.241707	2.162395
8	H	2.207858	1.074641	2.164882	3.245263	3.268407
9	H	3.394403	4.269378	3.891976	2.596050	2.080129
10	H	2.798803	4.023545	4.225554	3.270710	2.084683
11	Br	4.175271	4.173450	3.373287	2.729843	3.386687
12	H	3.252144	3.255108	2.151988	1.072157	2.149155
13	C	3.589376	2.522013	1.416019	2.438898	3.543439
14	C	4.334690	3.065021	2.421232	3.636604	4.586970
15	H	4.229812	3.351631	2.083541	2.612481	3.889459
16	H	5.386375	4.117652	3.390812	4.509829	5.566419
17	H	4.193321	2.893793	2.718873	4.021373	4.717284
18	C	3.304890	4.390049	4.461221	3.433943	2.538150
19	H	3.121353	4.278159	4.664934	3.883264	2.820923
20	H	3.600205	4.433715	4.295922	3.283756	2.772080
21	C	4.708620	5.857762	5.866998	4.715360	3.852180
22	O	5.458407	6.560264	6.385209	5.115954	4.405630
23	O	5.455258	6.656037	6.858973	5.823654	4.856968
24	H	6.339495	7.556236	7.710161	6.613382	5.672189

		6	7	8	9	10
6	C	0.000000				
7	H	2.842857	0.000000			
8	H	4.647609	2.751998	0.000000		
9	H	1.087795	3.852307	5.337744	0.000000	
10	H	1.093673	2.782952	4.976047	1.764824	0.000000
11	Br	3.752953	4.953374	4.951425	3.700310	4.838550
12	H	2.814271	4.226315	4.229392	2.495188	3.659768
13	C	4.872000	4.618074	2.833670	5.013423	5.577978
14	C	5.988932	5.264868	2.927129	6.199583	6.575836
15	H	5.039364	5.280333	3.783011	5.008978	5.882968
16	H	6.932503	6.323348	3.925277	7.062443	7.573333
17	H	6.159593	4.994054	2.483252	6.496908	6.592281
18	C	1.540000	3.358770	5.320206	2.129222	2.143565
19	H	2.148263	2.877480	5.073186	3.015656	2.447720
20	H	2.148263	3.863007	5.346085	2.474288	3.029412
21	C	2.514809	4.647414	6.807757	2.659425	2.725293
22	O	2.990228	5.510049	7.572347	2.689575	3.132978
23	O	3.625710	5.168913	7.507773	3.965746	3.662129
24	H	4.351770	6.050526	8.430526	4.536038	4.302056

		11	12	13	14	15
11	Br	0.000000				

12	H	2.675780	0.000000			
13	C	3.728078	2.783339	0.000000		
14	C	4.990873	4.027690	1.328249	0.000000	
15	H	3.165354	2.612689	1.084143	2.132438	0.000000
16	H	5.505647	4.744816	2.085393	1.081251	2.466637
17	H	5.709629	4.578801	2.122059	1.083461	3.104043
18	C	3.619308	3.792272	5.687695	6.853116	5.729170
19	H	4.168637	4.466563	5.948263	7.005090	6.126382
20	H	2.715924	3.545077	5.352289	6.578821	5.228915
21	C	4.715150	4.845284	7.068787	8.268819	7.028685
22	O	5.174373	5.006930	7.517312	8.749695	7.395058
23	O	5.636702	6.075457	8.092918	9.250863	8.096141
24	H	6.388086	6.770055	8.933484	10.112871	8.898454

		16	17	18	19	20
16	H	0.000000				
17	H	1.850986	0.000000			
18	C	7.751679	7.084819	0.000000		
19	H	7.945456	7.114864	1.070000	0.000000	
20	H	7.386232	6.950430	1.070000	1.747303	0.000000
21	C	9.150983	8.519871	1.540000	2.148263	2.148263
22	O	9.594678	9.056222	2.514864	3.300958	2.977012
23	O	10.151670	9.441438	2.408028	2.461211	2.961360
24	H	11.005975	10.318719	3.264865	3.415307	3.783470

		21	22	23	24
21	C	0.000000			
22	O	1.230269	0.000000		
23	O	1.356986	2.214392	0.000000	
24	H	1.926724	2.276596	0.971165	0.000000

Stoichiometry C8H11BrN2O2
Framework group C1[X(C8H11BrN2O2)]
Deg. of freedom 66
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.669700	-2.116625	-0.687753
2	6	0	-1.988414	-1.833413	-0.757585
3	7	0	-2.247846	-0.830947	0.178305
4	6	0	-1.076147	-0.461175	0.746221
5	7	0	-0.118999	-1.297821	0.293942

6	6	0	1.291112	-1.160423	0.622139
7	1	0	-0.067543	-2.792208	-1.268144
8	1	0	-2.755210	-2.216833	-1.405555
9	1	0	1.384741	-0.614847	1.558556
10	1	0	1.721428	-2.155493	0.766309
11	35	0	-0.501906	2.028417	-0.215143
12	1	0	-0.990154	0.147703	1.624511
13	6	0	-3.468579	-0.146050	0.392401
14	6	0	-4.664935	-0.692046	0.205675
15	1	0	-3.313472	0.886295	0.684926
16	1	0	-5.552664	-0.090428	0.343859
17	1	0	-4.801330	-1.726355	-0.086705
18	6	0	2.154450	-0.421545	-0.417239
19	1	0	2.163318	-0.975887	-1.332404
20	1	0	1.745670	0.551445	-0.593558
21	6	0	3.593365	-0.285208	0.114304
22	8	0	3.998719	-0.059819	1.253799
23	8	0	4.520700	-0.446647	-0.863140
24	1	0	5.417562	-0.355986	-0.501781

Rotational constants (GHZ): 0.8622240 0.3207182 0.2531844

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 404 symmetry adapted cartesian basis functions of A symmetry.

There are 389 symmetry adapted basis functions of A symmetry.

389 basis functions, 625 primitive gaussians, 404 cartesian basis functions

62 alpha electrons 62 beta electrons

nuclear repulsion energy 1075.2182428292 Hartrees.

NAtoms= 24 NActive= 24 NUniq= 24 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 389 RedAO= T EigKep= 6.28D-06 NBF= 389

NBsUse= 389 1.00D-06 EigRej= -1.00D+00 NBFU= 389

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0
NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=2910765817.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3145.72413531 A.U. after 15 cycles
NFock= 15 Conv=0.61D-08 -V/T= 2.0017

****

Population analysis using the SCF density.

****

Orbital symmetries:
Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A)
Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A)

The electronic state is 1-A.

Alpha occ. eigenvalues -- -482.71591 -62.36923 -56.18742 -56.18674 -56.18666
Alpha occ. eigenvalues -- -19.18309 -19.12999 -14.42793 -14.42384 -10.32983
Alpha occ. eigenvalues -- -10.30323 -10.25656 -10.25541 -10.25408 -10.25137
Alpha occ. eigenvalues -- -10.20622 -10.20560 -8.57833 -6.40277 -6.40050
Alpha occ. eigenvalues -- -6.40014 -2.51491 -2.51437 -2.51407 -2.51228
Alpha occ. eigenvalues -- -2.51228 -1.12241 -1.09728 -1.02432 -0.98774
Alpha occ. eigenvalues -- -0.84997 -0.81553 -0.80179 -0.73105 -0.69487
Alpha occ. eigenvalues -- -0.66265 -0.65061 -0.63372 -0.61857 -0.57690
Alpha occ. eigenvalues -- -0.54318 -0.52280 -0.51082 -0.50706 -0.50070
Alpha occ. eigenvalues -- -0.49552 -0.48981 -0.47349 -0.46698 -0.45511
Alpha occ. eigenvalues -- -0.42751 -0.41961 -0.40674 -0.39270 -0.36835
Alpha occ. eigenvalues -- -0.33642 -0.30859 -0.29829 -0.29267 -0.21266
Alpha occ. eigenvalues -- -0.20988 -0.20722
Alpha virt. eigenvalues -- -0.06520 -0.03688 -0.02534 -0.02191 -0.01381
Alpha virt. eigenvalues -- -0.00450 -0.00379 0.00162 0.01015 0.01585
Alpha virt. eigenvalues -- 0.02751 0.03221 0.03798 0.04482 0.05244
Alpha virt. eigenvalues -- 0.05536 0.06379 0.06652 0.06825 0.07876
Alpha virt. eigenvalues -- 0.08295 0.08822 0.08927 0.09216 0.09380
Alpha virt. eigenvalues -- 0.09873 0.10185 0.10394 0.10878 0.11218
Alpha virt. eigenvalues -- 0.11666 0.11980 0.12179 0.12612 0.12984
Alpha virt. eigenvalues -- 0.13264 0.13635 0.13902 0.14086 0.14971
Alpha virt. eigenvalues -- 0.15192 0.15386 0.16111 0.16687 0.17074
Alpha virt. eigenvalues -- 0.17238 0.17914 0.18233 0.18612 0.19135
Alpha virt. eigenvalues -- 0.20002 0.20401 0.20517 0.21299 0.21473
Alpha virt. eigenvalues -- 0.22021 0.22314 0.22687 0.23362 0.23632
Alpha virt. eigenvalues -- 0.24353 0.24667 0.24904 0.25621 0.26976
Alpha virt. eigenvalues -- 0.27288 0.28256 0.28397 0.28802 0.29011
Alpha virt. eigenvalues -- 0.29804 0.30598 0.31319 0.31581 0.32276
Alpha virt. eigenvalues -- 0.32718 0.33209 0.33552 0.33877 0.34801
Alpha virt. eigenvalues -- 0.35160 0.36060 0.36681 0.38044 0.38554
Alpha virt. eigenvalues -- 0.39319 0.40968 0.41751 0.42797 0.46097
Alpha virt. eigenvalues -- 0.46426 0.47556 0.47868 0.49167 0.49446
Alpha virt. eigenvalues -- 0.50781 0.51725 0.52607 0.54338 0.55514
Alpha virt. eigenvalues -- 0.56040 0.56639 0.57563 0.59215 0.59650
Alpha virt. eigenvalues -- 0.60434 0.61699 0.62197 0.62940 0.63874

Alpha virt. eigenvalues --	0.64011	0.65296	0.66573	0.67788	0.67809
Alpha virt. eigenvalues --	0.69057	0.69542	0.70467	0.71144	0.71946
Alpha virt. eigenvalues --	0.72834	0.73674	0.73786	0.74587	0.76314
Alpha virt. eigenvalues --	0.76862	0.77299	0.78304	0.79103	0.80931
Alpha virt. eigenvalues --	0.82417	0.83704	0.83724	0.86135	0.87291
Alpha virt. eigenvalues --	0.87462	0.89365	0.91437	0.92478	0.94747
Alpha virt. eigenvalues --	0.95601	0.97693	0.98406	1.01022	1.02497
Alpha virt. eigenvalues --	1.03086	1.04773	1.06620	1.08405	1.09345
Alpha virt. eigenvalues --	1.10937	1.11621	1.12797	1.14104	1.15916
Alpha virt. eigenvalues --	1.18080	1.19467	1.20563	1.21497	1.22958
Alpha virt. eigenvalues --	1.24319	1.27026	1.29652	1.30696	1.34312
Alpha virt. eigenvalues --	1.35283	1.39526	1.41249	1.45035	1.45845
Alpha virt. eigenvalues --	1.46875	1.48302	1.50589	1.51757	1.53051
Alpha virt. eigenvalues --	1.53502	1.53997	1.56452	1.57825	1.58597
Alpha virt. eigenvalues --	1.60011	1.60534	1.61982	1.62728	1.64977
Alpha virt. eigenvalues --	1.65574	1.68220	1.68727	1.69874	1.70965
Alpha virt. eigenvalues --	1.72769	1.73607	1.75409	1.76610	1.78372
Alpha virt. eigenvalues --	1.79156	1.79904	1.80609	1.83674	1.87491
Alpha virt. eigenvalues --	1.88772	1.91492	1.93375	1.96078	1.97323
Alpha virt. eigenvalues --	2.01056	2.02398	2.03088	2.05086	2.07463
Alpha virt. eigenvalues --	2.09444	2.11054	2.11316	2.11926	2.12514
Alpha virt. eigenvalues --	2.13547	2.18681	2.19967	2.21086	2.22439
Alpha virt. eigenvalues --	2.23730	2.28082	2.32365	2.35228	2.37200
Alpha virt. eigenvalues --	2.40127	2.42826	2.47072	2.48124	2.49871
Alpha virt. eigenvalues --	2.51919	2.52987	2.55177	2.55888	2.58679
Alpha virt. eigenvalues --	2.59326	2.60244	2.60471	2.61604	2.62796
Alpha virt. eigenvalues --	2.63665	2.69298	2.70940	2.72140	2.73032
Alpha virt. eigenvalues --	2.73947	2.75568	2.77403	2.78402	2.80787
Alpha virt. eigenvalues --	2.81941	2.83264	2.85616	2.86283	2.87272
Alpha virt. eigenvalues --	2.88235	2.91910	2.92662	2.97393	2.98391
Alpha virt. eigenvalues --	3.00037	3.03431	3.06318	3.11048	3.14754
Alpha virt. eigenvalues --	3.16085	3.16385	3.25237	3.30518	3.34388
Alpha virt. eigenvalues --	3.39669	3.50301	3.55173	3.56561	3.58875
Alpha virt. eigenvalues --	3.60523	3.63330	3.67575	3.73125	3.76127
Alpha virt. eigenvalues --	3.77981	3.78861	3.84283	3.88909	3.90041
Alpha virt. eigenvalues --	3.92646	4.05088	4.05611	4.08496	4.10560
Alpha virt. eigenvalues --	4.19885	4.27118	4.29112	4.32596	4.34649
Alpha virt. eigenvalues --	4.48482	4.69583	4.94758	4.97355	5.02660
Alpha virt. eigenvalues --	5.05051	5.17073	5.20846	5.35299	5.54499
Alpha virt. eigenvalues --	5.83728	6.77996	7.67905	7.72958	7.76784
Alpha virt. eigenvalues --	23.71206	23.73760	23.75018	23.84379	23.86555
Alpha virt. eigenvalues --	23.92430	24.17309	24.23182	35.46307	35.57225
Alpha virt. eigenvalues --	48.06168	49.84663	49.98337	289.88566	289.93675
Alpha virt. eigenvalues --	289.97127	1020.85690			

Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	7.626355	-1.903659	0.239146	-0.068078	-0.173921	-0.017657
2	C	-1.903659	7.692729	0.006223	-0.034777	0.318888	-0.286461
3	N	0.239146	0.006223	6.619636	0.246667	-0.168637	-0.114322
4	C	-0.068078	-0.034777	0.246667	5.970167	0.423645	-0.648354
5	N	-0.173921	0.318888	-0.168637	0.423645	6.722181	0.007711
6	C	-0.017657	-0.286461	-0.114322	-0.648354	0.007711	8.163472
7	H	0.610011	-0.221332	0.052224	-0.002725	-0.093340	-0.019166
8	H	-0.101863	0.494865	-0.075799	0.003167	0.030558	0.007211
9	H	0.012672	-0.004578	0.014240	0.049679	-0.043433	0.222642
10	H	-0.019157	-0.012528	-0.016775	-0.018043	-0.051703	0.600094
11	Br	0.034993	-0.012525	-0.026164	-0.060549	-0.033472	0.385996
12	H	-0.047857	0.074003	-0.053236	0.435634	-0.037793	-0.017110
13	C	0.285192	-0.373613	0.154979	-0.060024	-0.043744	-0.130806
14	C	-0.131632	0.200425	-0.069728	-0.156935	-0.019463	-0.058503
15	H	0.017604	-0.042131	-0.089232	0.045804	0.000367	-0.031032
16	H	-0.009662	0.014285	0.026740	-0.006980	0.000836	0.000147
17	H	0.019741	-0.021213	-0.035849	0.010603	-0.000623	-0.001527
18	C	0.030517	0.066083	0.055373	0.226499	-0.031229	-1.712723
19	H	0.041998	-0.033949	0.004464	-0.003054	-0.016344	-0.064530
20	H	-0.003228	0.001103	-0.002218	-0.025544	0.026402	0.046607
21	C	-0.199914	0.155535	-0.010052	-0.021864	0.012285	0.344706
22	O	0.004996	-0.003190	0.000044	-0.006531	0.003007	0.035070
23	O	-0.002741	0.000605	0.000068	-0.001055	-0.002257	-0.010469
24	H	-0.001593	0.000949	-0.000026	0.000202	0.000205	0.005798

		7	8	9	10	11	12
1	C	0.610011	-0.101863	0.012672	-0.019157	0.034993	-0.047857
2	C	-0.221332	0.494865	-0.004578	-0.012528	-0.012525	0.074003
3	N	0.052224	-0.075799	0.014240	-0.016775	-0.026164	-0.053236
4	C	-0.002725	0.003167	0.049679	-0.018043	-0.060549	0.435634
5	N	-0.093340	0.030558	-0.043433	-0.051703	-0.033472	-0.037793
6	C	-0.019166	0.007211	0.222642	0.600094	0.385996	-0.017110
7	H	0.516247	-0.010389	0.002895	-0.007688	0.002053	-0.003667
8	H	-0.010389	0.495233	0.000213	0.000182	0.000407	0.000728
9	H	0.002895	0.000213	0.525164	-0.049737	-0.026162	-0.009960
10	H	-0.007688	0.000182	-0.049737	0.554326	0.009203	0.006952
11	Br	0.002053	0.000407	-0.026162	0.009203	35.576519	-0.076935
12	H	-0.003667	0.000728	-0.009960	0.006952	-0.076935	0.487031
13	C	0.017223	-0.014416	0.008492	-0.010823	-0.046145	-0.032999
14	C	-0.005615	0.000230	0.000888	-0.000632	0.001942	0.032399
15	H	0.001460	-0.001307	0.005236	-0.002166	0.061555	-0.032659
16	H	-0.000087	0.001547	-0.000088	0.000021	0.001912	0.000002
17	H	0.000262	-0.004945	0.000053	0.000004	-0.001323	0.000667

18	C	0.016925	-0.000142	0.116543	-0.196086	-0.317789	-0.033799
19	H	0.001886	0.000351	0.013953	-0.016771	-0.007785	-0.000392
20	H	-0.000093	0.000077	-0.019736	0.011732	0.081630	0.009242
21	C	-0.020291	0.000725	-0.040490	0.012775	0.017615	0.015610
22	O	0.000701	-0.000051	0.000242	0.001605	-0.000092	0.001275
23	O	0.000089	0.000001	-0.000071	0.002628	0.000227	0.000392
24	H	-0.000267	0.000000	0.000799	-0.001426	-0.000133	0.000114
		13	14	15	16	17	18
1	C	0.285192	-0.131632	0.017604	-0.009662	0.019741	0.030517
2	C	-0.373613	0.200425	-0.042131	0.014285	-0.021213	0.066083
3	N	0.154979	-0.069728	-0.089232	0.026740	-0.035849	0.055373
4	C	-0.060024	-0.156935	0.045804	-0.006980	0.010603	0.226499
5	N	-0.043744	-0.019463	0.000367	0.000836	-0.000623	-0.031229
6	C	-0.130806	-0.058503	-0.031032	0.000147	-0.001527	-1.712723
7	H	0.017223	-0.005615	0.001460	-0.000087	0.000262	0.016925
8	H	-0.014416	0.000230	-0.001307	0.001547	-0.004945	-0.000142
9	H	0.008492	0.000888	0.005236	-0.000088	0.000053	0.116543
10	H	-0.010823	-0.000632	-0.002166	0.000021	0.000004	-0.196086
11	Br	-0.046145	0.001942	0.061555	0.001912	-0.001323	-0.317789
12	H	-0.032999	0.032399	-0.032659	0.000002	0.000667	-0.033799
13	C	5.784920	-0.035377	0.449636	-0.082564	0.046547	0.051576
14	C	-0.035377	5.905951	-0.079336	0.437403	0.333355	0.006106
15	H	0.449636	-0.079336	0.522711	-0.009577	0.004896	0.023150
16	H	-0.082564	0.437403	-0.009577	0.495089	-0.029032	-0.000221
17	H	0.046547	0.333355	0.004896	-0.029032	0.541702	0.000472
18	C	0.051576	0.006106	0.023150	-0.000221	0.000472	8.079069
19	H	0.000660	-0.000159	0.000062	-0.000045	0.000018	0.489434
20	H	-0.003888	0.000262	-0.007256	0.000162	-0.000077	0.225278
21	C	-0.009443	0.002541	-0.002962	0.000104	-0.000231	-1.004415
22	O	-0.000465	-0.000024	-0.000026	0.000000	-0.000001	-0.063925
23	O	-0.000137	0.000001	-0.000027	0.000001	-0.000003	-0.156856
24	H	-0.000064	0.000004	-0.000017	0.000000	-0.000001	-0.075266
		19	20	21	22	23	24
1	C	0.041998	-0.003228	-0.199914	0.004996	-0.002741	-0.001593
2	C	-0.033949	0.001103	0.155535	-0.003190	0.000605	0.000949
3	N	0.004464	-0.002218	-0.010052	0.000044	0.000068	-0.000026
4	C	-0.003054	-0.025544	-0.021864	-0.006531	-0.001055	0.000202
5	N	-0.016344	0.026402	0.012285	0.003007	-0.002257	0.000205
6	C	-0.064530	0.046607	0.344706	0.035070	-0.010469	0.005798
7	H	0.001886	-0.000093	-0.020291	0.000701	0.000089	-0.000267
8	H	0.000351	0.000077	0.000725	-0.000051	0.000001	0.000000
9	H	0.013953	-0.019736	-0.040490	0.000242	-0.000071	0.000799
10	H	-0.016771	0.011732	0.012775	0.001605	0.002628	-0.001426
11	Br	-0.007785	0.081630	0.017615	-0.000092	0.000227	-0.000133

12	H	-0.000392	0.009242	0.015610	0.001275	0.000392	0.000114
13	C	0.000660	-0.003888	-0.009443	-0.000465	-0.000137	-0.000064
14	C	-0.000159	0.000262	0.002541	-0.000024	0.000001	0.000004
15	H	0.000062	-0.007256	-0.002962	-0.000026	-0.000027	-0.000017
16	H	-0.000045	0.000162	0.000104	0.000000	0.000001	0.000000
17	H	0.000018	-0.000077	-0.000231	-0.000001	-0.000003	-0.000001
18	C	0.489434	0.225278	-1.004415	-0.063925	-0.156856	-0.075266
19	H	0.567126	-0.025521	-0.119696	0.000720	-0.020220	0.003051
20	H	-0.025521	0.505764	-0.020527	-0.000352	-0.004822	-0.000036
21	C	-0.119696	-0.020527	6.378316	0.376812	0.215901	0.079039
22	O	0.000720	-0.000352	0.376812	8.073579	-0.137211	-0.006456
23	O	-0.020220	-0.004822	0.215901	-0.137211	8.022937	0.244826
24	H	0.003051	-0.000036	0.079039	-0.006456	0.244826	0.462623

Mulliken charges:

		1
1	C	-0.242264
2	C	-0.075738
3	N	0.242233
4	C	-0.297554
5	N	0.169871
6	C	-0.706796
7	H	0.162688
8	H	0.173418
9	H	0.220546
10	H	0.204011
11	Br	-0.564979
12	H	0.282358
13	C	0.045284
14	C	-0.364105
15	H	0.165246
16	H	0.160006
17	H	0.136504
18	C	0.205425
19	H	0.184745
20	H	0.205040
21	C	-0.162079
22	O	-0.279727
23	O	-0.151808
24	H	0.287677

Sum of Mulliken charges = 0.00000

Mulliken charges with hydrogens summed into heavy atoms:

		1
1	C	-0.079576
2	C	0.097680

```
     3    N       0.242233
     4    C      -0.015197
     5    N       0.169871
     6    C      -0.282239
    11    Br     -0.564979
    13    C       0.210531
    14    C      -0.067596
    18    C       0.595209
    21    C      -0.162079
    22    O      -0.279727
    23    O       0.135868
 Electronic spatial extent (au):  <R**2>=           4109.9235
 Charge=                 0.0000 electrons
 Dipole moment (field-independent basis, Debye):
    X=              -2.4678    Y=              -8.8466    Z=              -0.1826
Tot=               9.1862
 Quadrupole moment (field-independent basis, Debye-Ang):
   XX=             -71.2779   YY=             -97.6478   ZZ=             -94.2160
   XY=               3.1249   XZ=              -6.2496   YZ=               5.4927
 Traceless Quadrupole moment (field-independent basis, Debye-Ang):
   XX=              16.4360   YY=              -9.9339   ZZ=              -6.5021
   XY=               3.1249   XZ=              -6.2496   YZ=               5.4927
 Octapole moment (field-independent basis, Debye-Ang**2):
  XXX=              -4.1096   YYY=               5.4972   ZZZ=              -4.3353
XYY=               8.4768
  XXY=              -0.1303   XXZ=             -30.6398   XZZ=             -13.1663
YZZ=              10.7590
  YYZ=             -10.6412   XYZ=             -14.2714
 Hexadecapole moment (field-independent basis, Debye-Ang**3):
 XXXX=           -2932.8804 YYYY=           -1141.4315 ZZZZ=            -323.4114
XXXY=             -28.9663
 XXXZ=            -121.4415 YYYX=             -16.5268 YYYZ=              22.4962
ZZZX=              -3.2578
 ZZZY=               1.5313 XXYY=            -781.3160 XXZZ=            -794.4060
YYZZ=            -228.7172
 XXYZ=              21.2425 YYXZ=              17.8909 ZZXY=              -6.2633
 N-N= 1.075218242829D+03 E-N=-9.638283007715D+03  KE= 3.140286911055D+03
 Calling FoFJK, ICntrl=           2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 -------------------------------------------------------------------
 Center         Atomic                     Forces (Hartrees/Bohr)
 Number         Number                X                    Y                    Z
 -------------------------------------------------------------------
```

1	6	0.002148022	0.002359798	0.000502463
2	6	-0.001725076	0.001226309	-0.000409685
3	7	0.000207225	-0.001103507	-0.001158102
4	6	0.000702062	-0.003535154	0.000305259
5	7	-0.000152932	0.004603076	-0.001551498
6	6	0.014975340	-0.001536042	0.007369878
7	1	-0.000135814	-0.001181894	0.000306103
8	1	-0.000168435	-0.000027726	0.000056249
9	1	-0.004196699	-0.001518618	0.002757625
10	1	-0.004862554	-0.000325070	0.002356527
11	35	-0.000413979	0.001775478	-0.001519076
12	1	0.000236806	-0.000072791	-0.000083835
13	6	-0.000514726	0.000022765	-0.000120896
14	6	0.000134216	0.000129406	0.000020867
15	1	-0.000254833	0.000023327	0.000154089
16	1	-0.000003686	0.000015655	0.000021889
17	1	-0.000012047	0.000027703	0.000045063
18	6	0.009635268	-0.011670756	0.021720154
19	1	0.004623826	-0.005011219	-0.013540280
20	1	-0.003536651	0.017149172	-0.004177389
21	6	0.027271936	0.004191110	0.025435527
22	8	-0.028802157	-0.004966493	-0.026770272
23	8	-0.008754949	-0.003520405	-0.016034291
24	1	-0.006400163	0.002945876	0.004313629

Cartesian Forces: Max 0.028802157 RMS 0.008373277

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.033610117 RMS 0.005473375

Search for a local minimum.

Step number 1 out of a maximum of 140

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Second derivative matrix not updated -- first step.

ITU= 0

Eigenvalues ---	0.00237	0.00377	0.00640	0.00809	0.01480
Eigenvalues ---	0.01761	0.01964	0.02032	0.02123	0.02207
Eigenvalues ---	0.02261	0.02317	0.02348	0.02435	0.03021
Eigenvalues ---	0.03038	0.03038	0.03376	0.03700	0.04440
Eigenvalues ---	0.05097	0.05603	0.06628	0.07629	0.09834
Eigenvalues ---	0.11054	0.12467	0.14721	0.15757	0.15969
Eigenvalues ---	0.15982	0.15992	0.16000	0.16000	0.16000

Eigenvalues ---	0.17619	0.18474	0.20652	0.22002	0.22812
Eigenvalues ---	0.24474	0.25000	0.25000	0.27824	0.28519
Eigenvalues ---	0.34392	0.35069	0.35498	0.35579	0.35613
Eigenvalues ---	0.35844	0.35939	0.36592	0.36627	0.36650
Eigenvalues ---	0.37230	0.41289	0.43066	0.43842	0.47825
Eigenvalues ---	0.52364	0.53140	0.53562	0.54471	0.59921
Eigenvalues ---	0.90974				

RFO step: Lambda=-1.27208050D-02 EMin= 2.36824093D-03

Linear search not attempted -- first point.

Iteration 1 RMS(Cart)= 0.04764848 RMS(Int)= 0.00107642

Iteration 2 RMS(Cart)= 0.00162624 RMS(Int)= 0.00030124

Iteration 3 RMS(Cart)= 0.00000253 RMS(Int)= 0.00030123

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00030123

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55224	0.00152	0.00000	0.00245	0.00247	2.55472
R2	2.63034	-0.00062	0.00000	-0.00131	-0.00132	2.62902
R3	2.03166	0.00062	0.00000	0.00163	0.00163	2.03329
R4	2.63760	-0.00154	0.00000	-0.00338	-0.00336	2.63424
R5	2.03078	0.00009	0.00000	0.00023	0.00023	2.03101
R6	2.55787	0.00077	0.00000	0.00154	0.00154	2.55941
R7	2.67589	0.00066	0.00000	0.00149	0.00149	2.67738
R8	2.54985	-0.00010	0.00000	-0.00134	-0.00125	2.54860
R9	5.15866	0.00087	0.00000	0.01376	0.01391	5.17257
R10	2.02608	-0.00001	0.00000	-0.00026	-0.00023	2.02586
R11	2.74824	0.00206	0.00000	0.00346	0.00342	2.75166
R12	2.05563	0.00132	0.00000	0.00364	0.00364	2.05927
R13	2.06674	-0.00061	0.00000	-0.00170	-0.00170	2.06504
R14	2.91018	0.00214	0.00000	0.00770	0.00780	2.91798
R15	5.05649	0.00085	0.00000	0.01545	0.01528	5.07177
R16	5.13235	-0.00108	0.00000	-0.00531	-0.00540	5.12695
R17	2.51003	-0.00018	0.00000	-0.00030	-0.00030	2.50972
R18	2.04873	0.00001	0.00000	0.00002	0.00002	2.04875
R19	2.04327	0.00001	0.00000	0.00003	0.00003	2.04330
R20	2.04744	-0.00003	0.00000	-0.00009	-0.00009	2.04735
R21	2.02201	0.01423	0.00000	0.03695	0.03695	2.05896
R22	2.02201	0.01743	0.00000	0.04767	0.04762	2.06962
R23	2.91018	-0.02073	0.00000	-0.06959	-0.06959	2.84059
R24	2.32487	-0.03361	0.00000	-0.03644	-0.03644	2.28844
R25	2.56433	-0.00352	0.00000	-0.00642	-0.00642	2.55791
R26	1.83524	-0.00362	0.00000	-0.00665	-0.00665	1.82859
A1	1.87488	0.00092	0.00000	0.00389	0.00384	1.87872
A2	2.27934	-0.00062	0.00000	-0.00270	-0.00274	2.27660
A3	2.12798	-0.00027	0.00000	-0.00052	-0.00055	2.12743

A4	1.87279	-0.00054	0.00000	-0.00269	-0.00268	1.87011
A5	2.28241	0.00040	0.00000	0.00222	0.00218	2.28459
A6	2.12696	0.00017	0.00000	0.00096	0.00093	2.12789
A7	1.89298	-0.00012	0.00000	-0.00022	-0.00020	1.89278
A8	2.22561	0.00004	0.00000	-0.00030	-0.00030	2.22531
A9	2.15398	0.00009	0.00000	0.00051	0.00049	2.15447
A10	1.87971	0.00084	0.00000	0.00255	0.00247	1.88218
A11	1.85821	-0.00317	0.00000	-0.00917	-0.00897	1.84924
A12	2.17520	-0.00035	0.00000	-0.00147	-0.00148	2.17373
A13	1.87362	0.00319	0.00000	0.00739	0.00746	1.88109
A14	2.17708	-0.00059	0.00000	-0.00121	-0.00116	2.17591
A15	1.89705	-0.00118	0.00000	-0.00429	-0.00423	1.89283
A16	2.21225	-0.00192	0.00000	-0.00952	-0.00950	2.20274
A17	2.15745	0.00324	0.00000	0.01551	0.01539	2.17284
A18	1.90192	-0.00109	0.00000	-0.01626	-0.01576	1.88617
A19	1.90212	-0.00062	0.00000	-0.01753	-0.01671	1.88541
A20	2.02260	-0.00788	0.00000	-0.04841	-0.04800	1.97460
A21	1.88492	-0.00220	0.00000	-0.00609	-0.00784	1.87708
A22	1.86723	0.00613	0.00000	0.04582	0.04509	1.91232
A23	1.88066	0.00600	0.00000	0.04576	0.04465	1.92531
A24	1.29449	-0.00196	0.00000	-0.01273	-0.01287	1.28161
A25	1.43494	-0.00104	0.00000	-0.00736	-0.00753	1.42741
A26	2.16085	0.00009	0.00000	0.00041	0.00041	2.16126
A27	1.95846	0.00020	0.00000	0.00128	0.00128	1.95974
A28	2.16303	-0.00029	0.00000	-0.00157	-0.00158	2.16146
A29	2.08611	-0.00003	0.00000	-0.00017	-0.00017	2.08594
A30	2.14569	0.00003	0.00000	0.00016	0.00016	2.14585
A31	2.05138	0.00000	0.00000	0.00001	0.00001	2.05139
A32	1.91063	0.00502	0.00000	0.04936	0.04936	1.95999
A33	1.91063	0.00083	0.00000	0.00627	0.00610	1.91674
A34	1.91063	-0.00302	0.00000	-0.01190	-0.01195	1.89868
A35	1.91063	-0.00186	0.00000	-0.01185	-0.01270	1.89793
A36	1.91063	-0.00125	0.00000	-0.01452	-0.01460	1.89604
A37	1.91063	0.00028	0.00000	-0.01736	-0.01735	1.89328
A38	2.47788	0.00003	0.00000	0.00435	0.00417	2.48205
A39	2.27021	-0.02084	0.00000	-0.07934	-0.07935	2.19086
A40	1.95991	-0.00702	0.00000	-0.02673	-0.02674	1.93317
A41	2.05307	0.02787	0.00000	0.10606	0.10605	2.15911
A42	1.93047	-0.01341	0.00000	-0.07764	-0.07764	1.85283
D1	0.00659	-0.00044	0.00000	-0.00400	-0.00403	0.00256
D2	3.09906	0.00043	0.00000	0.00773	0.00771	3.10678
D3	-3.08688	-0.00118	0.00000	-0.02026	-0.02022	-3.10710
D4	0.00560	-0.00030	0.00000	-0.00854	-0.00849	-0.00289
D5	-0.07474	0.00000	0.00000	-0.00035	-0.00032	-0.07506

D6	-3.02665	-0.00113	0.00000	-0.01195	-0.01182	-3.03847
D7	3.02380	0.00064	0.00000	0.01411	0.01411	3.03791
D8	0.07189	-0.00049	0.00000	0.00251	0.00261	0.07450
D9	0.06349	0.00074	0.00000	0.00702	0.00702	0.07051
D10	3.05175	0.00080	0.00000	0.00695	0.00698	3.05872
D11	-3.03431	-0.00005	0.00000	-0.00349	-0.00349	-3.03780
D12	-0.04606	0.00001	0.00000	-0.00356	-0.00353	-0.04959
D13	-0.10979	-0.00084	0.00000	-0.00756	-0.00756	-0.11735
D14	1.89529	0.00168	0.00000	-0.00233	-0.00221	1.89308
D15	-2.92530	-0.00047	0.00000	-0.00700	-0.00693	-2.93222
D16	-3.10574	-0.00089	0.00000	-0.00741	-0.00744	-3.11318
D17	-1.10066	0.00163	0.00000	-0.00218	-0.00209	-1.10274
D18	0.36194	-0.00052	0.00000	-0.00685	-0.00681	0.35514
D19	0.55265	-0.00002	0.00000	-0.00030	-0.00032	0.55233
D20	-2.54636	-0.00012	0.00000	-0.00318	-0.00320	-2.54955
D21	-2.76339	0.00002	0.00000	-0.00045	-0.00043	-2.76382
D22	0.42079	-0.00008	0.00000	-0.00333	-0.00331	0.41748
D23	0.11412	0.00048	0.00000	0.00475	0.00472	0.11884
D24	3.07331	0.00091	0.00000	0.01267	0.01273	3.08603
D25	-1.88072	0.00216	0.00000	0.01049	0.01023	-1.87049
D26	1.07846	0.00259	0.00000	0.01841	0.01824	1.09670
D27	2.92919	0.00016	0.00000	0.00413	0.00401	2.93320
D28	-0.39481	0.00059	0.00000	0.01205	0.01202	-0.38280
D29	-2.25996	0.00226	0.00000	0.01347	0.01342	-2.24654
D30	-0.25076	0.00320	0.00000	0.01546	0.01539	-0.23536
D31	-2.93566	0.00183	0.00000	0.01076	0.01085	-2.92480
D32	-0.88260	-0.00178	0.00000	-0.01575	-0.01615	-0.89874
D33	1.24134	0.00008	0.00000	-0.00334	-0.00356	1.23778
D34	0.42207	0.00109	0.00000	0.00009	0.00015	0.42222
D35	2.47513	-0.00252	0.00000	-0.02643	-0.02685	2.44828
D36	-1.68411	-0.00066	0.00000	-0.01402	-0.01426	-1.69837
D37	-1.10698	-0.00089	0.00000	-0.00404	-0.00435	-1.11133
D38	0.98741	0.00041	0.00000	0.01551	0.01539	1.00280
D39	3.08181	-0.00059	0.00000	-0.00920	-0.00932	3.07249
D40	3.05144	0.00105	0.00000	0.01409	0.01461	3.06604
D41	-1.13735	0.00236	0.00000	0.03365	0.03435	-1.10301
D42	0.95704	0.00136	0.00000	0.00894	0.00963	0.96668
D43	1.02836	-0.00245	0.00000	-0.02460	-0.02556	1.00280
D44	3.12275	-0.00115	0.00000	-0.00504	-0.00582	3.11693
D45	-1.06604	-0.00214	0.00000	-0.02975	-0.03053	-1.09657
D46	-0.04484	-0.00043	0.00000	0.00898	0.00903	-0.03581
D47	0.33697	-0.00073	0.00000	0.00646	0.00649	0.34346
D48	-3.08978	-0.00008	0.00000	-0.00215	-0.00215	-3.09194
D49	0.04769	-0.00003	0.00000	-0.00085	-0.00084	0.04684

D50	0.00429	0.00004	0.00000	0.00113	0.00113	0.00542
D51	-3.14143	0.00010	0.00000	0.00244	0.00244	-3.13899
D52	-0.27093	-0.00409	0.00000	-0.03844	-0.03846	-0.30939
D53	1.82347	0.00143	0.00000	0.01860	0.01819	1.84165
D54	-2.36532	-0.00107	0.00000	-0.01707	-0.01708	-2.38240
D55	-0.66641	0.00200	0.00000	0.05964	0.05965	-0.60676
D56	2.47524	0.00220	0.00000	0.06983	0.06955	2.54479
D57	-2.76080	-0.00153	0.00000	0.01537	0.01557	-2.74523
D58	0.38084	-0.00134	0.00000	0.02555	0.02547	0.40631
D59	1.42799	0.00135	0.00000	0.04941	0.04963	1.47762
D60	-1.71355	0.00154	0.00000	0.05959	0.05953	-1.65403
D61	3.14159	-0.00122	0.00000	-0.03655	-0.03700	3.10459
D62	0.00004	-0.00105	0.00000	-0.02775	-0.02731	-0.02727

Item	Value	Threshold	Converged?
Maximum Force	0.033610	0.000450	NO
RMS Force	0.005473	0.000300	NO
Maximum Displacement	0.222496	0.001800	NO
RMS Displacement	0.047764	0.001200	NO

Predicted change in Energy=-6.838759D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.296910	-2.130076	-0.451852
2	6	0	-1.564337	-1.723094	-0.687690
3	7	0	-1.824150	-0.663801	0.180397
4	6	0	-0.690011	-0.382968	0.865387
5	7	0	0.222216	-1.328019	0.559436
6	6	0	1.594746	-1.337370	1.045591
7	1	0	0.289728	-2.896801	-0.926934
8	1	0	-2.290374	-2.061879	-1.404076
9	1	0	1.628607	-0.766725	1.973334
10	1	0	1.862069	-2.369803	1.283861
11	35	0	0.214921	2.003452	-0.123747
12	1	0	-0.641316	0.256121	1.724722
13	6	0	-2.988356	0.141877	0.233850
14	6	0	-4.204932	-0.295647	-0.070021
15	1	0	-2.767203	1.165906	0.512853
16	1	0	-5.038939	0.392217	-0.049615
17	1	0	-4.409945	-1.323389	-0.344786
18	6	0	2.600177	-0.742756	0.035699

19	1	0	2.657701	-1.326194	-0.882678
20	1	0	2.310593	0.282908	-0.216519
21	6	0	3.962342	-0.710749	0.670531
22	8	0	4.187944	-0.504185	1.842251
23	8	0	4.927141	-0.934204	-0.252201
24	1	0	5.770257	-0.865599	0.217678

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.351897	0.000000			
3	N	2.209562	1.393979	0.000000		
4	C	2.223068	2.229895	1.354382	0.000000	
5	N	1.391220	2.214313	2.184598	1.348660	0.000000
6	C	2.539504	3.623928	3.590419	2.482634	1.456116
7	H	1.075971	2.207348	3.268172	3.239082	2.162159
8	H	2.210267	1.074762	2.163918	3.245052	3.272161
9	H	3.383470	4.265042	3.891882	2.598231	2.071737
10	H	2.780532	4.005685	4.209072	3.261249	2.073457
11	Br	4.177999	4.167846	3.371135	2.737205	3.400808
12	H	3.248081	3.254073	2.151812	1.072037	2.147808
13	C	3.588293	2.520949	1.416810	2.440634	3.546037
14	C	4.334001	3.064614	2.422059	3.638308	4.589297
15	H	4.230426	3.351792	2.085115	2.614961	3.893387
16	H	5.386149	4.117589	3.391600	4.511244	5.568654
17	H	4.192763	2.893929	2.719781	4.023285	4.719592
18	C	3.248919	4.339070	4.427396	3.412208	2.504302
19	H	3.092178	4.245134	4.653588	3.892631	2.830421
20	H	3.560469	4.388751	4.260270	3.258456	2.749275
21	C	4.627684	5.780466	5.807403	4.667954	3.792348
22	O	5.293425	6.401178	6.239593	4.976284	4.248684
23	O	5.362898	6.553723	6.770539	5.753717	4.790633
24	H	6.233593	7.439843	7.597179	6.510570	5.577759

		6	7	8	9	10
6	C	0.000000				
7	H	2.832976	0.000000			
8	H	4.649725	2.753486	0.000000		
9	H	1.089720	3.839450	5.333173	0.000000	
10	H	1.092773	2.763620	4.956068	1.760607	0.000000
11	Br	3.798995	4.966204	4.943953	3.751019	4.880555
12	H	2.828499	4.223629	4.228699	2.502114	3.654692
13	C	4.883843	4.618097	2.833112	5.016744	5.562166
14	C	5.997169	5.263294	2.926570	6.198983	6.553138
15	H	5.057351	5.284260	3.784254	5.019085	5.875871

16	H	6.942387	6.323134	3.925782	7.063402	7.551876
17	H	6.163575	4.990135	2.481943	6.492123	6.563965
18	C	1.544130	3.302233	5.265978	2.167706	2.179448
19	H	2.201867	2.841841	5.029567	3.086882	2.532990
20	H	2.175007	3.833945	5.298794	2.522358	3.080452
21	C	2.477666	4.562763	6.725028	2.673340	2.745865
22	O	2.837876	5.346876	7.411724	2.576105	3.033484
23	O	3.598842	5.080615	7.395336	3.982635	3.716866
24	H	4.282861	5.955847	8.308727	4.499485	4.321262

		11	12	13	14	15
11	Br	0.000000				
12	H	2.683868	0.000000			
13	C	3.722140	2.782868	0.000000		
14	C	4.982353	4.028016	1.328089	0.000000	
15	H	3.162248	2.610696	1.084152	2.131418	0.000000
16	H	5.495873	4.744037	2.085165	1.081269	2.464903
17	H	5.701413	4.580424	2.121965	1.083411	3.103342
18	C	3.640951	3.789172	5.661585	6.820600	5.716593
19	H	4.198773	4.492858	5.939683	6.987000	6.130877
20	H	2.713065	3.533115	5.319924	6.542802	5.205352
21	C	4.694777	4.820770	7.016400	8.211278	6.988095
22	O	5.092967	4.890157	7.382658	8.610496	7.275341
23	O	5.554399	6.027671	8.003081	9.156184	8.012410
24	H	6.261772	6.681146	8.816382	9.995599	8.780796

		16	17	18	19	20
16	H	0.000000				
17	H	1.850963	0.000000			
18	C	7.723440	7.044409	0.000000		
19	H	7.930019	7.088085	1.089553	0.000000	
20	H	7.352240	6.911025	1.095198	1.775798	0.000000
21	C	9.097154	8.455849	1.503173	2.119744	2.121906
22	O	9.461399	8.909429	2.416930	3.231498	2.895254
23	O	10.056003	9.345652	2.352510	2.387784	2.885993
24	H	10.885416	10.206000	3.177675	3.333307	3.671086

		21	22	23	24
21	C	0.000000			
22	O	1.210988	0.000000		
23	O	1.353590	2.262313	0.000000	
24	H	1.870190	2.296426	0.967646	0.000000

Stoichiometry C8H11BrN2O2

Framework group C1[X(C8H11BrN2O2)]

Deg. of freedom 66

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.622043	-2.107808	-0.683712
2	6	0	-1.941234	-1.827523	-0.777535
3	7	0	-2.219112	-0.837708	0.163862
4	6	0	-1.056682	-0.466902	0.751749
5	7	0	-0.088625	-1.297247	0.313257
6	6	0	1.319331	-1.181540	0.666168
7	1	0	-0.011117	-2.788436	-1.250482
8	1	0	-2.696948	-2.211592	-1.438217
9	1	0	1.387452	-0.648693	1.614283
10	1	0	1.711932	-2.188848	0.825378
11	35	0	-0.500286	2.039875	-0.196294
12	1	0	-0.987592	0.138297	1.633919
13	6	0	-3.447632	-0.162154	0.368105
14	6	0	-4.637944	-0.712834	0.158990
15	1	0	-3.304409	0.867296	0.676498
16	1	0	-5.530984	-0.118169	0.293136
17	1	0	-4.764394	-1.744443	-0.146907
18	6	0	2.154138	-0.443643	-0.402918
19	1	0	2.178704	-0.979945	-1.351022
20	1	0	1.738798	0.555157	-0.574230
21	6	0	3.562438	-0.293980	0.100890
22	8	0	3.881399	-0.112575	1.254947
23	8	0	4.448324	-0.376739	-0.919190
24	1	0	5.322718	-0.238750	-0.528379

Rotational constants (GHZ): 0.8538422 0.3284617 0.2577587

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 404 symmetry adapted cartesian basis functions of A symmetry.

There are 389 symmetry adapted basis functions of A symmetry.

389 basis functions, 625 primitive gaussians, 404 cartesian basis functions

62 alpha electrons 62 beta electrons

nuclear repulsion energy 1079.3291599661 Hartrees.

NAtoms= 24 NActive= 24 NUniq= 24 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 389 RedAO= T EigKep= 6.23D-06 NBF= 389
NBsUse= 389 1.00D-06 EigRej= -1.00D+00 NBFU= 389
Initial guess from the checkpoint file: "./cooh.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999985 -0.005028 0.001005 -0.001711 Ang= -0.62 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=2910765817.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3145.73012479 A.U. after 13 cycles
NFock= 13 Conv=0.48D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.001347054	0.000727614	-0.000239425
2	6	-0.000487444	0.000101073	0.000355180
3	7	0.000203941	0.000484071	-0.001080679
4	6	0.000915845	-0.003952013	0.001749388
5	7	-0.005759257	0.002357219	-0.002001749
6	6	0.005706208	0.001275699	-0.001088823
7	1	-0.000234576	-0.000374700	0.000271372
8	1	0.000046703	0.000039427	-0.000009179
9	1	-0.000033812	-0.000002232	-0.000814071
10	1	-0.000780651	0.000057159	0.000346232
11	35	-0.000014289	0.001677181	-0.001370463
12	1	0.000248513	0.000224560	-0.000100282
13	6	0.000127438	0.000124695	0.000039314

14	6	0.000033491	-0.000061896	0.000023176
15	1	-0.000070010	-0.000026672	0.000028018
16	1	0.000010858	0.000011011	0.000002281
17	1	-0.000015645	0.000014204	-0.000023342
18	6	-0.002631985	-0.005370618	0.006746027
19	1	-0.002302050	0.000126415	-0.001249352
20	1	-0.002136210	0.001270835	-0.000407513
21	6	-0.001523567	0.003055227	0.002591365
22	8	0.001461541	-0.003085585	-0.008208852
23	8	0.002068770	0.000904707	0.005281338
24	1	0.003819134	0.000422618	-0.000839960

Cartesian Forces: Max 0.008208852 RMS 0.002200841

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.008199739 RMS 0.001524577

Search for a local minimum.

Step number 2 out of a maximum of 140

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- RFO/linear search

Update second derivatives using D2CorX and points 1 2

DE= -5.99D-03 DEPred=-6.84D-03 R= 8.76D-01

TightC=F SS= 1.41D+00 RLast= 2.69D-01 DXNew= 5.0454D-01 8.0833D-01

Trust test= 8.76D-01 RLast= 2.69D-01 DXMaxT set to 5.05D-01

ITU= 1 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00235	0.00383	0.00727	0.00817	0.01480
Eigenvalues ---	0.01759	0.01963	0.02027	0.02122	0.02204
Eigenvalues ---	0.02254	0.02317	0.02346	0.02432	0.03038
Eigenvalues ---	0.03038	0.03068	0.03382	0.03712	0.04443
Eigenvalues ---	0.04961	0.05552	0.06690	0.07887	0.09603
Eigenvalues ---	0.10788	0.12340	0.14714	0.15767	0.15983
Eigenvalues ---	0.15991	0.15993	0.16000	0.16000	0.16527
Eigenvalues ---	0.17712	0.18072	0.20661	0.22002	0.22820
Eigenvalues ---	0.24112	0.24475	0.27079	0.27870	0.32861
Eigenvalues ---	0.34388	0.35069	0.35196	0.35498	0.35579
Eigenvalues ---	0.35764	0.35844	0.36496	0.36596	0.36650
Eigenvalues ---	0.37593	0.41372	0.43066	0.43825	0.47837
Eigenvalues ---	0.52379	0.53367	0.53732	0.54481	0.59921
Eigenvalues ---	0.86643				

RFO step: Lambda=-1.84727891D-03 EMin= 2.35200581D-03

Quartic linear search produced a step of -0.06087.

Iteration 1 RMS(Cart)= 0.06288918 RMS(Int)= 0.00372824

Iteration 2 RMS(Cart)= 0.00523158 RMS(Int)= 0.00005054

Iteration 3 RMS(Cart)= 0.00002036 RMS(Int)= 0.00004832

Iteration 4 RMS(Cart)= 0.00000000 RMS(Int)= 0.00004832

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55472	0.00022	-0.00015	0.00082	0.00068	2.55539
R2	2.62902	-0.00052	0.00008	-0.00122	-0.00114	2.62788
R3	2.03329	0.00002	-0.00010	0.00030	0.00020	2.03349
R4	2.63424	-0.00040	0.00020	-0.00126	-0.00105	2.63319
R5	2.03101	-0.00004	-0.00001	-0.00006	-0.00007	2.03093
R6	2.55941	0.00009	-0.00009	0.00032	0.00023	2.55964
R7	2.67738	-0.00003	-0.00009	0.00015	0.00006	2.67745
R8	2.54860	-0.00162	0.00008	-0.00364	-0.00356	2.54504
R9	5.17257	0.00081	-0.00085	0.01780	0.01698	5.18955
R10	2.02586	0.00023	0.00001	0.00027	0.00028	2.02613
R11	2.75166	0.00412	-0.00021	0.01118	0.01097	2.76263
R12	2.05927	-0.00070	-0.00022	-0.00129	-0.00151	2.05777
R13	2.06504	-0.00017	0.00010	-0.00072	-0.00061	2.06443
R14	2.91798	-0.00337	-0.00048	-0.00976	-0.01024	2.90775
R15	5.07177	0.00034	-0.00093	0.01317	0.01222	5.08400
R16	5.12695	-0.00006	0.00033	0.00781	0.00813	5.13508
R17	2.50972	-0.00002	0.00002	-0.00007	-0.00005	2.50967
R18	2.04875	-0.00003	0.00000	-0.00008	-0.00008	2.04867
R19	2.04330	0.00000	0.00000	0.00000	0.00000	2.04330
R20	2.04735	0.00000	0.00001	-0.00003	-0.00002	2.04733
R21	2.05896	0.00086	-0.00225	0.00783	0.00558	2.06454
R22	2.06962	0.00231	-0.00290	0.01397	0.01106	2.08068
R23	2.84059	0.00480	0.00424	0.00485	0.00909	2.84967
R24	2.28844	-0.00820	0.00222	-0.01393	-0.01171	2.27673
R25	2.55791	0.00096	0.00039	0.00067	0.00107	2.55898
R26	1.82859	0.00295	0.00040	0.00413	0.00454	1.83312
A1	1.87872	-0.00022	-0.00023	0.00019	-0.00006	1.87866
A2	2.27660	0.00000	0.00017	-0.00071	-0.00056	2.27604
A3	2.12743	0.00022	0.00003	0.00085	0.00087	2.12830
A4	1.87011	-0.00024	0.00016	-0.00088	-0.00071	1.86940
A5	2.28459	0.00011	-0.00013	0.00051	0.00038	2.28497
A6	2.12789	0.00013	-0.00006	0.00041	0.00036	2.12824
A7	1.89278	-0.00002	0.00001	0.00017	0.00018	1.89296
A8	2.22531	0.00016	0.00002	0.00051	0.00053	2.22584
A9	2.15447	-0.00012	-0.00003	-0.00026	-0.00029	2.15418
A10	1.88218	0.00001	-0.00015	0.00069	0.00051	1.88269
A11	1.84924	-0.00078	0.00055	-0.00870	-0.00812	1.84112

A12	2.17373	0.00008	0.00009	0.00101	0.00107	2.17479
A13	1.88109	0.00056	-0.00045	-0.00102	-0.00147	1.87961
A14	2.17591	0.00007	0.00007	0.00228	0.00233	2.17825
A15	1.89283	0.00051	0.00026	0.00056	0.00084	1.89367
A16	2.20274	-0.00074	0.00058	-0.00472	-0.00410	2.19864
A17	2.17284	0.00025	-0.00094	0.00518	0.00417	2.17701
A18	1.88617	-0.00011	0.00096	-0.00285	-0.00196	1.88421
A19	1.88541	0.00003	0.00102	-0.00591	-0.00485	1.88056
A20	1.97460	-0.00061	0.00292	-0.01202	-0.00913	1.96547
A21	1.87708	-0.00007	0.00048	0.00046	0.00099	1.87806
A22	1.91232	0.00009	-0.00274	0.00574	0.00304	1.91536
A23	1.92531	0.00067	-0.00272	0.01465	0.01194	1.93725
A24	1.28161	-0.00117	0.00078	-0.00907	-0.00829	1.27333
A25	1.42741	-0.00119	0.00046	-0.00864	-0.00817	1.41924
A26	2.16126	-0.00007	-0.00002	-0.00020	-0.00023	2.16103
A27	1.95974	0.00009	-0.00008	0.00071	0.00063	1.96037
A28	2.16146	-0.00003	0.00010	-0.00044	-0.00034	2.16111
A29	2.08594	-0.00004	0.00001	-0.00023	-0.00022	2.08573
A30	2.14585	0.00004	-0.00001	0.00025	0.00024	2.14609
A31	2.05139	0.00000	0.00000	-0.00002	-0.00002	2.05137
A32	1.95999	-0.00063	-0.00300	0.00374	0.00041	1.96040
A33	1.91674	-0.00103	-0.00037	-0.00783	-0.00817	1.90857
A34	1.89868	0.00252	0.00073	0.01820	0.01880	1.91748
A35	1.89793	-0.00055	0.00077	-0.01822	-0.01745	1.88048
A36	1.89604	0.00040	0.00089	0.01336	0.01408	1.91012
A37	1.89328	-0.00071	0.00106	-0.00950	-0.00831	1.88498
A38	2.48205	0.00197	-0.00025	0.01192	0.01162	2.49367
A39	2.19086	0.00003	0.00483	-0.01218	-0.00737	2.18349
A40	1.93317	0.00712	0.00163	0.02216	0.02377	1.95694
A41	2.15911	-0.00715	-0.00646	-0.01006	-0.01653	2.14258
A42	1.85283	0.00458	0.00473	0.01422	0.01895	1.87178
D1	0.00256	-0.00009	0.00025	0.00123	0.00147	0.00402
D2	3.10678	-0.00007	-0.00047	0.00266	0.00219	3.10897
D3	-3.10710	-0.00020	0.00123	-0.01081	-0.00957	-3.11667
D4	-0.00289	-0.00017	0.00052	-0.00937	-0.00884	-0.01173
D5	-0.07506	0.00022	0.00002	0.00221	0.00224	-0.07282
D6	-3.03847	0.00006	0.00072	-0.00454	-0.00380	-3.04227
D7	3.03791	0.00031	-0.00086	0.01297	0.01211	3.05002
D8	0.07450	0.00015	-0.00016	0.00622	0.00608	0.08058
D9	0.07051	-0.00013	-0.00043	-0.00435	-0.00477	0.06574
D10	3.05872	0.00001	-0.00042	-0.00137	-0.00178	3.05695
D11	-3.03780	-0.00016	0.00021	-0.00564	-0.00542	-3.04323
D12	-0.04959	-0.00002	0.00021	-0.00265	-0.00243	-0.05201
D13	-0.11735	0.00026	0.00046	0.00566	0.00612	-0.11123

D14	1.89308	0.00052	0.00013	0.00055	0.00072	1.89380
D15	-2.93222	-0.00025	0.00042	-0.00701	-0.00657	-2.93879
D16	-3.11318	0.00010	0.00045	0.00274	0.00319	-3.10999
D17	-1.10274	0.00036	0.00013	-0.00237	-0.00222	-1.10496
D18	0.35514	-0.00041	0.00041	-0.00993	-0.00950	0.34563
D19	0.55233	-0.00009	0.00002	-0.00237	-0.00236	0.54997
D20	-2.54955	-0.00012	0.00019	-0.00418	-0.00398	-2.55354
D21	-2.76382	0.00008	0.00003	0.00107	0.00110	-2.76272
D22	0.41748	0.00005	0.00020	-0.00073	-0.00052	0.41695
D23	0.11884	-0.00030	-0.00029	-0.00490	-0.00519	0.11365
D24	3.08603	-0.00026	-0.00077	0.00047	-0.00029	3.08574
D25	-1.87049	0.00033	-0.00062	0.00536	0.00469	-1.86580
D26	1.09670	0.00036	-0.00111	0.01073	0.00960	1.10630
D27	2.93320	0.00021	-0.00024	0.00749	0.00724	2.94044
D28	-0.38280	0.00025	-0.00073	0.01286	0.01214	-0.37066
D29	-2.24654	-0.00015	-0.00082	0.00255	0.00176	-2.24479
D30	-0.23536	-0.00026	-0.00094	-0.00139	-0.00227	-0.23764
D31	-2.92480	-0.00036	-0.00066	-0.00672	-0.00742	-2.93222
D32	-0.89874	-0.00048	0.00098	-0.01076	-0.00980	-0.90854
D33	1.23778	-0.00001	0.00022	-0.00424	-0.00406	1.23372
D34	0.42222	-0.00055	-0.00001	-0.01383	-0.01388	0.40835
D35	2.44828	-0.00067	0.00163	-0.01787	-0.01626	2.43203
D36	-1.69837	-0.00020	0.00087	-0.01135	-0.01052	-1.70889
D37	-1.11133	0.00076	0.00026	0.03124	0.03150	-1.07983
D38	1.00280	-0.00108	-0.00094	0.00513	0.00415	1.00695
D39	3.07249	-0.00104	0.00057	-0.00012	0.00040	3.07288
D40	3.06604	0.00124	-0.00089	0.03882	0.03791	3.10396
D41	-1.10301	-0.00060	-0.00209	0.01270	0.01056	-1.09245
D42	0.96668	-0.00057	-0.00059	0.00746	0.00681	0.97349
D43	1.00280	0.00087	0.00156	0.02593	0.02750	1.03030
D44	3.11693	-0.00097	0.00035	-0.00019	0.00015	3.11709
D45	-1.09657	-0.00094	0.00186	-0.00543	-0.00360	-1.10016
D46	-0.03581	-0.00076	-0.00055	0.01212	0.01160	-0.02421
D47	0.34346	-0.00066	-0.00040	0.01137	0.01101	0.35447
D48	-3.09194	-0.00003	0.00013	-0.00126	-0.00113	-3.09306
D49	0.04684	-0.00004	0.00005	-0.00137	-0.00132	0.04552
D50	0.00542	0.00001	-0.00007	0.00077	0.00070	0.00612
D51	-3.13899	0.00000	-0.00015	0.00066	0.00051	-3.13848
D52	-0.30939	0.00027	0.00234	-0.02013	-0.01785	-0.32725
D53	1.84165	-0.00153	-0.00111	-0.03242	-0.03352	1.80813
D54	-2.38240	-0.00176	0.00104	-0.03197	-0.03094	-2.41334
D55	-0.60676	0.00111	-0.00363	0.18552	0.18198	-0.42477
D56	2.54479	0.00120	-0.00423	0.19548	0.19136	2.73615
D57	-2.74523	0.00008	-0.00095	0.16145	0.16035	-2.58488

D58	0.40631	0.00016	-0.00155	0.17141	0.16974	0.57605
D59	1.47762	0.00092	-0.00302	0.18107	0.17806	1.65568
D60	-1.65403	0.00100	-0.00362	0.19103	0.18745	-1.46658
D61	3.10459	-0.00065	0.00225	-0.03474	-0.03244	3.07215
D62	-0.02727	-0.00061	0.00166	-0.02498	-0.02336	-0.05063

Item	Value	Threshold	Converged?
Maximum Force	0.008200	0.000450	NO
RMS Force	0.001525	0.000300	NO
Maximum Displacement	0.379578	0.001800	NO
RMS Displacement	0.062159	0.001200	NO

Predicted change in Energy=-1.131935D-03

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.305220	-2.143205	-0.430883
2	6	0	-1.569043	-1.729643	-0.676469
3	7	0	-1.824114	-0.660310	0.179741
4	6	0	-0.692274	-0.384950	0.870969
5	7	0	0.214203	-1.336139	0.575424
6	6	0	1.589941	-1.357927	1.069463
7	1	0	0.274931	-2.924160	-0.890747
8	1	0	-2.294785	-2.070680	-1.392027
9	1	0	1.626400	-0.772922	1.987174
10	1	0	1.835250	-2.391047	1.326234
11	35	0	0.229751	1.992354	-0.148766
12	1	0	-0.641331	0.265799	1.721562
13	6	0	-2.981297	0.156244	0.219894
14	6	0	-4.199736	-0.272787	-0.088469
15	1	0	-2.753484	1.180025	0.494237
16	1	0	-5.027758	0.422481	-0.077394
17	1	0	-4.412158	-1.300375	-0.358092
18	6	0	2.593484	-0.789836	0.050733
19	1	0	2.618748	-1.369994	-0.874656
20	1	0	2.307010	0.241458	-0.207486
21	6	0	3.973560	-0.752133	0.657347
22	8	0	4.210512	-0.704233	1.837637
23	8	0	4.945387	-0.754061	-0.285669
24	1	0	5.793993	-0.664735	0.175716

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.352255	0.000000			
3	N	2.208818	1.393424	0.000000		
4	C	2.221731	2.229683	1.354504	0.000000	
5	N	1.390614	2.214057	2.183586	1.346777	0.000000
6	C	2.541523	3.628448	3.596394	2.488893	1.461919
7	H	1.076077	2.207493	3.267561	3.238320	2.162211
8	H	2.210752	1.074723	2.163592	3.245131	3.271915
9	H	3.384646	4.268625	3.896863	2.602438	2.074742
10	H	2.780377	4.004683	4.207237	3.258845	2.074690
11	Br	4.179549	4.167420	3.370890	2.746190	3.406399
12	H	3.247967	3.254687	2.152641	1.072184	2.147505
13	C	3.587808	2.520813	1.416844	2.440578	3.544691
14	C	4.333932	3.064102	2.421919	3.638048	4.588500
15	H	4.230095	3.352554	2.085538	2.615275	3.891637
16	H	5.386099	4.117431	3.391443	4.510849	5.567501
17	H	4.193161	2.892911	2.719727	4.023199	4.719740
18	C	3.235127	4.328821	4.421379	3.410708	2.496944
19	H	3.056858	4.207876	4.621086	3.870451	2.808152
20	H	3.544047	4.373668	4.246095	3.248255	2.735252
21	C	4.628961	5.784033	5.818038	4.685132	3.805330
22	O	5.254394	6.385566	6.258375	5.007364	4.238275
23	O	5.433201	6.598658	6.786128	5.766912	4.844006
24	H	6.305096	7.488294	7.618110	6.529419	5.634235

		6	7	8	9	10
6	C	0.000000				
7	H	2.832802	0.000000			
8	H	4.653821	2.753752	0.000000		
9	H	1.088923	3.838844	5.336559	0.000000	
10	H	1.092449	2.762935	4.954671	1.760337	0.000000
11	Br	3.815570	4.972392	4.942390	3.762927	4.895656
12	H	2.835542	4.223687	4.229359	2.508405	3.653570
13	C	4.889858	4.617948	2.833510	5.021703	5.559839
14	C	6.003224	5.262706	2.925837	6.205021	6.550532
15	H	5.063342	5.285245	3.786222	5.022574	5.873777
16	H	6.948315	6.322979	3.925972	7.068893	7.548973
17	H	6.169799	4.988908	2.479044	6.499435	6.561755
18	C	1.538713	3.288984	5.255216	2.164565	2.183048
19	H	2.199588	2.812325	4.990134	3.087284	2.549575
20	H	2.168598	3.823262	5.284471	2.511719	3.083007
21	C	2.493684	4.560060	6.725373	2.697783	2.775935
22	O	2.807988	5.278348	7.390317	2.589346	2.957827
23	O	3.668794	5.185423	7.441612	4.022667	3.866640

24	H	4.353544	6.058250	8.358398	4.545538	4.469394
		11	12	13	14	15
11	Br	0.000000				
12	H	2.690334	0.000000			
13	C	3.717262	2.782526	0.000000		
14	C	4.975425	4.028465	1.328062	0.000000	
15	H	3.158009	2.608318	1.084108	2.131162	0.000000
16	H	5.487348	4.743577	2.085009	1.081268	2.464336
17	H	5.695015	4.582247	2.122067	1.083400	3.103232
18	C	3.656174	3.790787	5.657020	6.814291	5.715516
19	H	4.188032	4.477085	5.906603	6.950804	6.102241
20	H	2.717368	3.523427	5.306234	6.528121	5.194413
21	C	4.711489	4.844168	7.027557	8.221239	7.000926
22	O	5.202291	4.949224	7.421566	8.638767	7.338419
23	O	5.458824	6.023330	7.994784	9.159901	7.976312
24	H	6.174642	6.683482	8.813721	10.004901	8.750084
		16	17	18	19	20
16	H	0.000000				
17	H	1.850943	0.000000			
18	C	7.718125	7.036107	0.000000		
19	H	7.894153	7.050200	1.092505	0.000000	
20	H	7.338155	6.895444	1.101050	1.771743	0.000000
21	C	9.107320	8.464747	1.507982	2.136422	2.124275
22	O	9.501708	8.917794	2.411459	3.214574	2.949606
23	O	10.044463	9.373758	2.376109	2.477807	2.821028
24	H	10.879172	10.239849	3.205390	3.418019	3.623131
		21	22	23	24	
21	C	0.000000				
22	O	1.204793	0.000000			
23	O	1.354153	2.247433	0.000000		
24	H	1.885095	2.295856	0.970045	0.000000	

Stoichiometry C8H11BrN2O2
Framework group C1[X(C8H11BrN2O2)]
Deg. of freedom 66
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.631539	-2.095860	-0.715908
2	6	0	-1.949008	-1.806246	-0.810740

3	7	0	-2.224828	-0.833115	0.147680
4	6	0	-1.063603	-0.484901	0.751819
5	7	0	-0.099132	-1.308936	0.299524
6	6	0	1.314056	-1.215137	0.661889
7	1	0	-0.023755	-2.775185	-1.287797
8	1	0	-2.704021	-2.173698	-1.481534
9	1	0	1.382159	-0.694824	1.616032
10	1	0	1.687481	-2.230750	0.811982
11	35	0	-0.494283	2.043701	-0.155708
12	1	0	-0.994536	0.106846	1.643246
13	6	0	-3.449225	-0.152129	0.358767
14	6	0	-4.642378	-0.688754	0.130369
15	1	0	-3.300453	0.868814	0.691681
16	1	0	-5.531536	-0.090194	0.272724
17	1	0	-4.775058	-1.712125	-0.199576
18	6	0	2.148074	-0.471799	-0.396175
19	1	0	2.139806	-0.980056	-1.363219
20	1	0	1.733944	0.537623	-0.544072
21	6	0	3.570729	-0.326358	0.082270
22	8	0	3.918057	-0.335075	1.235878
23	8	0	4.438845	-0.156979	-0.943116
24	1	0	5.315721	-0.008099	-0.555930

Rotational constants (GHZ): 0.8529748 0.3275554 0.2570662

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 404 symmetry adapted cartesian basis functions of A symmetry.

There are 389 symmetry adapted basis functions of A symmetry.

389 basis functions, 625 primitive gaussians, 404 cartesian basis functions

62 alpha electrons 62 beta electrons

nuclear repulsion energy 1078.3771609217 Hartrees.

NAtoms= 24 NActive= 24 NUniq= 24 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 389 RedAO= T EigKep= 6.21D-06 NBF= 389

NBsUse= 389 1.00D-06 EigRej= -1.00D+00 NBFU= 389

Initial guess from the checkpoint file: "./cooh.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999883 -0.015240 -0.000550 0.000933 Ang= -1.75 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid=
0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0
NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=2910765817.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3145.73138015 A.U. after 13 cycles
NFock= 13 Conv=0.57D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000777045	0.000197116	-0.000255280
2	6	-0.000123760	0.000180762	0.000274351
3	7	0.000255358	0.000505349	-0.000513199
4	6	0.000294940	-0.003167741	0.001431026
5	7	-0.002710600	0.001450317	-0.001280767
6	6	0.003046222	0.000224674	-0.000896762
7	1	-0.000170099	-0.000121800	0.000180739
8	1	0.000064251	0.000062353	-0.000060926
9	1	-0.000107881	-0.000095371	-0.000282632
10	1	-0.000021321	0.000302901	0.000350582
11	35	0.000283542	0.001554689	-0.001118861
12	1	0.000281286	0.000237015	-0.000276087
13	6	-0.000106245	0.000071456	0.000178774
14	6	0.000042690	-0.000034697	0.000014293
15	1	0.000036796	-0.000024051	-0.000060168
16	1	0.000005262	0.000007379	-0.000023314
17	1	-0.000018720	0.000013319	-0.000013027
18	6	0.000112697	-0.001091080	0.002025999
19	1	-0.000745071	0.000535255	0.000202045
20	1	-0.000816452	-0.001479440	-0.000144354
21	6	-0.000475049	0.001107492	-0.003655594

22	8	0.001318458	-0.000791946	0.003574282
23	8	-0.000786170	0.000392897	0.000578688
24	1	-0.000437178	-0.000036849	-0.000229808

Cartesian Forces: Max 0.003655594 RMS 0.001051510

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.003724307 RMS 0.000581578
Search for a local minimum.
Step number 3 out of a maximum of 140
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Update second derivatives using D2CorX and points 2 3
DE= -1.26D-03 DEPred=-1.13D-03 R= 1.11D+00
TightC=F SS= 1.41D+00 RLast= 4.52D-01 DXNew= 8.4853D-01 1.3567D+00
Trust test= 1.11D+00 RLast= 4.52D-01 DXMaxT set to 8.49D-01
ITU= 1 1 0
Use linear search instead of GDIIS.

Eigenvalues ---	0.00195	0.00385	0.00731	0.00815	0.01480
Eigenvalues ---	0.01758	0.01962	0.02025	0.02120	0.02196
Eigenvalues ---	0.02256	0.02312	0.02346	0.02427	0.03038
Eigenvalues ---	0.03038	0.03077	0.03289	0.03689	0.04372
Eigenvalues ---	0.04699	0.05545	0.06591	0.08028	0.09569
Eigenvalues ---	0.10574	0.12271	0.14790	0.15808	0.15984
Eigenvalues ---	0.15993	0.15995	0.16000	0.16000	0.16546
Eigenvalues ---	0.17027	0.18005	0.20649	0.22002	0.22825
Eigenvalues ---	0.24479	0.24959	0.27288	0.27654	0.34251
Eigenvalues ---	0.34386	0.35110	0.35498	0.35571	0.35580
Eigenvalues ---	0.35844	0.35995	0.36481	0.36599	0.36650
Eigenvalues ---	0.37237	0.41322	0.43067	0.43826	0.47745
Eigenvalues ---	0.52339	0.53329	0.54461	0.54609	0.59921
Eigenvalues ---	0.94003				

RFO step: Lambda=-6.15153476D-04 EMin= 1.95421343D-03
Quartic linear search produced a step of 0.44619.
Iteration 1 RMS(Cart)= 0.06218259 RMS(Int)= 0.00569535
Iteration 2 RMS(Cart)= 0.00644933 RMS(Int)= 0.00009330
Iteration 3 RMS(Cart)= 0.00007896 RMS(Int)= 0.00005348
Iteration 4 RMS(Cart)= 0.00000001 RMS(Int)= 0.00005348

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55539	0.00010	0.00030	0.00042	0.00071	2.55611

R2	2.62788	-0.00028	-0.00051	-0.00064	-0.00116	2.62672
R3	2.03349	-0.00008	0.00009	-0.00031	-0.00022	2.03327
R4	2.63319	-0.00020	-0.00047	-0.00027	-0.00073	2.63246
R5	2.03093	-0.00002	-0.00003	-0.00006	-0.00010	2.03084
R6	2.55964	-0.00022	0.00010	-0.00074	-0.00063	2.55901
R7	2.67745	0.00005	0.00003	0.00019	0.00022	2.67767
R8	2.54504	-0.00101	-0.00159	-0.00250	-0.00409	2.54095
R9	5.18955	0.00081	0.00758	0.03051	0.03809	5.22764
R10	2.02613	0.00003	0.00012	-0.00010	0.00002	2.02615
R11	2.76263	0.00175	0.00489	0.00433	0.00921	2.77183
R12	2.05777	-0.00030	-0.00067	-0.00075	-0.00142	2.05634
R13	2.06443	-0.00021	-0.00027	-0.00075	-0.00102	2.06341
R14	2.90775	-0.00243	-0.00457	-0.00941	-0.01397	2.89377
R15	5.08400	0.00042	0.00545	0.01245	0.01790	5.10189
R16	5.13508	-0.00019	0.00363	-0.00582	-0.00218	5.13290
R17	2.50967	-0.00002	-0.00002	-0.00004	-0.00006	2.50961
R18	2.04867	-0.00003	-0.00004	-0.00010	-0.00014	2.04853
R19	2.04330	0.00000	0.00000	0.00000	0.00000	2.04330
R20	2.04733	-0.00001	-0.00001	-0.00002	-0.00003	2.04730
R21	2.06454	-0.00047	0.00249	-0.00201	0.00047	2.06501
R22	2.08068	-0.00087	0.00493	-0.00380	0.00115	2.08183
R23	2.84967	-0.00023	0.00405	-0.00480	-0.00074	2.84893
R24	2.27673	0.00372	-0.00522	0.00723	0.00201	2.27874
R25	2.55898	-0.00111	0.00048	-0.00325	-0.00277	2.55621
R26	1.83312	-0.00050	0.00202	-0.00242	-0.00040	1.83272
A1	1.87866	-0.00026	-0.00003	-0.00111	-0.00117	1.87749
A2	2.27604	0.00007	-0.00025	0.00025	-0.00001	2.27603
A3	2.12830	0.00018	0.00039	0.00091	0.00129	2.12959
A4	1.86940	-0.00005	-0.00032	0.00052	0.00021	1.86961
A5	2.28497	0.00000	0.00017	-0.00044	-0.00027	2.28470
A6	2.12824	0.00004	0.00016	-0.00015	0.00001	2.12825
A7	1.89296	-0.00010	0.00008	-0.00079	-0.00069	1.89227
A8	2.22584	0.00017	0.00024	0.00088	0.00111	2.22695
A9	2.15418	-0.00006	-0.00013	-0.00015	-0.00029	2.15388
A10	1.88269	0.00013	0.00023	0.00087	0.00104	1.88373
A11	1.84112	-0.00063	-0.00362	-0.00562	-0.00918	1.83194
A12	2.17479	-0.00001	0.00048	0.00151	0.00187	2.17666
A13	1.87961	0.00032	-0.00066	-0.00079	-0.00147	1.87815
A14	2.17825	0.00004	0.00104	0.00256	0.00351	2.18176
A15	1.89367	0.00030	0.00038	0.00089	0.00132	1.89498
A16	2.19864	-0.00022	-0.00183	0.00007	-0.00173	2.19691
A17	2.17701	-0.00008	0.00186	-0.00095	0.00082	2.17783
A18	1.88421	0.00004	-0.00087	-0.00181	-0.00273	1.88148
A19	1.88056	0.00041	-0.00216	0.00512	0.00303	1.88360

A20	1.96547	-0.00076	-0.00407	-0.00527	-0.00936	1.95611
A21	1.87806	-0.00020	0.00044	-0.00155	-0.00115	1.87691
A22	1.91536	0.00020	0.00136	-0.00007	0.00126	1.91662
A23	1.93725	0.00032	0.00533	0.00363	0.00893	1.94618
A24	1.27333	-0.00107	-0.00370	-0.00740	-0.01110	1.26223
A25	1.41924	-0.00110	-0.00365	-0.00825	-0.01191	1.40733
A26	2.16103	0.00001	-0.00010	0.00012	0.00002	2.16105
A27	1.96037	-0.00004	0.00028	-0.00048	-0.00020	1.96016
A28	2.16111	0.00003	-0.00015	0.00030	0.00014	2.16126
A29	2.08573	-0.00002	-0.00010	-0.00012	-0.00021	2.08551
A30	2.14609	0.00003	0.00011	0.00023	0.00033	2.14642
A31	2.05137	-0.00001	-0.00001	-0.00011	-0.00012	2.05125
A32	1.96040	-0.00015	0.00018	-0.00195	-0.00205	1.95835
A33	1.90857	-0.00011	-0.00364	0.00411	0.00048	1.90905
A34	1.91748	0.00086	0.00839	0.00741	0.01567	1.93315
A35	1.88048	-0.00041	-0.00779	-0.01100	-0.01883	1.86165
A36	1.91012	-0.00002	0.00628	0.00013	0.00628	1.91640
A37	1.88498	-0.00020	-0.00371	0.00107	-0.00261	1.88237
A38	2.49367	0.00145	0.00518	0.00824	0.01344	2.50711
A39	2.18349	0.00141	-0.00329	0.00756	0.00407	2.18757
A40	1.95694	-0.00147	0.01061	-0.01367	-0.00326	1.95369
A41	2.14258	0.00007	-0.00737	0.00680	-0.00077	2.14181
A42	1.87178	0.00000	0.00846	-0.00606	0.00240	1.87418
D1	0.00402	-0.00006	0.00065	-0.00010	0.00056	0.00458
D2	3.10897	-0.00009	0.00098	-0.00224	-0.00126	3.10771
D3	-3.11667	-0.00006	-0.00427	-0.00300	-0.00726	-3.12393
D4	-0.01173	-0.00010	-0.00395	-0.00514	-0.00907	-0.02081
D5	-0.07282	0.00013	0.00100	0.00187	0.00288	-0.06994
D6	-3.04227	0.00011	-0.00169	0.00187	0.00020	-3.04206
D7	3.05002	0.00014	0.00540	0.00447	0.00988	3.05990
D8	0.08058	0.00012	0.00271	0.00447	0.00721	0.08778
D9	0.06574	-0.00007	-0.00213	-0.00179	-0.00392	0.06182
D10	3.05695	-0.00003	-0.00079	-0.00228	-0.00307	3.05388
D11	-3.04323	-0.00004	-0.00242	0.00013	-0.00229	-3.04551
D12	-0.05201	0.00000	-0.00108	-0.00037	-0.00144	-0.05345
D13	-0.11123	0.00015	0.00273	0.00293	0.00567	-0.10556
D14	1.89380	0.00026	0.00032	-0.00030	0.00004	1.89384
D15	-2.93879	-0.00036	-0.00293	-0.01336	-0.01628	-2.95507
D16	-3.10999	0.00009	0.00142	0.00328	0.00471	-3.10528
D17	-1.10496	0.00020	-0.00099	0.00006	-0.00091	-1.10587
D18	0.34563	-0.00042	-0.00424	-0.01300	-0.01723	0.32840
D19	0.54997	-0.00001	-0.00105	0.00159	0.00054	0.55051
D20	-2.55354	0.00001	-0.00178	0.00346	0.00168	-2.55186
D21	-2.76272	0.00003	0.00049	0.00100	0.00150	-2.76122

D22	0.41695	0.00006	-0.00023	0.00286	0.00264	0.41959
D23	0.11365	-0.00016	-0.00232	-0.00288	-0.00520	0.10845
D24	3.08574	-0.00015	-0.00013	-0.00275	-0.00288	3.08286
D25	-1.86580	0.00035	0.00209	0.00360	0.00563	-1.86017
D26	1.10630	0.00036	0.00428	0.00372	0.00795	1.11425
D27	2.94044	0.00034	0.00323	0.01321	0.01645	2.95688
D28	-0.37066	0.00034	0.00542	0.01333	0.01877	-0.35189
D29	-2.24479	-0.00020	0.00078	-0.00075	0.00006	-2.24473
D30	-0.23764	-0.00021	-0.00101	-0.00282	-0.00380	-0.24143
D31	-2.93222	-0.00011	-0.00331	-0.00301	-0.00633	-2.93855
D32	-0.90854	-0.00012	-0.00437	-0.00311	-0.00751	-0.91606
D33	1.23372	0.00009	-0.00181	0.00165	-0.00021	1.23351
D34	0.40835	-0.00017	-0.00619	-0.00321	-0.00940	0.39895
D35	2.43203	-0.00018	-0.00725	-0.00331	-0.01059	2.42144
D36	-1.70889	0.00003	-0.00469	0.00145	-0.00329	-1.71218
D37	-1.07983	0.00017	0.01405	0.01122	0.02524	-1.05459
D38	1.00695	-0.00052	0.00185	-0.00106	0.00075	1.00769
D39	3.07288	-0.00032	0.00018	0.00711	0.00727	3.08015
D40	3.10396	0.00048	0.01692	0.01702	0.03394	3.13789
D41	-1.09245	-0.00021	0.00471	0.00475	0.00944	-1.08301
D42	0.97349	-0.00001	0.00304	0.01292	0.01596	0.98945
D43	1.03030	0.00040	0.01227	0.01673	0.02896	1.05927
D44	3.11709	-0.00029	0.00007	0.00445	0.00446	3.12155
D45	-1.10016	-0.00009	-0.00160	0.01262	0.01099	-1.08918
D46	-0.02421	-0.00045	0.00518	0.00251	0.00770	-0.01651
D47	0.35447	-0.00039	0.00491	0.00146	0.00641	0.36089
D48	-3.09306	0.00003	-0.00050	0.00168	0.00118	-3.09189
D49	0.04552	0.00001	-0.00059	0.00092	0.00033	0.04585
D50	0.00612	0.00000	0.00031	-0.00042	-0.00010	0.00602
D51	-3.13848	-0.00002	0.00023	-0.00117	-0.00094	-3.13942
D52	-0.32725	0.00006	-0.00797	-0.00393	-0.01197	-0.33921
D53	1.80813	-0.00045	-0.01496	-0.01063	-0.02561	1.78252
D54	-2.41334	-0.00080	-0.01380	-0.01583	-0.02961	-2.44294
D55	-0.42477	0.00059	0.08120	0.14317	0.22444	-0.20033
D56	2.73615	0.00038	0.08538	0.10328	0.18872	2.92487
D57	-2.58488	0.00021	0.07155	0.14058	0.21203	-2.37285
D58	0.57605	0.00001	0.07573	0.10070	0.17631	0.75236
D59	1.65568	0.00083	0.07945	0.15302	0.23253	1.88821
D60	-1.46658	0.00062	0.08364	0.11314	0.19681	-1.26977
D61	3.07215	0.00010	-0.01447	0.02462	0.01011	3.08226
D62	-0.05063	-0.00012	-0.01042	-0.01420	-0.02459	-0.07522

Item	Value	Threshold	Converged?
Maximum Force	0.003724	0.000450	NO
RMS Force	0.000582	0.000300	NO

Maximum Displacement 0.455355 0.001800 NO
RMS Displacement 0.064307 0.001200 NO
Predicted change in Energy=-5.015641D-04
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.308368	-2.158893	-0.408536
2	6	0	-1.568512	-1.738997	-0.664151
3	7	0	-1.820292	-0.659759	0.179887
4	6	0	-0.691181	-0.389064	0.876746
5	7	0	0.210133	-1.345453	0.592253
6	6	0	1.588175	-1.372371	1.093999
7	1	0	0.266302	-2.952081	-0.853848
8	1	0	-2.292564	-2.081350	-1.380714
9	1	0	1.623374	-0.773629	2.001955
10	1	0	1.825431	-2.401994	1.369411
11	35	0	0.248552	1.987926	-0.181318
12	1	0	-0.635360	0.279490	1.713119
13	6	0	-2.970089	0.167951	0.205267
14	6	0	-4.190581	-0.252566	-0.106544
15	1	0	-2.734004	1.192234	0.470299
16	1	0	-5.011749	0.450870	-0.108077
17	1	0	-4.411402	-1.280584	-0.367580
18	6	0	2.584428	-0.821342	0.069897
19	1	0	2.583822	-1.397854	-0.858407
20	1	0	2.301127	0.209028	-0.197926
21	6	0	3.976969	-0.782786	0.646236
22	8	0	4.255672	-0.945196	1.808146
23	8	0	4.911893	-0.560181	-0.305669
24	1	0	5.770195	-0.494171	0.141029

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.352633	0.000000			
3	N	2.208973	1.393036	0.000000		
4	C	2.220539	2.228541	1.354172	0.000000	
5	N	1.390002	2.212918	2.182395	1.344613	0.000000
6	C	2.544229	3.631829	3.600148	2.491898	1.466790
7	H	1.075963	2.207737	3.267602	3.237405	2.162318

8	H	2.210922	1.074672	2.163201	3.244131	3.270724
9	H	3.385417	4.269449	3.897658	2.602144	2.076413
10	H	2.788062	4.011707	4.212084	3.260053	2.080731
11	Br	4.190214	4.174303	3.379470	2.766347	3.422178
12	H	3.248701	3.255223	2.153382	1.072194	2.147472
13	C	3.588275	2.521260	1.416961	2.440199	3.543157
14	C	4.335535	3.065232	2.422007	3.637484	4.587919
15	H	4.229198	3.352232	2.085446	2.615115	3.888788
16	H	5.387293	4.118327	3.391433	4.510285	5.566443
17	H	4.196188	2.894844	2.720110	4.022835	4.720601
18	C	3.222764	4.315997	4.409055	3.401100	2.486931
19	H	3.024289	4.170850	4.584655	3.841101	2.782366
20	H	3.529996	4.357325	4.228904	3.235204	2.722692
21	C	4.622805	5.777873	5.817289	4.690392	3.809011
22	O	5.217011	6.376794	6.296828	5.064400	4.243229
23	O	5.460548	6.596497	6.750408	5.729034	4.850719
24	H	6.326313	7.486957	7.592392	6.503976	5.642922

		6	7	8	9	10
6	C	0.000000				
7	H	2.834950	0.000000			
8	H	4.656930	2.753826	0.000000		
9	H	1.088170	3.839649	5.337336	0.000000	
10	H	1.091909	2.770624	4.962246	1.758554	0.000000
11	Br	3.835703	4.985607	4.945182	3.779286	4.915557
12	H	2.838320	4.224378	4.229857	2.508858	3.655679
13	C	4.892873	4.618501	2.834383	5.021411	5.563889
14	C	6.007436	5.263996	2.927529	6.206396	6.556744
15	H	5.064330	5.284936	3.786485	5.019695	5.874975
16	H	6.951848	6.324087	3.927558	7.069405	7.554392
17	H	6.175724	4.991120	2.481359	6.503094	6.570601
18	C	1.531319	3.281320	5.241845	2.158413	2.182492
19	H	2.191769	2.790437	4.951677	3.081199	2.558637
20	H	2.162914	3.816197	5.267525	2.502886	3.082251
21	C	2.500888	4.552487	6.715790	2.716149	2.788177
22	O	2.794285	5.198930	7.371504	2.644993	2.867197
23	O	3.696732	5.253875	7.441363	4.023065	3.965403
24	H	4.378205	6.109332	8.357207	4.553819	4.550810

		11	12	13	14	15
11	Br	0.000000				
12	H	2.699805	0.000000			
13	C	3.717715	2.781550	0.000000		
14	C	4.973057	4.029126	1.328029	0.000000	
15	H	3.154897	2.604230	1.084036	2.131152	0.000000
16	H	5.480755	4.743301	2.084851	1.081268	2.464195

17	H	5.695000	4.584936	2.122214	1.083385	3.103310
18	C	3.662159	3.778762	5.643552	6.801131	5.700923
19	H	4.168385	4.448524	5.867629	6.911549	6.062449
20	H	2.716213	3.504285	5.286773	6.508740	5.173564
21	C	4.718345	4.851829	7.025665	8.219287	6.997773
22	O	5.349596	5.042924	7.484647	8.688209	7.430614
23	O	5.315549	5.962598	7.932016	9.109847	7.882439
24	H	6.062445	6.640870	8.765563	9.966781	8.676046

		16	17	18	19	20
16	H	0.000000				
17	H	1.850862	0.000000			
18	C	7.704031	7.024523	0.000000		
19	H	7.853246	7.013403	1.092756	0.000000	
20	H	7.317426	6.877920	1.101658	1.760177	0.000000
21	C	9.104282	8.464065	1.507589	2.140822	2.122440
22	O	9.565877	8.942285	2.414520	3.179700	3.029324
23	O	9.976971	9.351292	2.371993	2.535179	2.723856
24	H	10.826147	10.224580	3.203313	3.459550	3.555813

		21	22	23	24
21	C	0.000000			
22	O	1.205856	0.000000		
23	O	1.352686	2.246571	0.000000	
24	H	1.885256	2.297060	0.969834	0.000000

Stoichiometry C8H11BrN2O2
Framework group C1[X(C8H11BrN2O2)]
Deg. of freedom 66
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.632855	-2.085246	-0.752572
2	6	0	-1.949134	-1.788046	-0.845829
3	7	0	-2.225000	-0.836223	0.133191
4	6	0	-1.065475	-0.510862	0.752402
5	7	0	-0.103128	-1.324166	0.282925
6	6	0	1.313880	-1.244634	0.653380
7	1	0	-0.026905	-2.758160	-1.333698
8	1	0	-2.702426	-2.135993	-1.528766
9	1	0	1.378315	-0.741417	1.616050
10	1	0	1.683376	-2.263124	0.789093

11	35	0	-0.489408	2.053172	-0.111631
12	1	0	-0.995120	0.070990	1.650231
13	6	0	-3.446036	-0.152042	0.353974
14	6	0	-4.641502	-0.675114	0.107157
15	1	0	-3.292006	0.860126	0.710236
16	1	0	-5.527196	-0.073504	0.257997
17	1	0	-4.779639	-1.689640	-0.246933
18	6	0	2.138891	-0.482081	-0.387201
19	1	0	2.104319	-0.957310	-1.370602
20	1	0	1.724527	0.531119	-0.511208
21	6	0	3.570987	-0.343790	0.063134
22	8	0	3.981055	-0.590852	1.169883
23	8	0	4.376714	0.079850	-0.937412
24	1	0	5.264254	0.197517	-0.564579

Rotational constants (GHZ): 0.8467129 0.3286671 0.2565192

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 404 symmetry adapted cartesian basis functions of A symmetry.

There are 389 symmetry adapted basis functions of A symmetry.

389 basis functions, 625 primitive gaussians, 404 cartesian basis functions

62 alpha electrons 62 beta electrons

nuclear repulsion energy 1077.5686100860 Hartrees.

NAtoms= 24 NActive= 24 NUniq= 24 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 389 RedAO= T EigKep= 6.23D-06 NBF= 389

NBsUse= 389 1.00D-06 EigRej= -1.00D+00 NBFU= 389

Initial guess from the checkpoint file: "./cooh.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999855 -0.016991 -0.001386 0.000265 Ang= -1.95 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=2910765817.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3145.73186267 A.U. after 15 cycles
NFock= 15 Conv=0.30D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000138431	0.000101850	-0.000070209
2	6	-0.000112262	0.000248332	0.000065253
3	7	0.000601326	0.000280720	-0.000218065
4	6	-0.000443958	-0.002401481	0.001014879
5	7	0.000019821	0.000451028	-0.000171925
6	6	0.000515932	-0.000455443	-0.000113031
7	1	-0.000049887	-0.000038643	0.000079125
8	1	0.000003491	0.000014102	-0.000052330
9	1	-0.000441634	-0.000057998	0.000443990
10	1	-0.000002955	0.000240129	0.000162227
11	35	0.000257183	0.001255252	-0.000701313
12	1	0.000319664	0.000272120	-0.000339592
13	6	-0.000383438	0.000148065	0.000071414
14	6	0.000134227	-0.000036670	0.000020203
15	1	0.000096994	0.000032692	-0.000084235
16	1	-0.000001641	0.000005901	0.000007445
17	1	-0.000004303	-0.000004837	-0.000009911
18	6	0.000601294	0.004031774	0.000051494
19	1	0.000859744	-0.000144264	0.000201917
20	1	-0.001085561	-0.001620192	-0.000063852
21	6	0.000071194	-0.004809739	-0.003613064
22	8	0.000361144	0.001186513	0.003113026
23	8	-0.000998029	0.001744692	0.000368259
24	1	-0.000456777	-0.000443904	-0.000161706

Cartesian Forces: Max 0.004809739 RMS 0.001084625

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.

Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.002916373 RMS 0.000462695
Search for a local minimum.
Step number 4 out of a maximum of 140
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 3 4
DE= -4.83D-04 DEPred=-5.02D-04 R= 9.62D-01
TightC=F SS= 1.41D+00 RLast= 5.16D-01 DXNew= 1.4270D+00 1.5474D+00
Trust test= 9.62D-01 RLast= 5.16D-01 DXMaxT set to 1.43D+00
ITU= 1 1 1 0

Eigenvalues ---	0.00120	0.00387	0.00809	0.01319	0.01482
Eigenvalues ---	0.01759	0.01962	0.02033	0.02119	0.02196
Eigenvalues ---	0.02279	0.02315	0.02346	0.02421	0.02983
Eigenvalues ---	0.03038	0.03038	0.03106	0.03672	0.04474
Eigenvalues ---	0.04822	0.05562	0.06526	0.08235	0.09535
Eigenvalues ---	0.10709	0.12424	0.14918	0.15891	0.15981
Eigenvalues ---	0.15991	0.15997	0.16000	0.16000	0.16330
Eigenvalues ---	0.16735	0.17993	0.20666	0.22003	0.22838
Eigenvalues ---	0.24484	0.24700	0.27326	0.27650	0.34243
Eigenvalues ---	0.34378	0.35140	0.35462	0.35499	0.35579
Eigenvalues ---	0.35844	0.35930	0.36581	0.36600	0.36651
Eigenvalues ---	0.37451	0.41314	0.43073	0.43812	0.47671
Eigenvalues ---	0.52329	0.53314	0.54459	0.54478	0.59922
Eigenvalues ---	0.91957				

En-DIIS/RFO-DIIS IScMMF= 0 using points: 4 3
RFO step: Lambda=-9.54660338D-05.
DidBck=F Rises=F RFO-DIIS coefs: 1.10295 -0.10295
Iteration 1 RMS(Cart)= 0.06528669 RMS(Int)= 0.02207655
Iteration 2 RMS(Cart)= 0.03822911 RMS(Int)= 0.00175043
Iteration 3 RMS(Cart)= 0.00231333 RMS(Int)= 0.00082330
Iteration 4 RMS(Cart)= 0.00000398 RMS(Int)= 0.00082330
Iteration 5 RMS(Cart)= 0.00000001 RMS(Int)= 0.00082330

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55611	0.00008	0.00007	0.00105	0.00109	2.55719
R2	2.62672	-0.00004	-0.00012	-0.00121	-0.00135	2.62538
R3	2.03327	-0.00003	-0.00002	-0.00031	-0.00033	2.03294
R4	2.63246	-0.00022	-0.00008	-0.00108	-0.00117	2.63129
R5	2.03084	0.00003	-0.00001	-0.00002	-0.00003	2.03081
R6	2.55901	-0.00040	-0.00006	-0.00156	-0.00159	2.55742

R7	2.67767	0.00021	0.00002	0.00074	0.00076	2.67843
R8	2.54095	-0.00048	-0.00042	-0.00517	-0.00561	2.53534
R9	5.22764	0.00072	0.00392	0.06458	0.06841	5.29605
R10	2.02615	-0.00006	0.00000	-0.00007	-0.00007	2.02608
R11	2.77183	-0.00017	0.00095	0.00844	0.00937	2.78120
R12	2.05634	0.00032	-0.00015	-0.00042	-0.00057	2.05577
R13	2.06341	-0.00019	-0.00011	-0.00157	-0.00168	2.06173
R14	2.89377	0.00007	-0.00144	-0.01326	-0.01466	2.87911
R15	5.10189	0.00033	0.00184	0.02310	0.02497	5.12686
R16	5.13290	-0.00007	-0.00022	-0.00442	-0.00459	5.12831
R17	2.50961	-0.00011	-0.00001	-0.00026	-0.00027	2.50934
R18	2.04853	0.00003	-0.00001	-0.00004	-0.00005	2.04848
R19	2.04330	0.00000	0.00000	0.00001	0.00001	2.04331
R20	2.04730	0.00001	0.00000	0.00000	0.00000	2.04730
R21	2.06501	-0.00009	0.00005	0.00001	0.00006	2.06507
R22	2.08183	-0.00102	0.00012	-0.00190	-0.00171	2.08012
R23	2.84893	-0.00113	-0.00008	-0.00403	-0.00410	2.84483
R24	2.27874	0.00292	0.00021	0.00536	0.00557	2.28430
R25	2.55621	-0.00092	-0.00029	-0.00443	-0.00471	2.55150
R26	1.83272	-0.00051	-0.00004	-0.00121	-0.00126	1.83146
A1	1.87749	-0.00006	-0.00012	-0.00127	-0.00142	1.87607
A2	2.27603	0.00003	0.00000	0.00004	0.00004	2.27607
A3	2.12959	0.00003	0.00013	0.00132	0.00145	2.13104
A4	1.86961	-0.00009	0.00002	0.00022	0.00022	1.86983
A5	2.28470	0.00003	-0.00003	-0.00036	-0.00038	2.28432
A6	2.12825	0.00005	0.00000	0.00004	0.00004	2.12829
A7	1.89227	0.00001	-0.00007	-0.00097	-0.00100	1.89127
A8	2.22695	0.00003	0.00011	0.00134	0.00143	2.22838
A9	2.15388	-0.00003	-0.00003	-0.00028	-0.00034	2.15355
A10	1.88373	0.00023	0.00011	0.00212	0.00210	1.88583
A11	1.83194	-0.00053	-0.00095	-0.01266	-0.01351	1.81843
A12	2.17666	-0.00002	0.00019	0.00343	0.00328	2.17994
A13	1.87815	0.00021	-0.00015	-0.00126	-0.00148	1.87666
A14	2.18176	-0.00007	0.00036	0.00483	0.00489	2.18665
A15	1.89498	-0.00007	0.00014	0.00103	0.00125	1.89623
A16	2.19691	0.00015	-0.00018	-0.00013	-0.00029	2.19662
A17	2.17783	-0.00008	0.00008	-0.00061	-0.00062	2.17721
A18	1.88148	-0.00013	-0.00028	-0.00592	-0.00621	1.87527
A19	1.88360	0.00014	0.00031	0.00437	0.00472	1.88832
A20	1.95611	-0.00044	-0.00096	-0.01082	-0.01176	1.94435
A21	1.87691	-0.00021	-0.00012	-0.00268	-0.00283	1.87408
A22	1.91662	0.00045	0.00013	0.00499	0.00504	1.92167
A23	1.94618	0.00018	0.00092	0.00981	0.01072	1.95690
A24	1.26223	-0.00063	-0.00114	-0.01534	-0.01647	1.24575

A25	1.40733	-0.00067	-0.00123	-0.01659	-0.01788	1.38945
A26	2.16105	-0.00006	0.00000	-0.00031	-0.00031	2.16074
A27	1.96016	-0.00005	-0.00002	-0.00060	-0.00062	1.95955
A28	2.16126	0.00011	0.00001	0.00083	0.00085	2.16211
A29	2.08551	-0.00001	-0.00002	-0.00028	-0.00030	2.08521
A30	2.14642	0.00001	0.00003	0.00038	0.00041	2.14683
A31	2.05125	0.00000	-0.00001	-0.00011	-0.00012	2.05113
A32	1.95835	0.00043	-0.00021	-0.00359	-0.00382	1.95452
A33	1.90905	-0.00022	0.00005	0.00460	0.00453	1.91357
A34	1.93315	-0.00029	0.00161	0.01379	0.01522	1.94837
A35	1.86165	-0.00006	-0.00194	-0.01979	-0.02174	1.83991
A36	1.91640	-0.00073	0.00065	-0.00713	-0.00641	1.90999
A37	1.88237	0.00091	-0.00027	0.01161	0.01112	1.89349
A38	2.50711	0.00097	0.00138	0.01748	0.01906	2.52617
A39	2.18757	0.00049	0.00042	0.00739	0.00241	2.18998
A40	1.95369	-0.00136	-0.00034	-0.00703	-0.01273	1.94096
A41	2.14181	0.00089	-0.00008	0.00248	-0.00300	2.13882
A42	1.87418	-0.00022	0.00025	0.00229	0.00254	1.87672
D1	0.00458	-0.00002	0.00006	0.00017	0.00024	0.00482
D2	3.10771	-0.00007	-0.00013	-0.00296	-0.00309	3.10462
D3	-3.12393	0.00002	-0.00075	-0.00745	-0.00818	-3.13211
D4	-0.02081	-0.00003	-0.00093	-0.01058	-0.01150	-0.03231
D5	-0.06994	0.00010	0.00030	0.00543	0.00573	-0.06421
D6	-3.04206	0.00012	0.00002	0.00361	0.00365	-3.03841
D7	3.05990	0.00006	0.00102	0.01227	0.01329	3.07319
D8	0.08778	0.00009	0.00074	0.01044	0.01120	0.09899
D9	0.06182	-0.00006	-0.00040	-0.00581	-0.00622	0.05560
D10	3.05388	-0.00005	-0.00032	-0.00524	-0.00556	3.04832
D11	-3.04551	-0.00002	-0.00024	-0.00301	-0.00324	-3.04876
D12	-0.05345	-0.00001	-0.00015	-0.00244	-0.00259	-0.05604
D13	-0.10556	0.00010	0.00058	0.00908	0.00970	-0.09587
D14	1.89384	0.00019	0.00000	0.00254	0.00251	1.89635
D15	-2.95507	-0.00036	-0.00168	-0.02761	-0.02930	-2.98437
D16	-3.10528	0.00009	0.00049	0.00837	0.00889	-3.09639
D17	-1.10587	0.00018	-0.00009	0.00182	0.00170	-1.10417
D18	0.32840	-0.00037	-0.00177	-0.02832	-0.03011	0.29829
D19	0.55051	0.00005	0.00006	0.00484	0.00489	0.55540
D20	-2.55186	0.00006	0.00017	0.00682	0.00699	-2.54487
D21	-2.76122	0.00006	0.00015	0.00546	0.00562	-2.75560
D22	0.41959	0.00008	0.00027	0.00744	0.00772	0.42731
D23	0.10845	-0.00012	-0.00054	-0.00887	-0.00944	0.09901
D24	3.08286	-0.00012	-0.00030	-0.00701	-0.00735	3.07551
D25	-1.86017	0.00028	0.00058	0.00535	0.00587	-1.85430
D26	1.11425	0.00028	0.00082	0.00720	0.00796	1.12221

D27	2.95688	0.00035	0.00169	0.02766	0.02940	2.98629
D28	-0.35189	0.00035	0.00193	0.02952	0.03150	-0.32039
D29	-2.24473	-0.00014	0.00001	0.00053	0.00058	-2.24415
D30	-0.24143	-0.00004	-0.00039	-0.00360	-0.00399	-0.24543
D31	-2.93855	0.00024	-0.00065	-0.00232	-0.00294	-2.94149
D32	-0.91606	-0.00001	-0.00077	-0.00625	-0.00704	-0.92310
D33	1.23351	0.00003	-0.00002	0.00210	0.00204	1.23555
D34	0.39895	0.00026	-0.00097	-0.00458	-0.00552	0.39342
D35	2.42144	0.00002	-0.00109	-0.00852	-0.00962	2.41182
D36	-1.71218	0.00006	-0.00034	-0.00017	-0.00055	-1.71272
D37	-1.05459	-0.00026	0.00260	0.02327	0.02586	-1.02873
D38	1.00769	-0.00022	0.00008	-0.00058	-0.00052	1.00717
D39	3.08015	0.00059	0.00075	0.02498	0.02576	3.10591
D40	3.13789	-0.00011	0.00349	0.03436	0.03785	-3.10744
D41	-1.08301	-0.00008	0.00097	0.01051	0.01148	-1.07153
D42	0.98945	0.00074	0.00164	0.03607	0.03776	1.02721
D43	1.05927	-0.00026	0.00298	0.02825	0.03120	1.09046
D44	3.12155	-0.00022	0.00046	0.00440	0.00482	3.12637
D45	-1.08918	0.00059	0.00113	0.02996	0.03110	-1.05808
D46	-0.01651	-0.00005	0.00079	0.00468	0.00547	-0.01104
D47	0.36089	-0.00004	0.00066	0.00234	0.00303	0.36392
D48	-3.09189	0.00000	0.00012	0.00109	0.00121	-3.09068
D49	0.04585	0.00001	0.00003	0.00084	0.00088	0.04673
D50	0.00602	-0.00003	-0.00001	-0.00115	-0.00116	0.00486
D51	-3.13942	-0.00001	-0.00010	-0.00140	-0.00150	-3.14092
D52	-0.33921	-0.00001	-0.00123	-0.00881	-0.01006	-0.34928
D53	1.78252	0.00034	-0.00264	-0.02233	-0.02492	1.75760
D54	-2.44294	-0.00008	-0.00305	-0.03509	-0.03818	-2.48112
D55	-0.20033	-0.00076	0.02311	0.12770	0.15083	-0.04951
D56	2.92487	0.00072	0.01943	0.32057	0.33977	-3.01855
D57	-2.37285	-0.00059	0.02183	0.12772	0.14967	-2.22318
D58	0.75236	0.00089	0.01815	0.32059	0.33861	1.09097
D59	1.88821	-0.00064	0.02394	0.14859	0.17277	2.06098
D60	-1.26977	0.00084	0.02026	0.34146	0.36171	-0.90806
D61	3.08226	-0.00037	0.00104	-0.08411	-0.08259	2.99967
D62	-0.07522	0.00106	-0.00253	0.10295	0.09994	0.02472

Item	Value	Threshold	Converged?
Maximum Force	0.002916	0.000450	NO
RMS Force	0.000463	0.000300	NO
Maximum Displacement	0.598684	0.001800	NO
RMS Displacement	0.096772	0.001200	NO

Predicted change in Energy=-4.621332D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.321695	-2.194297	-0.379702
2	6	0	-1.574697	-1.757119	-0.644342
3	7	0	-1.809524	-0.660713	0.181234
4	6	0	-0.679666	-0.403808	0.880462
5	7	0	0.207022	-1.373244	0.608456
6	6	0	1.589184	-1.411367	1.112658
7	1	0	0.237584	-3.008214	-0.806395
8	1	0	-2.302163	-2.097265	-1.358473
9	1	0	1.626476	-0.795940	2.008937
10	1	0	1.814624	-2.436170	1.411465
11	35	0	0.296828	1.971832	-0.240735
12	1	0	-0.605186	0.294006	1.691034
13	6	0	-2.942019	0.191536	0.188387
14	6	0	-4.170163	-0.209317	-0.118632
15	1	0	-2.684048	1.215602	0.432960
16	1	0	-4.976141	0.511266	-0.136376
17	1	0	-4.412277	-1.237264	-0.360342
18	6	0	2.574026	-0.886298	0.075533
19	1	0	2.537258	-1.462652	-0.852181
20	1	0	2.300289	0.141623	-0.207485
21	6	0	3.983714	-0.876697	0.603711
22	8	0	4.315528	-1.188960	1.723351
23	8	0	4.825046	-0.269957	-0.260608
24	1	0	5.681970	-0.177361	0.182559

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.353208	0.000000			
3	N	2.209110	1.392418	0.000000		
4	C	2.218560	2.226557	1.353329	0.000000	
5	N	1.389290	2.211648	2.180981	1.341645	0.000000
6	C	2.547857	3.635482	3.603089	2.493345	1.471748
7	H	1.075788	2.208135	3.267541	3.235701	2.162374
8	H	2.211258	1.074658	2.162654	3.242395	3.269407
9	H	3.384726	4.267465	3.894211	2.597213	2.075928
10	H	2.798328	4.021809	4.219025	3.260973	2.087826
11	Br	4.214085	4.191728	3.397804	2.802551	3.452351
12	H	3.249611	3.255925	2.154395	1.072156	2.147413

13	C	3.589014	2.521957	1.417365	2.439599	3.541392
14	C	4.338088	3.067329	2.422043	3.635874	4.587279
15	H	4.227120	3.350867	2.085357	2.615395	3.884741
16	H	5.389170	4.119882	3.391441	4.508993	5.565190
17	H	4.201090	2.898753	2.720302	4.020775	4.721757
18	C	3.209875	4.299820	4.390624	3.386329	2.474638
19	H	2.988670	4.127720	4.539335	3.804182	2.751627
20	H	3.515818	4.337232	4.205402	3.218890	2.709677
21	C	4.608656	5.764435	5.812636	4.695458	3.809197
22	O	5.190122	6.373658	6.338251	5.126294	4.261076
23	O	5.496017	6.581459	6.660738	5.623328	4.826868
24	H	6.358314	7.472523	7.507071	6.403808	5.620194

		6	7	8	9	10
6	C	0.000000				
7	H	2.838927	0.000000			
8	H	4.660421	2.754075	0.000000		
9	H	1.087868	3.840478	5.335457	0.000000	
10	H	1.091022	2.780862	4.973465	1.755769	0.000000
11	Br	3.866251	5.012419	4.955971	3.806514	4.946105
12	H	2.838675	4.225171	4.230532	2.503869	3.658893
13	C	4.894423	4.619293	2.835631	5.016040	5.570136
14	C	6.010913	5.266410	2.931037	6.202556	6.566410
15	H	5.061963	5.283233	3.785520	5.011050	5.876305
16	H	6.954142	6.326025	3.930409	7.064397	7.562915
17	H	6.182037	4.995641	2.487659	6.501907	6.584146
18	C	1.523562	3.277085	5.224944	2.155009	2.182546
19	H	2.182216	2.771165	4.907041	3.075715	2.567884
20	H	2.158756	3.812469	5.245947	2.499115	3.082513
21	C	2.505728	4.534893	6.697178	2.745496	2.790944
22	O	2.802742	5.132146	7.356391	2.732585	2.811996
23	O	3.695874	5.370358	7.439185	3.957062	4.068285
24	H	4.374786	6.215553	8.355069	4.490582	4.644221

		11	12	13	14	15
11	Br	0.000000				
12	H	2.713017	0.000000			
13	C	3.720716	2.780151	0.000000		
14	C	4.972558	4.029551	1.327886	0.000000	
15	H	3.148233	2.598799	1.084009	2.131475	0.000000
16	H	5.472509	4.742561	2.084551	1.081275	2.464534
17	H	5.699849	4.587688	2.122318	1.083383	3.103652
18	C	3.668047	3.756375	5.621496	6.780862	5.673895
19	H	4.145970	4.407804	5.817352	6.862829	6.007217
20	H	2.713784	3.474101	5.257470	6.480571	5.138795
21	C	4.735012	4.859096	7.019928	8.212970	6.990416

22	O	5.477060	5.139421	7.545453	8.738395	7.512728
23	O	5.052798	5.797791	7.793707	8.996533	7.685988
24	H	5.813601	6.482747	8.631877	9.856787	8.484886

		16	17	18	19	20
16	H	0.000000				
17	H	1.850800	0.000000			
18	C	7.681349	7.008681	0.000000		
19	H	7.801275	6.970562	1.092790	0.000000	
20	H	7.286160	6.854432	1.100752	1.745132	0.000000
21	C	9.096877	8.458846	1.505418	2.134292	2.128130
22	O	9.627277	8.973221	2.416554	3.141738	3.091888
23	O	9.833057	9.288367	2.357956	2.646971	2.558636
24	H	10.685095	10.164249	3.189570	3.551320	3.419013

		21	22	23	24
21	C	0.000000			
22	O	1.208802	0.000000		
23	O	1.350193	2.245055	0.000000	
24	H	1.884281	2.294458	0.969169	0.000000

Stoichiometry C8H11BrN2O2
Framework group C1[X(C8H11BrN2O2)]
Deg. of freedom 66
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.657436	-2.086680	-0.787664
2	6	0	-1.969103	-1.765016	-0.872733
3	7	0	-2.227890	-0.830382	0.126424
4	6	0	-1.063910	-0.545027	0.755091
5	7	0	-0.115882	-1.357044	0.263276
6	6	0	1.307648	-1.305055	0.633279
7	1	0	-0.065202	-2.762021	-1.379688
8	1	0	-2.728009	-2.083423	-1.563796
9	1	0	1.374458	-0.821701	1.605576
10	1	0	1.666109	-2.328544	0.752882
11	35	0	-0.455979	2.061820	-0.075007
12	1	0	-0.977571	0.035705	1.652206
13	6	0	-3.434553	-0.124855	0.361201
14	6	0	-4.640542	-0.618323	0.105540
15	1	0	-3.258466	0.877571	0.734309

16	1	0	-5.513297	-0.000861	0.267385
17	1	0	-4.800249	-1.623129	-0.266722
18	6	0	2.121260	-0.528606	-0.394536
19	1	0	2.047733	-0.969059	-1.391924
20	1	0	1.716329	0.490124	-0.493903
21	6	0	3.569637	-0.429872	0.003886
22	8	0	4.045551	-0.855893	1.030148
23	8	0	4.250799	0.385915	-0.828899
24	1	0	5.135019	0.514063	-0.453367

Rotational constants (GHZ): 0.8371659 0.3333551 0.2564918

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 404 symmetry adapted cartesian basis functions of A symmetry.

There are 389 symmetry adapted basis functions of A symmetry.

389 basis functions, 625 primitive gaussians, 404 cartesian basis functions

62 alpha electrons 62 beta electrons

nuclear repulsion energy 1077.2388817761 Hartrees.

NAtoms= 24 NActive= 24 NUniq= 24 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 389 RedAO= T EigKep= 6.15D-06 NBF= 389

NBsUse= 389 1.00D-06 EigRej= -1.00D+00 NBFU= 389

Initial guess from the checkpoint file: "./cooh.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999836 -0.017732 -0.002274 0.002723 Ang= -2.07 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Keep R1 ints in memory in canonical form, NReq=2910765817.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3145.73030746 A.U. after 15 cycles

NFock= 15 Conv=0.42D-08 -V/T= 2.0017

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000574811	-0.000023188	0.000055084
2	6	-0.000008795	0.000260967	-0.000191292
3	7	0.000985141	-0.000047968	0.000220242
4	6	-0.001275191	-0.000992224	0.000267018
5	7	0.002507302	-0.000925529	0.001119818
6	6	-0.002745850	-0.001831248	0.000811234
7	1	0.000135462	0.000045306	-0.000068421
8	1	-0.000075129	-0.000067152	0.000013530
9	1	-0.000264241	0.000342492	0.000782635
10	1	-0.000071030	-0.000180997	-0.000201676
11	35	0.000024040	0.000616025	-0.000136553
12	1	0.000336982	0.000333785	-0.000344348
13	6	-0.000675409	0.000333030	-0.000067483
14	6	0.000211048	-0.000079304	0.000057442
15	1	0.000175688	0.000086067	-0.000092267
16	1	-0.000006539	0.000010433	0.000021005
17	1	0.000012090	-0.000038275	-0.000019733
18	6	0.001178401	-0.001149318	-0.005770019
19	1	0.000033931	-0.001619047	-0.000676573
20	1	0.000642239	-0.001020501	0.001377926
21	6	-0.002983952	0.020034694	0.008594147
22	8	0.000511301	-0.007533867	-0.002442918
23	8	0.001657454	-0.005658549	-0.003128972
24	1	0.000269866	-0.000895630	-0.000179826

Cartesian Forces: Max 0.020034694 RMS 0.003031001

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.005265062 RMS 0.001187115

Search for a local minimum.

Step number 5 out of a maximum of 140
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- RFO/linear search
Update second derivatives using D2CorX and points 3 5 4
DE= 1.56D-03 DEPred=-4.62D-04 R=-3.37D+00
Trust test=-3.37D+00 RLast= 6.89D-01 DXMaxT set to 7.14D-01
ITU= -1 1 1 1 0
Use linear search instead of GDIIS.
Energy rises -- skip Quadratic/GDIIS search.
Quartic linear search produced a step of -0.80866.
Iteration 1 RMS(Cart)= 0.05897749 RMS(Int)= 0.01259790
Iteration 2 RMS(Cart)= 0.02166986 RMS(Int)= 0.00053834
Iteration 3 RMS(Cart)= 0.00077519 RMS(Int)= 0.00012672
Iteration 4 RMS(Cart)= 0.00000046 RMS(Int)= 0.00012672

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55719	0.00002	-0.00088	0.00000	-0.00087	2.55632
R2	2.62538	0.00020	0.00109	0.00000	0.00109	2.62647
R3	2.03294	0.00006	0.00027	0.00000	0.00027	2.03321
R4	2.63129	-0.00010	0.00094	0.00000	0.00095	2.63223
R5	2.03081	0.00006	0.00002	0.00000	0.00002	2.03083
R6	2.55742	-0.00062	0.00129	0.00000	0.00128	2.55870
R7	2.67843	0.00041	-0.00062	0.00000	-0.00062	2.67782
R8	2.53534	0.00026	0.00454	0.00000	0.00454	2.53988
R9	5.29605	0.00062	-0.05532	0.00000	-0.05531	5.24074
R10	2.02608	-0.00008	0.00006	0.00000	0.00006	2.02614
R11	2.78120	-0.00203	-0.00758	0.00000	-0.00757	2.77363
R12	2.05577	0.00083	0.00046	0.00000	0.00046	2.05623
R13	2.06173	0.00010	0.00136	0.00000	0.00136	2.06309
R14	2.87911	0.00290	0.01185	0.00000	0.01185	2.89096
R15	5.12686	0.00008	-0.02019	0.00000	-0.02019	5.10667
R16	5.12831	0.00015	0.00371	0.00000	0.00370	5.13201
R17	2.50934	-0.00018	0.00022	0.00000	0.00022	2.50956
R18	2.04848	0.00010	0.00004	0.00000	0.00004	2.04852
R19	2.04331	0.00001	-0.00001	0.00000	-0.00001	2.04330
R20	2.04730	0.00004	0.00000	0.00000	0.00000	2.04730
R21	2.06507	0.00143	-0.00005	0.00000	-0.00005	2.06502
R22	2.08012	-0.00143	0.00139	0.00000	0.00137	2.08149
R23	2.84483	0.00051	0.00332	0.00000	0.00332	2.84814
R24	2.28430	-0.00018	-0.00450	0.00000	-0.00450	2.27980
R25	2.55150	0.00039	0.00381	0.00000	0.00381	2.55531
R26	1.83146	0.00007	0.00102	0.00000	0.00102	1.83248
A1	1.87607	0.00005	0.00115	0.00000	0.00116	1.87723
A2	2.27607	0.00005	-0.00003	0.00000	-0.00003	2.27604

A3	2.13104	-0.00010	-0.00117	0.00000	-0.00117	2.12987
A4	1.86983	-0.00007	-0.00018	0.00000	-0.00017	1.86965
A5	2.28432	0.00004	0.00030	0.00000	0.00030	2.28462
A6	2.12829	0.00003	-0.00004	0.00000	-0.00004	2.12826
A7	1.89127	0.00015	0.00081	0.00000	0.00080	1.89207
A8	2.22838	-0.00014	-0.00116	0.00000	-0.00115	2.22723
A9	2.15355	-0.00001	0.00027	0.00000	0.00028	2.15382
A10	1.88583	0.00019	-0.00170	0.00000	-0.00168	1.88415
A11	1.81843	-0.00020	0.01092	0.00000	0.01091	1.82934
A12	2.17994	0.00007	-0.00265	0.00000	-0.00260	2.17734
A13	1.87666	0.00011	0.00120	0.00000	0.00121	1.87787
A14	2.18665	-0.00018	-0.00396	0.00000	-0.00391	2.18274
A15	1.89623	-0.00032	-0.00101	0.00000	-0.00102	1.89521
A16	2.19662	0.00063	0.00024	0.00000	0.00023	2.19685
A17	2.17721	-0.00033	0.00050	0.00000	0.00051	2.17773
A18	1.87527	-0.00008	0.00502	0.00000	0.00502	1.88030
A19	1.88832	-0.00017	-0.00382	0.00000	-0.00382	1.88449
A20	1.94435	0.00000	0.00951	0.00000	0.00951	1.95386
A21	1.87408	0.00003	0.00229	0.00000	0.00229	1.87637
A22	1.92167	0.00008	-0.00408	0.00000	-0.00406	1.91760
A23	1.95690	0.00013	-0.00867	0.00000	-0.00866	1.94824
A24	1.24575	0.00021	0.01332	0.00000	0.01332	1.25907
A25	1.38945	0.00011	0.01446	0.00000	0.01447	1.40392
A26	2.16074	-0.00019	0.00025	0.00000	0.00025	2.16099
A27	1.95955	-0.00005	0.00050	0.00000	0.00050	1.96005
A28	2.16211	0.00023	-0.00069	0.00000	-0.00069	2.16142
A29	2.08521	0.00000	0.00024	0.00000	0.00024	2.08545
A30	2.14683	-0.00002	-0.00033	0.00000	-0.00033	2.14650
A31	2.05113	0.00002	0.00010	0.00000	0.00010	2.05123
A32	1.95452	-0.00045	0.00309	0.00000	0.00309	1.95762
A33	1.91357	0.00041	-0.00366	0.00000	-0.00364	1.90993
A34	1.94837	-0.00118	-0.01231	0.00000	-0.01228	1.93609
A35	1.83991	0.00059	0.01758	0.00000	0.01758	1.85749
A36	1.90999	0.00045	0.00519	0.00000	0.00517	1.91516
A37	1.89349	0.00031	-0.00900	0.00000	-0.00896	1.88453
A38	2.52617	-0.00047	-0.01541	0.00000	-0.01544	2.51073
A39	2.18998	-0.00105	-0.00195	0.00000	-0.00112	2.18886
A40	1.94096	0.00181	0.01029	0.00000	0.01112	1.95208
A41	2.13882	0.00060	0.00242	0.00000	0.00325	2.14207
A42	1.87672	-0.00025	-0.00205	0.00000	-0.00205	1.87467
D1	0.00482	0.00004	-0.00019	0.00000	-0.00019	0.00462
D2	3.10462	0.00000	0.00250	0.00000	0.00250	3.10712
D3	-3.13211	0.00013	0.00661	0.00000	0.00661	-3.12550
D4	-0.03231	0.00009	0.00930	0.00000	0.00930	-0.02301

D5	-0.06421	0.00001	-0.00464	0.00000	-0.00464	-0.06885
D6	-3.03841	0.00018	-0.00295	0.00000	-0.00295	-3.04137
D7	3.07319	-0.00007	-0.01074	0.00000	-0.01075	3.06244
D8	0.09899	0.00010	-0.00906	0.00000	-0.00906	0.08993
D9	0.05560	-0.00005	0.00503	0.00000	0.00503	0.06063
D10	3.04832	-0.00007	0.00450	0.00000	0.00450	3.05282
D11	-3.04876	-0.00002	0.00262	0.00000	0.00262	-3.04614
D12	-0.05604	-0.00003	0.00209	0.00000	0.00209	-0.05395
D13	-0.09587	0.00004	-0.00784	0.00000	-0.00784	-0.10371
D14	1.89635	0.00015	-0.00203	0.00000	-0.00203	1.89432
D15	-2.98437	-0.00027	0.02369	0.00000	0.02370	-2.96067
D16	-3.09639	0.00007	-0.00719	0.00000	-0.00719	-3.10358
D17	-1.10417	0.00018	-0.00138	0.00000	-0.00137	-1.10554
D18	0.29829	-0.00024	0.02435	0.00000	0.02435	0.32264
D19	0.55540	0.00009	-0.00396	0.00000	-0.00396	0.55145
D20	-2.54487	0.00011	-0.00565	0.00000	-0.00565	-2.55052
D21	-2.75560	0.00008	-0.00454	0.00000	-0.00455	-2.76015
D22	0.42731	0.00010	-0.00624	0.00000	-0.00624	0.42107
D23	0.09901	-0.00004	0.00763	0.00000	0.00764	0.10664
D24	3.07551	-0.00009	0.00594	0.00000	0.00595	3.08146
D25	-1.85430	0.00005	-0.00474	0.00000	-0.00473	-1.85903
D26	1.12221	0.00000	-0.00644	0.00000	-0.00643	1.11578
D27	2.98629	0.00032	-0.02378	0.00000	-0.02379	2.96250
D28	-0.32039	0.00027	-0.02547	0.00000	-0.02548	-0.34587
D29	-2.24415	-0.00011	-0.00047	0.00000	-0.00048	-2.24463
D30	-0.24543	0.00006	0.00323	0.00000	0.00323	-0.24220
D31	-2.94149	0.00022	0.00238	0.00000	0.00237	-2.93912
D32	-0.92310	0.00012	0.00569	0.00000	0.00570	-0.91740
D33	1.23555	0.00017	-0.00165	0.00000	-0.00164	1.23390
D34	0.39342	0.00039	0.00447	0.00000	0.00446	0.39788
D35	2.41182	0.00029	0.00778	0.00000	0.00778	2.41960
D36	-1.71272	0.00034	0.00044	0.00000	0.00045	-1.71228
D37	-1.02873	-0.00035	-0.02091	0.00000	-0.02091	-1.04964
D38	1.00717	0.00037	0.00042	0.00000	0.00042	1.00760
D39	3.10591	0.00027	-0.02083	0.00000	-0.02084	3.08508
D40	-3.10744	-0.00031	-0.03061	0.00000	-0.03061	-3.13805
D41	-1.07153	0.00041	-0.00928	0.00000	-0.00928	-1.08081
D42	1.02721	0.00031	-0.03053	0.00000	-0.03054	0.99667
D43	1.09046	-0.00048	-0.02523	0.00000	-0.02522	1.06524
D44	3.12637	0.00024	-0.00390	0.00000	-0.00389	3.12248
D45	-1.05808	0.00014	-0.02515	0.00000	-0.02515	-1.08323
D46	-0.01104	0.00030	-0.00442	0.00000	-0.00442	-0.01546
D47	0.36392	0.00027	-0.00245	0.00000	-0.00245	0.36146
D48	-3.09068	-0.00001	-0.00098	0.00000	-0.00098	-3.09166

D49	0.04673	0.00001	-0.00071	0.00000	-0.00071	0.04602
D50	0.00486	-0.00003	0.00094	0.00000	0.00094	0.00580
D51	-3.14092	-0.00001	0.00121	0.00000	0.00121	-3.13971
D52	-0.34928	-0.00002	0.00814	0.00000	0.00814	-0.34114
D53	1.75760	0.00000	0.02015	0.00000	0.02015	1.77775
D54	-2.48112	0.00099	0.03087	0.00000	0.03088	-2.45024
D55	-0.04951	0.00349	-0.12197	0.00000	-0.12194	-0.17145
D56	-3.01855	-0.00524	-0.27476	0.00000	-0.27475	2.98989
D57	-2.22318	0.00457	-0.12103	0.00000	-0.12102	-2.34420
D58	1.09097	-0.00415	-0.27382	0.00000	-0.27383	0.81714
D59	2.06098	0.00346	-0.13971	0.00000	-0.13972	1.92126
D60	-0.90806	-0.00527	-0.29250	0.00000	-0.29253	-1.20059
D61	2.99967	0.00494	0.06679	0.00000	0.06674	3.06641
D62	0.02472	-0.00329	-0.08082	0.00000	-0.08077	-0.05605

Item	Value	Threshold	Converged?
Maximum Force	0.005265	0.000450	NO
RMS Force	0.001187	0.000300	NO
Maximum Displacement	0.479296	0.001800	NO
RMS Displacement	0.078193	0.001200	NO

Predicted change in Energy=-1.225580D-04

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.311143	-2.166063	-0.402143
2	6	0	-1.569766	-1.742725	-0.660162
3	7	0	-1.818587	-0.659937	0.180004
4	6	0	-0.689600	-0.391895	0.877771
5	7	0	0.208939	-1.350993	0.596308
6	6	0	1.587538	-1.380134	1.099180
7	1	0	0.260720	-2.963450	-0.843473
8	1	0	-2.294179	-2.084721	-1.376527
9	1	0	1.622769	-0.777986	2.004809
10	1	0	1.822240	-2.408859	1.379418
11	35	0	0.257960	1.984644	-0.192406
12	1	0	-0.630574	0.282552	1.709168
13	6	0	-2.965014	0.172682	0.201197
14	6	0	-4.186909	-0.243994	-0.110159
15	1	0	-2.724732	1.197018	0.462199
16	1	0	-5.005104	0.462882	-0.115318
17	1	0	-4.411817	-1.272089	-0.367374

18	6	0	2.582194	-0.834433	0.072897
19	1	0	2.575029	-1.411195	-0.855233
20	1	0	2.301019	0.195470	-0.198206
21	6	0	3.977948	-0.801379	0.640656
22	8	0	4.267300	-0.992354	1.796187
23	8	0	4.898417	-0.502821	-0.303839
24	1	0	5.757321	-0.430994	0.140521

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.352746	0.000000			
3	N	2.209004	1.392918	0.000000		
4	C	2.220153	2.228154	1.354008	0.000000	
5	N	1.389867	2.212683	2.182139	1.344046	0.000000
6	C	2.544925	3.632537	3.600729	2.492186	1.467741
7	H	1.075929	2.207816	3.267597	3.237079	2.162330
8	H	2.210989	1.074669	2.163096	3.243793	3.270479
9	H	3.385291	4.269083	3.897022	2.601217	2.076325
10	H	2.790024	4.013643	4.213424	3.260235	2.082086
11	Br	4.194787	4.177639	3.382979	2.773281	3.427965
12	H	3.248906	3.255388	2.153602	1.072187	2.147489
13	C	3.588423	2.521397	1.417039	2.440084	3.542835
14	C	4.336031	3.065637	2.422014	3.637176	4.587812
15	H	4.228808	3.351974	2.085429	2.615169	3.888029
16	H	5.387661	4.118629	3.391434	4.510038	5.566219
17	H	4.197133	2.895596	2.720146	4.022441	4.720837
18	C	3.220294	4.312904	4.405541	3.398278	2.484578
19	H	3.017467	4.162607	4.576021	3.834068	2.776505
20	H	3.527296	4.353503	4.224443	3.232108	2.720220
21	C	4.620183	5.775412	5.816529	4.691471	3.809129
22	O	5.212714	6.377151	6.305598	5.076898	4.247190
23	O	5.469511	6.595583	6.736239	5.712655	4.849830
24	H	6.334919	7.486517	7.579469	6.489056	5.642577

		6	7	8	9	10
6	C	0.000000				
7	H	2.835707	0.000000			
8	H	4.657605	2.753873	0.000000		
9	H	1.088112	3.839810	5.336991	0.000000	
10	H	1.091739	2.772573	4.964393	1.758024	0.000000
11	Br	3.841575	4.990744	4.947251	3.784519	4.921430
12	H	2.838420	4.224560	4.230021	2.507927	3.656327
13	C	4.893193	4.618660	2.834625	5.020412	5.565102
14	C	6.008123	5.264465	2.928206	6.205690	6.558609

15	H	5.063904	5.284619	3.786304	5.018072	5.875253
16	H	6.952311	6.324465	3.928109	7.068478	7.556041
17	H	6.176950	4.991991	2.482570	6.502893	6.573203
18	C	1.529832	3.280501	5.238612	2.157770	2.182509
19	H	2.189939	2.786694	4.943134	3.080194	2.560409
20	H	2.162127	3.815490	5.263417	2.502183	3.082314
21	C	2.501851	4.549172	6.712344	2.721825	2.788698
22	O	2.795947	5.187071	7.369693	2.661395	2.856309
23	O	3.701359	5.277701	7.442210	4.016894	3.991140
24	H	4.382577	6.131411	8.358402	4.548681	4.575115

		11	12	13	14	15
11	Br	0.000000				
12	H	2.702331	0.000000			
13	C	3.718292	2.781305	0.000000		
14	C	4.972972	4.029233	1.328002	0.000000	
15	H	3.153619	2.603205	1.084031	2.131214	0.000000
16	H	5.479192	4.743182	2.084793	1.081269	2.464260
17	H	5.695941	4.585492	2.122234	1.083385	3.103376
18	C	3.663283	3.774508	5.639349	6.797270	5.695771
19	H	4.164117	4.440813	5.858053	6.902267	6.051931
20	H	2.715745	3.498556	5.281207	6.503391	5.166953
21	C	4.721676	4.853359	7.024716	8.218228	6.996524
22	O	5.375112	5.061831	7.497178	8.698727	7.447240
23	O	5.266283	5.936223	7.908534	9.091075	7.847844
24	H	6.015739	6.616267	8.743410	9.949146	8.642865

		16	17	18	19	20
16	H	0.000000				
17	H	1.850850	0.000000			
18	C	7.699710	7.021507	0.000000		
19	H	7.843344	7.005239	1.092763	0.000000	
20	H	7.311485	6.873465	1.101479	1.757310	0.000000
21	C	9.103025	8.463205	1.507173	2.139565	2.123555
22	O	9.578572	8.949096	2.415420	3.173206	3.042169
23	O	9.952278	9.342176	2.369976	2.554860	2.691698
24	H	10.802511	10.216494	3.201370	3.475529	3.528911

		21	22	23	24
21	C	0.000000			
22	O	1.206420	0.000000		
23	O	1.352209	2.246788	0.000000	
24	H	1.885070	2.297067	0.969707	0.000000

Stoichiometry C8H11BrN2O2

Framework group C1[X(C8H11BrN2O2)]

Deg. of freedom 66

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.638307	-2.084967	-0.760713
2	6	0	-1.953563	-1.782420	-0.852845
3	7	0	-2.226234	-0.834575	0.130752
4	6	0	-1.065970	-0.517890	0.752712
5	7	0	-0.106472	-1.331006	0.278722
6	6	0	1.311663	-1.257677	0.649908
7	1	0	-0.034966	-2.758128	-1.344201
8	1	0	-2.707770	-2.123814	-1.538071
9	1	0	1.376312	-0.759118	1.614920
10	1	0	1.678534	-2.277431	0.781830
11	35	0	-0.482363	2.054906	-0.102399
12	1	0	-0.992777	0.062965	1.650952
13	6	0	-3.444376	-0.145941	0.354157
14	6	0	-4.641995	-0.662647	0.104533
15	1	0	-3.285864	0.864038	0.714625
16	1	0	-5.525060	-0.057724	0.257531
17	1	0	-4.784523	-1.674998	-0.254010
18	6	0	2.135314	-0.491916	-0.387201
19	1	0	2.093532	-0.959719	-1.373885
20	1	0	1.723267	0.522679	-0.505820
21	6	0	3.570591	-0.362383	0.054129
22	8	0	3.993925	-0.645400	1.147810
23	8	0	4.354652	0.141867	-0.925387
24	1	0	5.242205	0.261927	-0.553681

Rotational constants (GHZ): 0.8449103 0.3293854 0.2565044
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 404 symmetry adapted cartesian basis functions of A symmetry.
There are 389 symmetry adapted basis functions of A symmetry.
389 basis functions, 625 primitive gaussians, 404 cartesian basis functions
62 alpha electrons 62 beta electrons
nuclear repulsion energy 1077.4263942086 Hartrees.
NAtoms= 24 NActive= 24 NUniq= 24 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.
NBasis= 389 RedAO= T EigKep= 6.22D-06 NBF= 389
NBsUse= 389 1.00D-06 EigRej= -1.00D+00 NBFU= 389
Lowest energy guess from the checkpoint file: "./cooh.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999992 -0.003872 -0.000419 0.000650 Ang= -0.45 deg.
B after Tr= 0.000000 0.000000 0.000000
Rot= 0.999899 0.013917 0.001859 -0.002068 Ang= 1.63 deg.
Keep R1 ints in memory in canonical form, NReq=2910765817.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3145.73195190 A.U. after 11 cycles
NFock= 11 Conv=0.47D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000002962	0.000081683	-0.000039050
2	6	-0.000095530	0.000254280	0.000016457
3	7	0.000692225	0.000216428	-0.000140650
4	6	-0.000608370	-0.002166252	0.000881491
5	7	0.000468989	0.000208960	0.000067287
6	6	-0.000094053	-0.000672413	0.000026656
7	1	-0.000016374	-0.000021686	0.000051264
8	1	-0.000011148	-0.000000455	-0.000040211
9	1	-0.000412632	0.000000934	0.000514337
10	1	-0.000020597	0.000168911	0.000100932
11	35	0.000231233	0.001125208	-0.000594435
12	1	0.000324963	0.000282250	-0.000346104
13	6	-0.000443507	0.000184128	0.000045072
14	6	0.000150685	-0.000043988	0.000027679
15	1	0.000110737	0.000042586	-0.000085083
16	1	-0.000002465	0.000006683	0.000009957
17	1	-0.000000948	-0.000011066	-0.000011272
18	6	0.000778298	0.002893565	-0.000642062
19	1	0.000764128	-0.000399456	0.000017419
20	1	-0.000718877	-0.001445956	0.000191326
21	6	-0.000079590	0.000268067	-0.002120017
22	8	0.000184463	-0.000579830	0.002124492

23	8	-0.000843046	0.000128828	0.000085410
24	1	-0.000361544	-0.000521411	-0.000140894

Cartesian Forces: Max 0.002893565 RMS 0.000680344

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.002163776 RMS 0.000368384

Search for a local minimum.

Step number 6 out of a maximum of 140

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Update second derivatives using D2CorX and points 5 4 6

ITU= 0 -1 1 1 1 0

Use linear search instead of GDIIS.

Eigenvalues ---	0.00197	0.00387	0.00808	0.01479	0.01754
Eigenvalues ---	0.01960	0.02030	0.02117	0.02192	0.02274
Eigenvalues ---	0.02278	0.02346	0.02418	0.02820	0.03038
Eigenvalues ---	0.03038	0.03104	0.03586	0.04444	0.04650
Eigenvalues ---	0.04980	0.05593	0.06523	0.08303	0.09509
Eigenvalues ---	0.10667	0.12404	0.14960	0.15913	0.15979
Eigenvalues ---	0.15991	0.15996	0.16000	0.16000	0.16254
Eigenvalues ---	0.16730	0.17957	0.20664	0.22003	0.22837
Eigenvalues ---	0.24485	0.24718	0.27384	0.27731	0.34214
Eigenvalues ---	0.34377	0.35130	0.35435	0.35499	0.35579
Eigenvalues ---	0.35844	0.35902	0.36375	0.36592	0.36650
Eigenvalues ---	0.37449	0.41317	0.43069	0.43792	0.47639
Eigenvalues ---	0.52334	0.53307	0.54332	0.54462	0.59921
Eigenvalues ---	0.91231				

RFO step: Lambda=-1.54902734D-04 EMin= 1.97033827D-03

Quartic linear search produced a step of -0.00369.

Iteration 1 RMS(Cart)= 0.01191707 RMS(Int)= 0.00022196

Iteration 2 RMS(Cart)= 0.00019934 RMS(Int)= 0.00001624

Iteration 3 RMS(Cart)= 0.00000011 RMS(Int)= 0.00001624

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55632	0.00006	0.00000	0.00047	0.00046	2.55678
R2	2.62647	0.00000	0.00000	-0.00018	-0.00018	2.62629
R3	2.03321	-0.00001	0.00000	-0.00007	-0.00007	2.03314
R4	2.63223	-0.00021	0.00000	-0.00054	-0.00054	2.63169
R5	2.03083	0.00003	0.00000	0.00009	0.00009	2.03092

R6	2.55870	-0.00045	0.00000	-0.00120	-0.00119	2.55752
R7	2.67782	0.00025	0.00000	0.00070	0.00070	2.67851
R8	2.53988	-0.00036	0.00000	-0.00166	-0.00166	2.53822
R9	5.24074	0.00071	-0.00005	0.03428	0.03421	5.27496
R10	2.02614	-0.00007	0.00000	-0.00007	-0.00006	2.02608
R11	2.77363	-0.00052	-0.00001	0.00020	0.00019	2.77382
R12	2.05623	0.00041	0.00000	0.00107	0.00107	2.05731
R13	2.06309	-0.00014	0.00000	-0.00064	-0.00064	2.06245
R14	2.89096	0.00059	0.00001	0.00020	0.00022	2.89118
R15	5.10667	0.00028	-0.00002	0.00732	0.00731	5.11397
R16	5.13201	-0.00005	0.00000	-0.00244	-0.00243	5.12958
R17	2.50956	-0.00013	0.00000	-0.00026	-0.00026	2.50930
R18	2.04852	0.00004	0.00000	0.00013	0.00013	2.04865
R19	2.04330	0.00001	0.00000	0.00002	0.00002	2.04332
R20	2.04730	0.00001	0.00000	0.00004	0.00004	2.04734
R21	2.06502	0.00019	0.00000	0.00059	0.00059	2.06561
R22	2.08149	-0.00106	0.00000	-0.00277	-0.00276	2.07874
R23	2.84814	-0.00106	0.00000	-0.00277	-0.00277	2.84537
R24	2.27980	0.00216	0.00000	0.00249	0.00249	2.28229
R25	2.55531	-0.00085	0.00000	-0.00198	-0.00198	2.55333
R26	1.83248	-0.00043	0.00000	-0.00049	-0.00049	1.83199
A1	1.87723	-0.00004	0.00000	-0.00014	-0.00014	1.87708
A2	2.27604	0.00003	0.00000	0.00004	0.00004	2.27608
A3	2.12987	0.00001	0.00000	0.00011	0.00011	2.12998
A4	1.86965	-0.00009	0.00000	-0.00006	-0.00006	1.86959
A5	2.28462	0.00004	0.00000	-0.00005	-0.00005	2.28457
A6	2.12826	0.00005	0.00000	0.00006	0.00007	2.12832
A7	1.89207	0.00004	0.00000	-0.00031	-0.00029	1.89177
A8	2.22723	0.00000	0.00000	0.00033	0.00032	2.22755
A9	2.15382	-0.00003	0.00000	-0.00003	-0.00003	2.15379
A10	1.88415	0.00022	0.00000	0.00138	0.00135	1.88550
A11	1.82934	-0.00046	0.00001	-0.00510	-0.00507	1.82426
A12	2.17734	0.00000	0.00000	0.00210	0.00201	2.17935
A13	1.87787	0.00019	0.00000	0.00022	0.00021	1.87809
A14	2.18274	-0.00010	0.00000	0.00192	0.00184	2.18457
A15	1.89521	-0.00011	0.00000	-0.00028	-0.00027	1.89494
A16	2.19685	0.00025	0.00000	0.00153	0.00153	2.19838
A17	2.17773	-0.00014	0.00000	-0.00131	-0.00132	2.17641
A18	1.88030	-0.00013	0.00000	-0.00384	-0.00383	1.87646
A19	1.88449	0.00008	0.00000	0.00093	0.00093	1.88542
A20	1.95386	-0.00035	0.00001	-0.00243	-0.00240	1.95145
A21	1.87637	-0.00017	0.00000	-0.00150	-0.00151	1.87487
A22	1.91760	0.00039	0.00000	0.00410	0.00409	1.92169
A23	1.94824	0.00017	-0.00001	0.00248	0.00247	1.95071

A24	1.25907	-0.00046	0.00001	-0.00586	-0.00585	1.25322
A25	1.40392	-0.00052	0.00001	-0.00668	-0.00669	1.39723
A26	2.16099	-0.00009	0.00000	-0.00049	-0.00049	2.16051
A27	1.96005	-0.00005	0.00000	-0.00043	-0.00043	1.95961
A28	2.16142	0.00013	0.00000	0.00088	0.00088	2.16230
A29	2.08545	-0.00001	0.00000	-0.00010	-0.00010	2.08536
A30	2.14650	0.00000	0.00000	0.00008	0.00008	2.14657
A31	2.05123	0.00000	0.00000	0.00002	0.00002	2.05125
A32	1.95762	0.00028	0.00000	-0.00267	-0.00269	1.95493
A33	1.90993	-0.00010	0.00000	0.00448	0.00446	1.91439
A34	1.93609	-0.00038	-0.00001	-0.00016	-0.00025	1.93584
A35	1.85749	0.00006	0.00002	-0.00197	-0.00192	1.85557
A36	1.91516	-0.00055	0.00000	-0.01110	-0.01110	1.90406
A37	1.88453	0.00073	-0.00001	0.01206	0.01204	1.89656
A38	2.51073	0.00068	-0.00001	0.00587	0.00588	2.51661
A39	2.18886	0.00013	0.00000	0.00159	0.00157	2.19043
A40	1.95208	-0.00108	0.00001	-0.00287	-0.00288	1.94920
A41	2.14207	0.00096	0.00000	0.00146	0.00144	2.14351
A42	1.87467	-0.00024	0.00000	0.00143	0.00143	1.87610
D1	0.00462	-0.00001	0.00000	-0.00013	-0.00013	0.00449
D2	3.10712	-0.00005	0.00000	-0.00161	-0.00161	3.10551
D3	-3.12550	0.00004	0.00001	-0.00108	-0.00108	-3.12658
D4	-0.02301	0.00000	0.00001	-0.00256	-0.00255	-0.02556
D5	-0.06885	0.00009	0.00000	0.00312	0.00311	-0.06573
D6	-3.04137	0.00014	0.00000	0.00366	0.00365	-3.03771
D7	3.06244	0.00004	-0.00001	0.00397	0.00396	3.06641
D8	0.08993	0.00009	-0.00001	0.00451	0.00450	0.09443
D9	0.06063	-0.00006	0.00000	-0.00289	-0.00288	0.05775
D10	3.05282	-0.00005	0.00000	-0.00297	-0.00297	3.04985
D11	-3.04614	-0.00002	0.00000	-0.00156	-0.00156	-3.04770
D12	-0.05395	-0.00001	0.00000	-0.00165	-0.00165	-0.05560
D13	-0.10371	0.00009	-0.00001	0.00474	0.00474	-0.09897
D14	1.89432	0.00019	0.00000	0.00317	0.00316	1.89748
D15	-2.96067	-0.00034	0.00002	-0.01474	-0.01473	-2.97541
D16	-3.10358	0.00008	-0.00001	0.00478	0.00479	-3.09880
D17	-1.10554	0.00018	0.00000	0.00321	0.00320	-1.10234
D18	0.32264	-0.00035	0.00002	-0.01470	-0.01469	0.30795
D19	0.55145	0.00006	0.00000	0.00517	0.00517	0.55662
D20	-2.55052	0.00007	0.00000	0.00603	0.00603	-2.54449
D21	-2.76015	0.00007	0.00000	0.00506	0.00506	-2.75509
D22	0.42107	0.00008	-0.00001	0.00592	0.00592	0.42698
D23	0.10664	-0.00011	0.00001	-0.00483	-0.00483	0.10182
D24	3.08146	-0.00011	0.00001	-0.00502	-0.00502	3.07644
D25	-1.85903	0.00023	0.00000	0.00030	0.00028	-1.85875

D26	1.11578	0.00022	-0.00001	0.00010	0.00009	1.11588
D27	2.96250	0.00035	-0.00002	0.01477	0.01475	2.97725
D28	-0.34587	0.00034	-0.00002	0.01458	0.01456	-0.33131
D29	-2.24463	-0.00015	0.00000	-0.00003	-0.00001	-2.24464
D30	-0.24220	-0.00002	0.00000	-0.00076	-0.00077	-0.24297
D31	-2.93912	0.00024	0.00000	0.00427	0.00428	-2.93484
D32	-0.91740	0.00001	0.00000	0.00102	0.00102	-0.91638
D33	1.23390	0.00005	0.00000	0.00321	0.00321	1.23711
D34	0.39788	0.00029	0.00000	0.00474	0.00474	0.40263
D35	2.41960	0.00006	0.00001	0.00148	0.00148	2.42109
D36	-1.71228	0.00010	0.00000	0.00367	0.00367	-1.70861
D37	-1.04964	-0.00028	-0.00002	0.00023	0.00020	-1.04944
D38	1.00760	-0.00010	0.00000	-0.00096	-0.00096	1.00664
D39	3.08508	0.00050	-0.00002	0.01668	0.01666	3.10174
D40	-3.13805	-0.00015	-0.00003	0.00387	0.00384	-3.13421
D41	-1.08081	0.00003	-0.00001	0.00268	0.00268	-1.07813
D42	0.99667	0.00063	-0.00003	0.02033	0.02030	1.01697
D43	1.06524	-0.00030	-0.00002	0.00148	0.00145	1.06669
D44	3.12248	-0.00012	0.00000	0.00029	0.00029	3.12277
D45	-1.08323	0.00048	-0.00002	0.01794	0.01791	-1.06532
D46	-0.01546	0.00001	0.00000	-0.00042	-0.00043	-0.01589
D47	0.36146	0.00001	0.00000	-0.00167	-0.00169	0.35977
D48	-3.09166	-0.00001	0.00000	-0.00014	-0.00014	-3.09180
D49	0.04602	0.00001	0.00000	0.00045	0.00045	0.04648
D50	0.00580	-0.00003	0.00000	-0.00113	-0.00113	0.00466
D51	-3.13971	-0.00001	0.00000	-0.00054	-0.00054	-3.14025
D52	-0.34114	0.00000	0.00001	0.00026	0.00028	-0.34085
D53	1.77775	0.00031	0.00002	-0.00160	-0.00159	1.77615
D54	-2.45024	0.00007	0.00003	-0.00949	-0.00950	-2.45974
D55	-0.17145	0.00005	-0.00011	0.02783	0.02772	-0.14372
D56	2.98989	-0.00038	-0.00024	0.01766	0.01742	3.00731
D57	-2.34420	0.00034	-0.00011	0.03923	0.03909	-2.30510
D58	0.81714	-0.00008	-0.00024	0.02907	0.02880	0.84593
D59	1.92126	0.00015	-0.00012	0.04080	0.04071	1.96197
D60	-1.20059	-0.00027	-0.00026	0.03064	0.03041	-1.17018
D61	3.06641	0.00061	0.00006	0.02333	0.02339	3.08980
D62	-0.05605	0.00021	-0.00007	0.01348	0.01341	-0.04265

Item	Value	Threshold	Converged?
Maximum Force	0.002164	0.000450	NO
RMS Force	0.000368	0.000300	NO
Maximum Displacement	0.089801	0.001800	NO
RMS Displacement	0.011928	0.001200	NO

Predicted change in Energy=-7.834230D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.308663	-2.169372	-0.397186
2	6	0	-1.566983	-1.746182	-0.658179
3	7	0	-1.817368	-0.662875	0.180378
4	6	0	-0.691201	-0.397028	0.882311
5	7	0	0.209253	-1.353260	0.601408
6	6	0	1.587560	-1.377184	1.105647
7	1	0	0.263790	-2.967672	-0.835996
8	1	0	-2.289510	-2.088084	-1.376562
9	1	0	1.614652	-0.777300	2.013738
10	1	0	1.827056	-2.404568	1.385432
11	35	0	0.256170	1.997523	-0.194930
12	1	0	-0.629294	0.286757	1.705790
13	6	0	-2.962461	0.172312	0.196713
14	6	0	-4.184494	-0.243854	-0.114195
15	1	0	-2.719838	1.197430	0.452706
16	1	0	-5.001573	0.464286	-0.123315
17	1	0	-4.410818	-1.272825	-0.366712
18	6	0	2.577912	-0.823039	0.079552
19	1	0	2.570749	-1.399216	-0.849305
20	1	0	2.294127	0.204480	-0.191960
21	6	0	3.976354	-0.805286	0.637402
22	8	0	4.277422	-1.039875	1.783242
23	8	0	4.886134	-0.477788	-0.306360
24	1	0	5.752996	-0.438152	0.125854

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.352988	0.000000			
3	N	2.208914	1.392633	0.000000		
4	C	2.219156	2.227178	1.353379	0.000000	
5	N	1.389772	2.212683	2.181992	1.343170	0.000000
6	C	2.545925	3.632959	3.599985	2.490650	1.467842
7	H	1.075890	2.208028	3.267464	3.236170	2.162274
8	H	2.211230	1.074716	2.162915	3.242957	3.270496
9	H	3.383720	4.266225	3.892693	2.596477	2.074018
10	H	2.791835	4.016133	4.215148	3.259597	2.082602
11	Br	4.209864	4.189728	3.393838	2.791386	3.444431

12	H	3.249290	3.255834	2.154112	1.072153	2.147668
13	C	3.588710	2.521670	1.417407	2.439839	3.542728
14	C	4.337023	3.066638	2.421908	3.635874	4.587797
15	H	4.227462	3.350820	2.085510	2.615765	3.886863
16	H	5.388373	4.119303	3.391443	4.509152	5.566094
17	H	4.199095	2.897657	2.719804	4.020277	4.721100
18	C	3.220591	4.310058	4.399352	3.393082	2.482743
19	H	3.014725	4.156651	4.567058	3.826643	2.771885
20	H	3.528712	4.350933	4.218451	3.229250	2.720788
21	C	4.614377	5.769957	5.813464	4.691772	3.806918
22	O	5.202135	6.373106	6.313300	5.090397	4.247934
23	O	5.464030	6.585995	6.723698	5.703169	4.843936
24	H	6.325694	7.477149	7.573894	6.488574	5.638853

		6	7	8	9	10
6	C	0.000000				
7	H	2.837604	0.000000			
8	H	4.658155	2.754128	0.000000		
9	H	1.088679	3.839732	5.334301	0.000000	
10	H	1.091402	2.774100	4.967382	1.757238	0.000000
11	Br	3.853926	5.006414	4.956705	3.797806	4.933927
12	H	2.836073	4.224877	4.230494	2.502468	3.657803
13	C	4.891809	4.618948	2.835039	5.015308	5.567122
14	C	6.007417	5.265682	2.930140	6.200223	6.561730
15	H	5.060499	5.283073	3.784971	5.012403	5.875255
16	H	6.951117	6.325369	3.929441	7.062787	7.558890
17	H	6.177319	4.994466	2.486844	6.497567	6.577380
18	C	1.529949	3.285246	5.235685	2.161258	2.184111
19	H	2.188375	2.789676	4.937070	3.081869	2.560832
20	H	2.164412	3.820942	5.260120	2.508123	3.084389
21	C	2.500532	4.542020	6.705421	2.733628	2.781499
22	O	2.794328	5.165854	7.362587	2.685595	2.832831
23	O	3.699091	5.276941	7.431571	4.021835	3.991567
24	H	4.380940	6.120050	8.346342	4.561252	4.567968

		11	12	13	14	15
11	Br	0.000000				
12	H	2.706198	0.000000			
13	C	3.720802	2.781022	0.000000		
14	C	4.974916	4.029062	1.327864	0.000000	
15	H	3.149001	2.601907	1.084097	2.131641	0.000000
16	H	5.477208	4.742780	2.084621	1.081279	2.464876
17	H	5.701357	4.585573	2.122170	1.083406	3.103711
18	C	3.663522	3.763305	5.630291	6.789928	5.682226
19	H	4.162129	4.428464	5.846390	6.892645	6.035571
20	H	2.714457	3.486347	5.271036	6.494581	5.151834

21	C	4.731626	4.852423	7.021187	8.214594	6.991708
22	O	5.413817	5.083485	7.510152	8.708498	7.465756
23	O	5.251299	5.920577	7.891525	9.075679	7.825174
24	H	6.020839	6.614780	8.737098	9.942288	8.635443

		16	17	18	19	20
16	H	0.000000				
17	H	1.850889	0.000000			
18	C	7.690705	7.017393	0.000000		
19	H	7.831971	6.999368	1.093072	0.000000	
20	H	7.300647	6.867988	1.100021	1.755125	0.000000
21	C	9.099103	8.459994	1.505707	2.130440	2.130107
22	O	9.591517	8.953328	2.416177	3.157873	3.063217
23	O	9.934172	9.331080	2.365591	2.550456	2.682737
24	H	10.795241	10.209917	3.198663	3.464285	3.532386

		21	22	23	24
21	C	0.000000			
22	O	1.207735	0.000000		
23	O	1.351163	2.247868	0.000000	
24	H	1.884920	2.299201	0.969448	0.000000

Stoichiometry C8H11BrN2O2
Framework group C1[X(C8H11BrN2O2)]
Deg. of freedom 66
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.629892	-2.088834	-0.764051
2	6	0	-1.945762	-1.788462	-0.858060
3	7	0	-2.222224	-0.844496	0.127801
4	6	0	-1.064787	-0.530758	0.755132
5	7	0	-0.101918	-1.337033	0.278784
6	6	0	1.315347	-1.257211	0.652347
7	1	0	-0.024181	-2.759583	-1.347789
8	1	0	-2.697573	-2.128238	-1.546788
9	1	0	1.371348	-0.765723	1.622155
10	1	0	1.688905	-2.274762	0.779632
11	35	0	-0.489344	2.065101	-0.094701
12	1	0	-0.991788	0.057216	1.648703
13	6	0	-3.441263	-0.156044	0.349213
14	6	0	-4.637931	-0.673853	0.098051

15	1	0	-3.283160	0.854477	0.708539
16	1	0	-5.521700	-0.069551	0.249492
17	1	0	-4.779151	-1.686670	-0.259759
18	6	0	2.132304	-0.477906	-0.380130
19	1	0	2.091409	-0.941312	-1.369266
20	1	0	1.715762	0.533664	-0.495309
21	6	0	3.570551	-0.360727	0.049830
22	8	0	4.009629	-0.687647	1.126379
23	8	0	4.340046	0.176177	-0.922412
24	1	0	5.237357	0.267210	-0.566919

Rotational constants (GHZ): 0.8384115 0.3298318 0.2559545

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 404 symmetry adapted cartesian basis functions of A symmetry.

There are 389 symmetry adapted basis functions of A symmetry.

389 basis functions, 625 primitive gaussians, 404 cartesian basis functions

62 alpha electrons 62 beta electrons

nuclear repulsion energy 1076.5183507765 Hartrees.

NAtoms= 24 NActive= 24 NUniq= 24 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 389 RedAO= T EigKep= 6.23D-06 NBF= 389

NBsUse= 389 1.00D-06 EigRej= -1.00D+00 NBFU= 389

Initial guess from the checkpoint file: "./cooh.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 0.999996 -0.002697 -0.000274 -0.000951 Ang= -0.33 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Keep R1 ints in memory in canonical form, NReq=2910765817.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3145.73206461 A.U. after 11 cycles
NFock= 11 Conv=0.49D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000019593	0.000034670	-0.000051230
2	6	-0.000008083	0.000227476	-0.000044808
3	7	0.000806063	0.000140235	0.000001966
4	6	-0.000705597	-0.001709147	0.000562308
5	7	0.000163181	0.000102440	-0.000012368
6	6	-0.000487497	-0.000104995	0.000308496
7	1	0.000016160	-0.000021156	0.000021043
8	1	-0.000018632	-0.000025970	0.000016877
9	1	0.000008764	-0.000033215	0.000155954
10	1	0.000129664	0.000041404	-0.000086241
11	35	0.000127282	0.000819806	-0.000385346
12	1	0.000285873	0.000314208	-0.000318379
13	6	-0.000466907	0.000273708	0.000028493
14	6	0.000124161	-0.000080843	0.000061962
15	1	0.000109826	0.000038023	-0.000080841
16	1	-0.000001162	0.000010960	-0.000014192
17	1	0.000004745	-0.000009939	-0.000011416
18	6	0.000505221	0.001251129	-0.000585614
19	1	0.000267489	-0.000372741	-0.000103224
20	1	-0.000636583	-0.000614513	0.000442993
21	6	0.000450530	-0.000033624	-0.000215080
22	8	-0.000187591	-0.000103037	0.000331353
23	8	-0.000267665	0.000049424	-0.000068451
24	1	-0.000199651	-0.000194302	0.000045745

Cartesian Forces: Max 0.001709147 RMS 0.000377945

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000573743 RMS 0.000169569
Search for a local minimum.

Step number 7 out of a maximum of 140
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 5 4 6 7
DE= -1.13D-04 DEPred=-7.83D-05 R= 1.44D+00
TightC=F SS= 1.41D+00 RLast= 1.04D-01 DXNew= 1.2000D+00 3.1335D-01
Trust test= 1.44D+00 RLast= 1.04D-01 DXMaxT set to 7.14D-01
ITU= 1 0 -1 1 1 1 0

Eigenvalues ---	0.00195	0.00387	0.00810	0.01291	0.01616
Eigenvalues ---	0.01796	0.01978	0.02038	0.02129	0.02197
Eigenvalues ---	0.02314	0.02346	0.02416	0.02485	0.03038
Eigenvalues ---	0.03038	0.03158	0.03668	0.04335	0.04598
Eigenvalues ---	0.05040	0.05579	0.06541	0.08447	0.09862
Eigenvalues ---	0.10513	0.12251	0.15045	0.15461	0.15975
Eigenvalues ---	0.15992	0.15996	0.16000	0.16000	0.16085
Eigenvalues ---	0.16777	0.17863	0.20670	0.21999	0.22833
Eigenvalues ---	0.24484	0.25089	0.27319	0.27701	0.34303
Eigenvalues ---	0.34389	0.35139	0.35390	0.35502	0.35579
Eigenvalues ---	0.35843	0.35869	0.36306	0.36597	0.36650
Eigenvalues ---	0.37238	0.41323	0.43053	0.43696	0.47518
Eigenvalues ---	0.52410	0.53288	0.54007	0.54601	0.59914
Eigenvalues ---	0.93017				

En-DIIS/RFO-DIIS IScMMF= 0 using points: 7 6
RFO step: Lambda=-1.54389816D-05.
DidBck=F Rises=F RFO-DIIS coefs: 1.84219 -0.84219
Iteration 1 RMS(Cart)= 0.01163542 RMS(Int)= 0.00017470
Iteration 2 RMS(Cart)= 0.00015795 RMS(Int)= 0.00004356
Iteration 3 RMS(Cart)= 0.00000007 RMS(Int)= 0.00004356

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55678	0.00000	0.00039	0.00017	0.00053	2.55730
R2	2.62629	-0.00002	-0.00015	-0.00005	-0.00022	2.62607
R3	2.03314	0.00001	-0.00006	0.00008	0.00002	2.03316
R4	2.63169	-0.00012	-0.00045	-0.00027	-0.00074	2.63096
R5	2.03092	0.00001	0.00007	-0.00002	0.00006	2.03098
R6	2.55752	-0.00055	-0.00100	-0.00163	-0.00261	2.55491
R7	2.67851	0.00032	0.00059	0.00108	0.00167	2.68018
R8	2.53822	-0.00022	-0.00140	-0.00083	-0.00221	2.53601
R9	5.27496	0.00057	0.02881	0.02098	0.04975	5.32471
R10	2.02608	-0.00002	-0.00005	0.00014	0.00010	2.02617
R11	2.77382	-0.00023	0.00016	0.00048	0.00063	2.77445
R12	2.05731	0.00011	0.00090	-0.00015	0.00076	2.05806
R13	2.06245	-0.00003	-0.00054	-0.00004	-0.00058	2.06187

R14	2.89118	0.00031	0.00019	0.00034	0.00054	2.89172
R15	5.11397	0.00010	0.00615	-0.00225	0.00392	5.11789
R16	5.12958	-0.00001	-0.00205	0.00115	-0.00089	5.12869
R17	2.50930	-0.00010	-0.00022	-0.00021	-0.00043	2.50887
R18	2.04865	0.00004	0.00011	0.00014	0.00025	2.04889
R19	2.04332	0.00001	0.00001	0.00003	0.00005	2.04337
R20	2.04734	0.00001	0.00003	0.00004	0.00007	2.04741
R21	2.06561	0.00029	0.00049	0.00123	0.00172	2.06733
R22	2.07874	-0.00039	-0.00232	0.00006	-0.00224	2.07650
R23	2.84537	-0.00017	-0.00233	0.00100	-0.00133	2.84404
R24	2.28229	0.00028	0.00209	-0.00071	0.00139	2.28368
R25	2.55333	-0.00032	-0.00166	-0.00041	-0.00208	2.55125
R26	1.83199	-0.00017	-0.00041	-0.00013	-0.00054	1.83145
A1	1.87708	-0.00009	-0.00012	-0.00030	-0.00044	1.87664
A2	2.27608	0.00007	0.00004	0.00030	0.00035	2.27643
A3	2.12998	0.00003	0.00009	0.00000	0.00010	2.13008
A4	1.86959	-0.00005	-0.00005	0.00008	0.00001	1.86960
A5	2.28457	0.00003	-0.00004	-0.00003	-0.00007	2.28450
A6	2.12832	0.00003	0.00006	-0.00004	0.00002	2.12835
A7	1.89177	0.00006	-0.00025	-0.00011	-0.00032	1.89145
A8	2.22755	-0.00004	0.00027	0.00000	0.00025	2.22780
A9	2.15379	-0.00002	-0.00003	0.00013	0.00009	2.15388
A10	1.88550	0.00015	0.00114	0.00102	0.00206	1.88755
A11	1.82426	-0.00029	-0.00427	-0.00307	-0.00729	1.81697
A12	2.17935	0.00001	0.00169	0.00148	0.00289	2.18224
A13	1.87809	0.00017	0.00018	0.00050	0.00067	1.87875
A14	2.18457	-0.00006	0.00155	0.00147	0.00275	2.18733
A15	1.89494	-0.00005	-0.00023	-0.00023	-0.00041	1.89454
A16	2.19838	0.00015	0.00129	0.00052	0.00182	2.20020
A17	2.17641	-0.00011	-0.00111	-0.00032	-0.00149	2.17491
A18	1.87646	0.00006	-0.00323	0.00238	-0.00086	1.87560
A19	1.88542	0.00013	0.00078	0.00062	0.00139	1.88681
A20	1.95145	-0.00016	-0.00202	0.00066	-0.00133	1.95012
A21	1.87487	-0.00003	-0.00127	-0.00006	-0.00133	1.87354
A22	1.92169	0.00007	0.00344	-0.00068	0.00275	1.92444
A23	1.95071	-0.00006	0.00208	-0.00274	-0.00066	1.95004
A24	1.25322	-0.00033	-0.00493	-0.00388	-0.00879	1.24444
A25	1.39723	-0.00038	-0.00563	-0.00460	-0.01030	1.38693
A26	2.16051	-0.00013	-0.00041	-0.00091	-0.00132	2.15919
A27	1.95961	-0.00003	-0.00036	-0.00033	-0.00070	1.95892
A28	2.16230	0.00016	0.00074	0.00120	0.00194	2.16425
A29	2.08536	0.00000	-0.00008	0.00000	-0.00008	2.08528
A30	2.14657	-0.00001	0.00006	-0.00006	0.00001	2.14658
A31	2.05125	0.00001	0.00002	0.00005	0.00007	2.05132

A32	1.95493	0.00011	-0.00227	-0.00081	-0.00313	1.95180
A33	1.91439	-0.00020	0.00375	-0.00054	0.00319	1.91758
A34	1.93584	-0.00025	-0.00021	-0.00208	-0.00243	1.93341
A35	1.85557	0.00012	-0.00162	0.00235	0.00079	1.85636
A36	1.90406	-0.00015	-0.00935	0.00022	-0.00915	1.89491
A37	1.89656	0.00040	0.01014	0.00111	0.01123	1.90779
A38	2.51661	0.00053	0.00495	0.00537	0.01036	2.52697
A39	2.19043	-0.00020	0.00132	-0.00154	-0.00023	2.19020
A40	1.94920	-0.00021	-0.00242	0.00088	-0.00156	1.94764
A41	2.14351	0.00041	0.00121	0.00062	0.00182	2.14533
A42	1.87610	-0.00030	0.00121	-0.00211	-0.00091	1.87519
D1	0.00449	-0.00001	-0.00011	0.00064	0.00054	0.00503
D2	3.10551	-0.00001	-0.00136	0.00082	-0.00054	3.10497
D3	-3.12658	0.00003	-0.00091	-0.00004	-0.00094	-3.12752
D4	-0.02556	0.00002	-0.00215	0.00013	-0.00202	-0.02758
D5	-0.06573	0.00007	0.00262	0.00192	0.00454	-0.06119
D6	-3.03771	0.00011	0.00308	0.00216	0.00525	-3.03247
D7	3.06641	0.00003	0.00334	0.00254	0.00587	3.07228
D8	0.09443	0.00008	0.00379	0.00278	0.00658	0.10100
D9	0.05775	-0.00005	-0.00243	-0.00294	-0.00538	0.05237
D10	3.04985	-0.00003	-0.00250	-0.00275	-0.00525	3.04459
D11	-3.04770	-0.00004	-0.00132	-0.00310	-0.00441	-3.05211
D12	-0.05560	-0.00002	-0.00139	-0.00290	-0.00429	-0.05989
D13	-0.09897	0.00007	0.00399	0.00409	0.00811	-0.09086
D14	1.89748	0.00019	0.00266	0.00364	0.00629	1.90377
D15	-2.97541	-0.00026	-0.01241	-0.01139	-0.02383	-2.99923
D16	-3.09880	0.00006	0.00403	0.00392	0.00797	-3.09082
D17	-1.10234	0.00018	0.00270	0.00347	0.00615	-1.09619
D18	0.30795	-0.00027	-0.01237	-0.01157	-0.02396	0.28399
D19	0.55662	0.00006	0.00435	0.00674	0.01109	0.56771
D20	-2.54449	0.00007	0.00508	0.00786	0.01293	-2.53156
D21	-2.75509	0.00008	0.00426	0.00694	0.01121	-2.74388
D22	0.42698	0.00010	0.00498	0.00806	0.01304	0.44003
D23	0.10182	-0.00008	-0.00407	-0.00369	-0.00778	0.09404
D24	3.07644	-0.00010	-0.00423	-0.00383	-0.00807	3.06837
D25	-1.85875	0.00010	0.00024	-0.00088	-0.00065	-1.85940
D26	1.11588	0.00008	0.00008	-0.00101	-0.00095	1.11493
D27	2.97725	0.00027	0.01243	0.01185	0.02430	3.00156
D28	-0.33131	0.00025	0.01226	0.01172	0.02401	-0.30730
D29	-2.24464	-0.00012	-0.00001	-0.00093	-0.00088	-2.24552
D30	-0.24297	-0.00002	-0.00065	-0.00100	-0.00168	-0.24464
D31	-2.93484	0.00003	0.00360	0.00336	0.00697	-2.92787
D32	-0.91638	0.00010	0.00086	0.00482	0.00568	-0.91070
D33	1.23711	0.00001	0.00270	0.00224	0.00494	1.24206

D34	0.40263	0.00008	0.00399	0.00361	0.00761	0.41024
D35	2.42109	0.00014	0.00125	0.00507	0.00632	2.42741
D36	-1.70861	0.00005	0.00309	0.00249	0.00558	-1.70303
D37	-1.04944	-0.00012	0.00017	-0.00226	-0.00210	-1.05154
D38	1.00664	-0.00004	-0.00081	-0.00019	-0.00100	1.00564
D39	3.10174	0.00017	0.01403	-0.00048	0.01354	3.11528
D40	-3.13421	-0.00014	0.00324	-0.00523	-0.00199	-3.13620
D41	-1.07813	-0.00005	0.00226	-0.00316	-0.00089	-1.07902
D42	1.01697	0.00016	0.01710	-0.00345	0.01365	1.03062
D43	1.06669	-0.00011	0.00122	-0.00294	-0.00172	1.06497
D44	3.12277	-0.00002	0.00024	-0.00087	-0.00062	3.12215
D45	-1.06532	0.00019	0.01508	-0.00116	0.01392	-1.05140
D46	-0.01589	0.00003	-0.00036	0.00273	0.00237	-0.01353
D47	0.35977	0.00004	-0.00142	0.00227	0.00079	0.36056
D48	-3.09180	0.00002	-0.00012	0.00134	0.00123	-3.09057
D49	0.04648	0.00001	0.00038	0.00061	0.00099	0.04747
D50	0.00466	-0.00001	-0.00095	0.00006	-0.00090	0.00377
D51	-3.14025	-0.00001	-0.00045	-0.00068	-0.00113	-3.14138
D52	-0.34085	-0.00003	0.00024	-0.00222	-0.00197	-0.34282
D53	1.77615	0.00006	-0.00134	-0.00209	-0.00346	1.77269
D54	-2.45974	0.00015	-0.00800	-0.00003	-0.00808	-2.46783
D55	-0.14372	0.00003	0.02335	-0.00254	0.02082	-0.12290
D56	3.00731	-0.00009	0.01467	0.00219	0.01687	3.02419
D57	-2.30510	0.00016	0.03293	-0.00027	0.03260	-2.27250
D58	0.84593	0.00005	0.02425	0.00446	0.02866	0.87459
D59	1.96197	-0.00011	0.03429	-0.00378	0.03056	1.99253
D60	-1.17018	-0.00023	0.02561	0.00095	0.02661	-1.14357
D61	3.08980	0.00019	0.01970	-0.00191	0.01779	3.10758
D62	-0.04265	0.00008	0.01129	0.00268	0.01397	-0.02868

Item	Value	Threshold	Converged?
Maximum Force	0.000574	0.000450	NO
RMS Force	0.000170	0.000300	YES
Maximum Displacement	0.074039	0.001800	NO
RMS Displacement	0.011654	0.001200	NO

Predicted change in Energy=-5.172143D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.308369	-2.176327	-0.392983
2	6	0	-1.566149	-1.751795	-0.655834

3	7	0	-1.815790	-0.667134	0.180547
4	6	0	-0.692954	-0.406572	0.887125
5	7	0	0.208915	-1.359523	0.605214
6	6	0	1.587881	-1.377920	1.108858
7	1	0	0.263435	-2.976492	-0.829264
8	1	0	-2.288142	-2.093365	-1.374958
9	1	0	1.610567	-0.783660	2.021237
10	1	0	1.835033	-2.404644	1.383154
11	35	0	0.255135	2.014612	-0.198466
12	1	0	-0.623931	0.292066	1.697533
13	6	0	-2.957766	0.173897	0.190909
14	6	0	-4.181387	-0.241170	-0.114200
15	1	0	-2.709040	1.200577	0.435066
16	1	0	-4.995911	0.469824	-0.130141
17	1	0	-4.411613	-1.271990	-0.355558
18	6	0	2.573185	-0.812607	0.083573
19	1	0	2.567240	-1.388264	-0.846687
20	1	0	2.284938	0.213097	-0.185289
21	6	0	3.973443	-0.807625	0.635195
22	8	0	4.280620	-1.079055	1.772017
23	8	0	4.875818	-0.450109	-0.303193
24	1	0	5.746813	-0.436596	0.121618

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.353267	0.000000			
3	N	2.208828	1.392244	0.000000		
4	C	2.217795	2.225493	1.352001	0.000000	
5	N	1.389658	2.212459	2.181553	1.341997	0.000000
6	C	2.547301	3.633432	3.598882	2.488954	1.468177
7	H	1.075901	2.208470	3.267419	3.234990	2.162241
8	H	2.211483	1.074747	2.162602	3.241437	3.270305
9	H	3.383829	4.265621	3.891226	2.595114	2.073974
10	H	2.793020	4.018921	4.218259	3.260223	2.083681
11	Br	4.233125	4.208573	3.409421	2.817714	3.468837
12	H	3.250046	3.256298	2.154493	1.072203	2.148148
13	C	3.589399	2.522272	1.418291	2.439473	3.542723
14	C	4.338528	3.068358	2.421646	3.633066	4.587267
15	H	4.225206	3.348546	2.085910	2.617611	3.885553
16	H	5.389272	4.120098	3.391514	4.507587	5.565741
17	H	4.201886	2.901214	2.718742	4.015176	4.720172
18	C	3.223381	4.308466	4.392456	3.387953	2.482136
19	H	3.015960	4.153732	4.559187	3.820823	2.769574

20	H	3.532382	4.348918	4.210062	3.225198	2.721746
21	C	4.611334	5.765873	5.808757	4.690370	3.804887
22	O	5.191344	6.366455	6.314164	5.096244	4.244864
23	O	5.464767	6.581617	6.712580	5.694732	4.840684
24	H	6.321131	7.470850	7.566345	6.485175	5.635066

		6	7	8	9	10
6	C	0.000000				
7	H	2.840054	0.000000			
8	H	4.658836	2.754676	0.000000		
9	H	1.089080	3.840395	5.333798	0.000000	
10	H	1.091093	2.773395	4.970376	1.756452	0.000000
11	Br	3.872284	5.030814	4.972712	3.820289	4.952517
12	H	2.833285	4.225587	4.230848	2.500991	3.663002
13	C	4.890160	4.619722	2.835632	5.013649	5.571466
14	C	6.006040	5.267802	2.933345	6.196864	6.566581
15	H	5.056300	5.280344	3.781983	5.011202	5.877507
16	H	6.949503	6.326656	3.930842	7.060114	7.564021
17	H	6.176541	4.998580	2.494587	6.492633	6.582295
18	C	1.530233	3.294026	5.234515	2.163797	2.183658
19	H	2.187100	2.798265	4.934670	3.083141	2.557606
20	H	2.166112	3.830751	5.258150	2.513376	3.084639
21	C	2.498099	4.540130	6.700842	2.739502	2.771771
22	O	2.789255	5.148272	7.353972	2.697879	2.808790
23	O	3.696654	5.285209	7.427738	4.021952	3.988778
24	H	4.376922	6.117408	8.339371	4.564815	4.557051

		11	12	13	14	15
11	Br	0.000000				
12	H	2.708271	0.000000			
13	C	3.723248	2.780407	0.000000		
14	C	4.977789	4.027680	1.327637	0.000000	
15	H	3.138527	2.601325	1.084227	2.132635	0.000000
16	H	5.473986	4.741961	2.084390	1.081303	2.466422
17	H	5.710076	4.583447	2.122001	1.083442	3.104420
18	C	3.666888	3.747895	5.619263	6.781584	5.663776
19	H	4.164803	4.413630	5.834607	6.884499	6.015323
20	H	2.713988	3.465945	5.256330	6.482652	5.128331
21	C	4.741923	4.844970	7.014444	8.208758	6.980581
22	O	5.445926	5.093146	7.514254	8.710076	7.472583
23	O	5.237989	5.899234	7.873916	9.061585	7.797426
24	H	6.022408	6.603092	8.726235	9.932922	8.618586

		16	17	18	19	20
16	H	0.000000				
17	H	1.850981	0.000000			
18	C	7.679942	7.013649	0.000000		

19	H	7.820945	6.997079	1.093983	0.000000	
20	H	7.285583	6.861361	1.098837	1.755420	0.000000
21	C	9.092135	8.456145	1.505003	2.123799	2.136847
22	O	9.595377	8.950906	2.416025	3.144661	3.079521
23	O	9.916010	9.323873	2.362861	2.550501	2.677014
24	H	10.783835	10.203881	3.196052	3.457307	3.535657

		21	22	23	24
21	C	0.000000			
22	O	1.208469	0.000000		
23	O	1.350063	2.248629	0.000000	
24	H	1.883153	2.299194	0.969164	0.000000

Stoichiometry C8H11BrN2O2
Framework group C1[X(C8H11BrN2O2)]
Deg. of freedom 66
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.624238	-2.097510	-0.767732
2	6	0	-1.940397	-1.797278	-0.862155
3	7	0	-2.217796	-0.855558	0.125041
4	6	0	-1.062994	-0.548363	0.757473
5	7	0	-0.097997	-1.347910	0.277409
6	6	0	1.319209	-1.261576	0.651060
7	1	0	-0.017763	-2.767451	-1.351626
8	1	0	-2.691382	-2.135328	-1.552681
9	1	0	1.371296	-0.779999	1.626491
10	1	0	1.701334	-2.276777	0.768672
11	35	0	-0.494788	2.078709	-0.088190
12	1	0	-0.986639	0.053590	1.641465
13	6	0	-3.436027	-0.162983	0.343675
14	6	0	-4.633020	-0.681572	0.096909
15	1	0	-3.274790	0.850165	0.694508
16	1	0	-5.516187	-0.075286	0.244044
17	1	0	-4.775233	-1.696936	-0.253319
18	6	0	2.128643	-0.467026	-0.376130
19	1	0	2.089302	-0.926178	-1.368315
20	1	0	1.706538	0.541657	-0.484883
21	6	0	3.569308	-0.360744	0.046035
22	8	0	4.018157	-0.725311	1.107178

```
      23                8                0        4.327794       0.208890      -0.914634
      24                1                0        5.231149       0.275685      -0.570008
 ---------------------------------------------------------------------
 Rotational constants (GHZ):           0.8294984           0.3305261           0.2552823
 Standard basis: 6-311++G(d,p) (5D, 7F)
 There are     404 symmetry adapted cartesian basis functions of A      symmetry.
 There are     389 symmetry adapted basis functions of A      symmetry.
    389 basis functions,      625 primitive gaussians,      404 cartesian basis functions
     62 alpha electrons              62 beta electrons
          nuclear repulsion energy           1075.2453694523 Hartrees.
 NAtoms=       24 NActive=       24 NUniq=       24 SFac= 1.00D+00 NAtFMM=       60 NAOKFM=F
Big=F
 Integral buffers will be        131072 words long.
 Raffenetti 2 integral format.
 Two-electron integral symmetry is turned on.
 One-electron integrals computed using PRISM.
 NBasis=      389 RedAO= T EigKep=    6.27D-06    NBF=      389
 NBsUse=      389 1.00D-06 EigRej= -1.00D+00 NBFU=      389
 Initial guess from the checkpoint file:    "./cooh.chk"
 B after Tr=          0.000000        0.000000        0.000000
             Rot=        0.999997      -0.002463      -0.000246      -0.000737 Ang=    -0.30 deg.
 ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn=                5 AccDes=
0.00D+00
 Harris functional with IExCor=    402 and IRadAn=             5 diagonalized for initial guess.
 HarFok:    IExCor=    402 AccDes= 0.00D+00 IRadAn=                5 IDoV= 1 UseB2=F ITyADJ=14
 ICtDFT=    3500011 ScaDFX=    1.000000    1.000000    1.000000    1.000000
 FoFCou: FMM=F IPFlag=                  0 FMFlag=           100000 FMFlg1=                  0
             NFxFlg=                  0 DoJE=T BraDBF=F KetDBF=T FulRan=T
             wScrn=      0.000000  ICntrl=             500  IOpCl=      0  I1Cent=        200000004  NGrid=
0
             NMat0=         1 NMatS0=            1 NMatT0=         0 NMatD0=         1 NMtDS0=         0
NMtDT0=         0
 Petite list used in FoFCou.
 Keep R1 ints in memory in canonical form, NReq=2910765817.
 Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
 Requested convergence on MAX density matrix=1.00D-06.
 Requested convergence on                      energy=1.00D-06.
 No special actions if energy rises.
 SCF Done:    E(RB3LYP) =    -3145.73213043          A.U. after      11 cycles
                  NFock= 11    Conv=0.79D-08         -V/T= 2.0017
 Calling FoFJK, ICntrl=              2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
 ***** Axes restored to original set *****
 ---------------------------------------------------------------------
```

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000010375	-0.000062714	0.000001869
2	6	0.000042837	0.000181055	-0.000206371
3	7	0.000579188	-0.000053893	0.000145657
4	6	-0.000438360	-0.000869097	0.000255049
5	7	0.000086137	0.000108941	0.000095866
6	6	-0.000508053	0.000050272	0.000330584
7	1	0.000020404	0.000002285	0.000005783
8	1	-0.000031056	-0.000031191	0.000044757
9	1	0.000096956	-0.000017841	-0.000146214
10	1	0.000028458	-0.000108246	-0.000123377
11	35	0.000030027	0.000456611	-0.000145679
12	1	0.000220788	0.000258242	-0.000267343
13	6	-0.000390285	0.000276183	-0.000038435
14	6	0.000081505	-0.000086279	0.000056594
15	1	0.000102930	0.000023946	-0.000053802
16	1	-0.000008220	0.000007640	-0.000006694
17	1	0.000011290	-0.000012891	-0.000003975
18	6	0.000266158	-0.000580935	-0.000677422
19	1	-0.000172786	0.000022304	0.000052956
20	1	-0.000437160	0.000076333	0.000488145
21	6	0.000143320	0.000431225	0.000860351
22	8	-0.000132026	0.000039792	-0.000636417
23	8	0.000244866	-0.000242824	-0.000125665
24	1	0.000152708	0.000131084	0.000093784

Cartesian Forces: Max 0.000869097 RMS 0.000276004

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
Internal Forces: Max 0.000647687 RMS 0.000136268
Search for a local minimum.
Step number 8 out of a maximum of 140
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 5 4 6 7 8
DE= -6.58D-05 DEPred=-5.17D-05 R= 1.27D+00
TightC=F SS= 1.41D+00 RLast= 1.11D-01 DXNew= 1.2000D+00 3.3239D-01
Trust test= 1.27D+00 RLast= 1.11D-01 DXMaxT set to 7.14D-01

ITU= 1 1 0 -1 1 1 1 0

Eigenvalues ---	0.00197	0.00388	0.00808	0.00854	0.01591
Eigenvalues ---	0.01777	0.01979	0.02034	0.02127	0.02197
Eigenvalues ---	0.02347	0.02364	0.02430	0.02484	0.03038
Eigenvalues ---	0.03039	0.03156	0.03790	0.04388	0.04755
Eigenvalues ---	0.05010	0.05680	0.06506	0.08481	0.09828
Eigenvalues ---	0.10717	0.12214	0.15005	0.15319	0.15972
Eigenvalues ---	0.15994	0.15997	0.16000	0.16002	0.16067
Eigenvalues ---	0.16743	0.17859	0.20753	0.21987	0.22835
Eigenvalues ---	0.24484	0.25018	0.27191	0.27714	0.34360
Eigenvalues ---	0.34531	0.35189	0.35493	0.35579	0.35618
Eigenvalues ---	0.35843	0.36070	0.36590	0.36650	0.37082
Eigenvalues ---	0.37632	0.41323	0.43011	0.43654	0.47491
Eigenvalues ---	0.52391	0.53327	0.54229	0.55130	0.59908
Eigenvalues ---	0.95179				

En-DIIS/RFO-DIIS IScMMF= 0 using points: 8 7 6

RFO step: Lambda=-6.68589574D-06.

DidBck=F Rises=F RFO-DIIS coefs: 1.56428 -0.78088 0.21659

Iteration 1 RMS(Cart)= 0.00717002 RMS(Int)= 0.00004091

Iteration 2 RMS(Cart)= 0.00004626 RMS(Int)= 0.00002369

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00002369

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55730	0.00000	0.00020	0.00018	0.00036	2.55767
R2	2.62607	-0.00001	-0.00008	0.00000	-0.00009	2.62598
R3	2.03316	0.00001	0.00003	-0.00003	0.00000	2.03316
R4	2.63096	0.00000	-0.00030	-0.00009	-0.00039	2.63057
R5	2.03098	0.00000	0.00001	0.00002	0.00003	2.03101
R6	2.55491	-0.00035	-0.00121	-0.00080	-0.00199	2.55292
R7	2.68018	0.00029	0.00079	0.00079	0.00158	2.68176
R8	2.53601	-0.00006	-0.00089	-0.00053	-0.00142	2.53459
R9	5.32471	0.00037	0.02066	0.01351	0.03416	5.35887
R10	2.02617	0.00001	0.00007	0.00002	0.00009	2.02626
R11	2.77445	-0.00021	0.00032	-0.00051	-0.00020	2.77425
R12	2.05806	-0.00013	0.00020	-0.00026	-0.00006	2.05800
R13	2.06187	0.00008	-0.00019	0.00013	-0.00006	2.06181
R14	2.89172	0.00017	0.00025	0.00086	0.00111	2.89283
R15	5.11789	-0.00007	0.00063	-0.00364	-0.00300	5.11489
R16	5.12869	-0.00002	0.00003	-0.00034	-0.00031	5.12839
R17	2.50887	-0.00006	-0.00019	-0.00015	-0.00033	2.50854
R18	2.04889	0.00003	0.00011	0.00012	0.00023	2.04913
R19	2.04337	0.00001	0.00002	0.00004	0.00006	2.04343
R20	2.04741	0.00001	0.00003	0.00004	0.00007	2.04748
R21	2.06733	-0.00005	0.00084	-0.00040	0.00045	2.06778

R22	2.07650	0.00015	-0.00067	0.00047	-0.00019	2.07631
R23	2.84404	0.00044	-0.00015	0.00069	0.00054	2.84458
R24	2.28368	-0.00065	0.00024	-0.00016	0.00009	2.28376
R25	2.55125	0.00027	-0.00075	0.00023	-0.00051	2.55074
R26	1.83145	0.00018	-0.00020	0.00030	0.00011	1.83156
A1	1.87664	-0.00008	-0.00022	-0.00010	-0.00033	1.87632
A2	2.27643	0.00006	0.00019	0.00016	0.00035	2.27678
A3	2.13008	0.00002	0.00004	-0.00007	-0.00003	2.13005
A4	1.86960	-0.00004	0.00002	-0.00015	-0.00014	1.86945
A5	2.28450	0.00004	-0.00003	0.00021	0.00019	2.28469
A6	2.12835	0.00001	0.00000	0.00001	0.00001	2.12836
A7	1.89145	0.00008	-0.00012	0.00007	-0.00003	1.89143
A8	2.22780	-0.00007	0.00007	-0.00022	-0.00016	2.22764
A9	2.15388	-0.00001	0.00006	0.00002	0.00007	2.15395
A10	1.88755	0.00002	0.00087	0.00039	0.00120	1.88876
A11	1.81697	-0.00012	-0.00302	-0.00179	-0.00478	1.81219
A12	2.18224	0.00004	0.00120	0.00101	0.00204	2.18428
A13	1.87875	0.00020	0.00033	0.00122	0.00154	1.88030
A14	2.18733	-0.00002	0.00116	0.00089	0.00188	2.18921
A15	1.89454	0.00003	-0.00017	-0.00003	-0.00017	1.89436
A16	2.20020	0.00001	0.00069	-0.00013	0.00057	2.20076
A17	2.17491	-0.00004	-0.00056	0.00026	-0.00033	2.17458
A18	1.87560	0.00006	0.00035	-0.00084	-0.00050	1.87511
A19	1.88681	0.00007	0.00058	-0.00045	0.00013	1.88695
A20	1.95012	-0.00008	-0.00023	-0.00038	-0.00061	1.94951
A21	1.87354	0.00006	-0.00043	0.00067	0.00025	1.87378
A22	1.92444	-0.00009	0.00067	0.00005	0.00072	1.92516
A23	1.95004	0.00000	-0.00091	0.00092	0.00001	1.95006
A24	1.24444	-0.00025	-0.00369	-0.00339	-0.00707	1.23737
A25	1.38693	-0.00026	-0.00436	-0.00389	-0.00829	1.37864
A26	2.15919	-0.00014	-0.00064	-0.00070	-0.00134	2.15785
A27	1.95892	-0.00002	-0.00030	-0.00038	-0.00068	1.95824
A28	2.16425	0.00016	0.00090	0.00109	0.00200	2.16624
A29	2.08528	0.00001	-0.00002	0.00007	0.00005	2.08532
A30	2.14658	-0.00002	-0.00001	-0.00013	-0.00015	2.14644
A31	2.05132	0.00001	0.00004	0.00007	0.00010	2.05142
A32	1.95180	-0.00004	-0.00118	0.00037	-0.00081	1.95099
A33	1.91758	-0.00021	0.00084	-0.00006	0.00079	1.91837
A34	1.93341	0.00006	-0.00132	0.00017	-0.00114	1.93227
A35	1.85636	0.00009	0.00086	0.00009	0.00094	1.85730
A36	1.89491	0.00016	-0.00276	0.00152	-0.00125	1.89366
A37	1.90779	-0.00006	0.00373	-0.00215	0.00158	1.90938
A38	2.52697	0.00038	0.00457	0.00492	0.00949	2.53646
A39	2.19020	-0.00017	-0.00047	-0.00020	-0.00067	2.18953

A40	1.94764	0.00040	-0.00026	0.00071	0.00045	1.94810
A41	2.14533	-0.00023	0.00071	-0.00049	0.00023	2.14556
A42	1.87519	0.00005	-0.00082	0.00104	0.00022	1.87541
D1	0.00503	-0.00003	0.00033	-0.00149	-0.00116	0.00387
D2	3.10497	0.00002	0.00004	0.00048	0.00052	3.10549
D3	-3.12752	0.00000	-0.00030	-0.00116	-0.00146	-3.12898
D4	-0.02758	0.00005	-0.00059	0.00081	0.00022	-0.02736
D5	-0.06119	0.00004	0.00189	0.00223	0.00411	-0.05708
D6	-3.03247	0.00006	0.00217	0.00159	0.00376	-3.02870
D7	3.07228	0.00001	0.00246	0.00193	0.00438	3.07666
D8	0.10100	0.00004	0.00274	0.00129	0.00403	0.10504
D9	0.05237	0.00002	-0.00241	0.00026	-0.00215	0.05022
D10	3.04459	0.00002	-0.00232	-0.00067	-0.00300	3.04160
D11	-3.05211	-0.00003	-0.00215	-0.00150	-0.00365	-3.05576
D12	-0.05989	-0.00002	-0.00207	-0.00243	-0.00450	-0.06439
D13	-0.09086	0.00000	0.00355	0.00110	0.00466	-0.08621
D14	1.90377	0.00017	0.00286	0.00180	0.00466	1.90843
D15	-2.99923	-0.00016	-0.01025	-0.00909	-0.01935	-3.01859
D16	-3.09082	0.00000	0.00346	0.00201	0.00549	-3.08534
D17	-1.09619	0.00018	0.00278	0.00271	0.00548	-1.09071
D18	0.28399	-0.00015	-0.01034	-0.00818	-0.01853	0.26546
D19	0.56771	0.00007	0.00514	0.00716	0.01230	0.58002
D20	-2.53156	0.00007	0.00599	0.00687	0.01286	-2.51870
D21	-2.74388	0.00008	0.00523	0.00610	0.01133	-2.73255
D22	0.44003	0.00008	0.00608	0.00581	0.01188	0.45191
D23	0.09404	-0.00002	-0.00334	-0.00204	-0.00539	0.08865
D24	3.06837	-0.00004	-0.00347	-0.00146	-0.00494	3.06343
D25	-1.85940	0.00002	-0.00043	-0.00074	-0.00118	-1.86059
D26	1.11493	0.00000	-0.00056	-0.00017	-0.00073	1.11420
D27	3.00156	0.00015	0.01052	0.00821	0.01874	3.02029
D28	-0.30730	0.00013	0.01039	0.00878	0.01919	-0.28811
D29	-2.24552	-0.00002	-0.00050	-0.00069	-0.00114	-2.24666
D30	-0.24464	0.00002	-0.00078	-0.00056	-0.00136	-0.24600
D31	-2.92787	-0.00007	0.00301	0.00322	0.00622	-2.92164
D32	-0.91070	0.00006	0.00299	0.00334	0.00632	-0.90437
D33	1.24206	0.00006	0.00209	0.00393	0.00603	1.24809
D34	0.41024	-0.00005	0.00327	0.00252	0.00579	0.41602
D35	2.42741	0.00008	0.00324	0.00264	0.00588	2.43329
D36	-1.70303	0.00008	0.00235	0.00323	0.00559	-1.69743
D37	-1.05154	0.00001	-0.00123	-0.00246	-0.00370	-1.05524
D38	1.00564	-0.00004	-0.00036	-0.00216	-0.00252	1.00312
D39	3.11528	-0.00021	0.00403	-0.00478	-0.00075	3.11452
D40	-3.13620	0.00005	-0.00196	-0.00120	-0.00315	-3.13935
D41	-1.07902	0.00000	-0.00108	-0.00089	-0.00198	-1.08100

D42	1.03062	-0.00016	0.00330	-0.00351	-0.00021	1.03041
D43	1.06497	0.00004	-0.00128	-0.00267	-0.00395	1.06102
D44	3.12215	-0.00001	-0.00041	-0.00236	-0.00277	3.11938
D45	-1.05140	-0.00017	0.00398	-0.00498	-0.00100	-1.05240
D46	-0.01353	0.00001	0.00143	0.00111	0.00256	-0.01097
D47	0.36056	0.00002	0.00081	0.00090	0.00167	0.36224
D48	-3.09057	0.00000	0.00072	-0.00051	0.00021	-3.09036
D49	0.04747	0.00001	0.00046	0.00015	0.00061	0.04808
D50	0.00377	0.00000	-0.00026	-0.00022	-0.00048	0.00329
D51	-3.14138	0.00001	-0.00052	0.00044	-0.00008	-3.14146
D52	-0.34282	-0.00001	-0.00117	-0.00027	-0.00146	-0.34428
D53	1.77269	-0.00013	-0.00161	0.00019	-0.00143	1.77127
D54	-2.46783	0.00008	-0.00250	0.00093	-0.00157	-2.46940
D55	-0.12290	0.00013	0.00574	-0.00426	0.00149	-0.12142
D56	3.02419	0.00003	0.00575	-0.00722	-0.00147	3.02271
D57	-2.27250	0.00004	0.00993	-0.00585	0.00408	-2.26842
D58	0.87459	-0.00006	0.00993	-0.00882	0.00112	0.87571
D59	1.99253	-0.00012	0.00843	-0.00564	0.00278	1.99531
D60	-1.14357	-0.00023	0.00843	-0.00860	-0.00018	-1.14374
D61	3.10758	-0.00006	0.00497	-0.00172	0.00325	3.11084
D62	-0.02868	-0.00016	0.00498	-0.00460	0.00038	-0.02829

Item	Value	Threshold	Converged?
Maximum Force	0.000648	0.000450	NO
RMS Force	0.000136	0.000300	YES
Maximum Displacement	0.029066	0.001800	NO
RMS Displacement	0.007191	0.001200	NO

Predicted change in Energy=-1.811842D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.310031	-2.182812	-0.392012
2	6	0	-1.566615	-1.755072	-0.656370
3	7	0	-1.814316	-0.670004	0.179714
4	6	0	-0.693296	-0.414366	0.888952
5	7	0	0.208254	-1.366177	0.605737
6	6	0	1.587538	-1.383800	1.108228
7	1	0	0.260152	-2.985051	-0.826598
8	1	0	-2.289244	-2.095561	-1.375392
9	1	0	1.608746	-0.794836	2.024031
10	1	0	1.837853	-2.411403	1.376170

11	35	0	0.256020	2.025928	-0.199843
12	1	0	-0.617462	0.295341	1.689134
13	6	0	-2.953374	0.176412	0.186528
14	6	0	-4.179096	-0.237891	-0.110307
15	1	0	-2.698599	1.204296	0.419685
16	1	0	-4.991620	0.475332	-0.130420
17	1	0	-4.413118	-1.270458	-0.340448
18	6	0	2.570245	-0.809585	0.084520
19	1	0	2.566848	-1.382851	-0.847506
20	1	0	2.277907	0.215831	-0.180582
21	6	0	3.970733	-0.803387	0.636325
22	8	0	4.278079	-1.081555	1.771521
23	8	0	4.872533	-0.440046	-0.299988
24	1	0	5.743834	-0.429057	0.124395

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.353459	0.000000			
3	N	2.208695	1.392036	0.000000		
4	C	2.217016	2.224454	1.350946	0.000000	
5	N	1.389609	2.212309	2.181041	1.341248	0.000000
6	C	2.547529	3.633225	3.597812	2.487988	1.468071
7	H	1.075900	2.208825	3.267342	3.234284	2.162182
8	H	2.211772	1.074765	2.162435	3.240482	3.270224
9	H	3.383111	4.264916	3.890300	2.594717	2.073491
10	H	2.791438	4.019003	4.219278	3.260713	2.083664
11	Br	4.250980	4.222129	3.420293	2.835791	3.486777
12	H	3.250680	3.256758	2.154692	1.072253	2.148534
13	C	3.589973	2.522738	1.419127	2.439338	3.542768
14	C	4.339556	3.070029	2.421368	3.630491	4.586348
15	H	4.223341	3.346212	2.086275	2.619450	3.884808
16	H	5.389938	4.120920	3.391642	4.506248	5.565228
17	H	4.203614	2.904692	2.717515	4.010161	4.718210
18	C	3.226271	4.307723	4.387815	3.384377	2.482028
19	H	3.020571	4.154588	4.556088	3.818611	2.770408
20	H	3.534914	4.346399	4.202476	3.220108	2.721123
21	C	4.613592	5.765326	5.804574	4.687038	3.804461
22	O	5.190799	6.364647	6.310349	5.092999	4.243058
23	O	5.468516	6.581711	6.707976	5.691457	4.840822
24	H	6.323892	7.470647	7.562191	6.482391	5.634938

		6	7	8	9	10
6	C	0.000000				
7	H	2.840688	0.000000			

8	H	4.658799	2.755320	0.000000		
9	H	1.089046	3.839509	5.333131	0.000000	
10	H	1.091062	2.769548	4.970289	1.756559	0.000000
11	Br	3.887188	5.050024	4.984672	3.838254	4.967485
12	H	2.831782	4.226119	4.231145	2.501328	3.667830
13	C	4.889138	4.620392	2.835935	5.013250	5.573857
14	C	6.004332	5.269430	2.936481	6.193925	6.567910
15	H	5.054038	5.278073	3.778747	5.012352	5.879416
16	H	6.948088	6.327719	3.932211	7.058315	7.566026
17	H	6.174089	5.001562	2.502548	6.486896	6.582033
18	C	1.530822	3.301411	5.234473	2.164809	2.184165
19	H	2.187224	2.808617	4.936421	3.083739	2.556187
20	H	2.167132	3.838531	5.256327	2.515858	3.085366
21	C	2.497838	4.546230	6.701047	2.739487	2.771690
22	O	2.787530	5.149491	7.352619	2.696537	2.807045
23	O	3.696612	5.294188	7.428881	4.022343	3.988112
24	H	4.376558	6.124398	8.340080	4.565234	4.555581

		11	12	13	14	15
11	Br	0.000000				
12	H	2.706684	0.000000			
13	C	3.724272	2.780009	0.000000		
14	C	4.980277	4.025862	1.327462	0.000000	
15	H	3.128685	2.601698	1.084351	2.133698	0.000000
16	H	5.472376	4.740931	2.084288	1.081335	2.468187
17	H	5.717236	4.580167	2.121790	1.083478	3.105122
18	C	3.671053	3.735924	5.611859	6.776312	5.650555
19	H	4.168833	4.403488	5.828669	6.882018	6.002003
20	H	2.713825	3.447510	5.244294	6.473306	5.109109
21	C	4.743763	4.833958	7.007538	8.203473	6.968337
22	O	5.451576	5.086153	7.509234	8.704991	7.465026
23	O	5.234810	5.885358	7.865210	9.055873	7.780991
24	H	6.020646	6.590845	8.718478	9.927546	8.604051

		16	17	18	19	20
16	H	0.000000				
17	H	1.851097	0.000000			
18	C	7.673266	7.011445	0.000000		
19	H	7.816489	6.999262	1.094221	0.000000	
20	H	7.274330	6.855978	1.098736	1.756149	0.000000
21	C	9.085527	8.453473	1.505289	2.123306	2.138178
22	O	9.590026	8.946117	2.415913	3.142992	3.081332
23	O	9.907985	9.322796	2.363246	2.550459	2.678902
24	H	10.776493	10.202338	3.196569	3.456523	3.538579

		21	22	23	24
21	C	0.000000			

22 O 1.208516 0.000000

23 O 1.349793 2.248568 0.000000

24 H 1.883103 2.299394 0.969220 0.000000

Stoichiometry C8H11BrN2O2

Framework group C1[X(C8H11BrN2O2)]

Deg. of freedom 66

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.625153	-2.106201	-0.769029
2	6	0	-1.940633	-1.802296	-0.863928
3	7	0	-2.215739	-0.860614	0.123652
4	6	0	-1.061676	-0.559378	0.758042
5	7	0	-0.097499	-1.357418	0.275920
6	6	0	1.319965	-1.270554	0.648050
7	1	0	-0.020162	-2.778203	-1.352091
8	1	0	-2.692635	-2.138787	-1.554134
9	1	0	1.371907	-0.795504	1.626647
10	1	0	1.704611	-2.285617	0.758102
11	35	0	-0.494690	2.087631	-0.086694
12	1	0	-0.980435	0.054841	1.633176
13	6	0	-3.431879	-0.162014	0.340176
14	6	0	-4.630322	-0.680785	0.101921
15	1	0	-3.265692	0.854061	0.680456
16	1	0	-5.512066	-0.071598	0.245817
17	1	0	-4.775175	-1.699372	-0.237818
18	6	0	2.125741	-0.467036	-0.375912
19	1	0	2.088078	-0.922582	-1.370085
20	1	0	1.700058	0.540553	-0.479727
21	6	0	3.566687	-0.359994	0.046121
22	8	0	4.016609	-0.731819	1.104339
23	8	0	4.323895	0.215711	-0.911553
24	1	0	5.227910	0.279764	-0.567983

Rotational constants (GHZ): 0.8234172 0.3310278 0.2549279

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 404 symmetry adapted cartesian basis functions of A symmetry.

There are 389 symmetry adapted basis functions of A symmetry.

389 basis functions, 625 primitive gaussians, 404 cartesian basis functions

62 alpha electrons 62 beta electrons
nuclear repulsion energy 1074.3522779495 Hartrees.
NAtoms= 24 NActive= 24 NUniq= 24 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 389 RedAO= T EigKep= 6.33D-06 NBF= 389
NBsUse= 389 1.00D-06 EigRej= -1.00D+00 NBFU= 389
Initial guess from the checkpoint file: "./cooh.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 -0.000609 -0.000097 0.000001 Ang= -0.07 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=2910765817.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3145.73216317 A.U. after 11 cycles
NFock= 11 Conv=0.63D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000033128	-0.000024408	-0.000045941
2	6	0.000024909	0.000041733	-0.000112922
3	7	0.000300625	-0.000070014	0.000055879
4	6	-0.000150798	-0.000339881	0.000064068
5	7	-0.000081866	0.000000202	0.000041863

6	6	-0.000255399	0.000157442	0.000192988
7	1	0.000033001	0.000020137	-0.000017998
8	1	-0.000039419	-0.000020268	0.000052211
9	1	0.000190522	-0.000006543	-0.000140981
10	1	0.000016787	-0.000088425	-0.000110301
11	35	-0.000008970	0.000249900	-0.000022582
12	1	0.000151231	0.000176365	-0.000176749
13	6	-0.000247116	0.000215607	-0.000046611
14	6	0.000040946	-0.000066902	0.000065026
15	1	0.000068733	0.000021390	-0.000040370
16	1	-0.000004954	0.000005882	-0.000017762
17	1	0.000017486	-0.000012355	-0.000009713
18	6	0.000334000	-0.000942633	-0.000499443
19	1	-0.000242117	0.000171950	0.000126074
20	1	-0.000479478	0.000184736	0.000460614
21	6	-0.000022564	0.000171961	0.000865994
22	8	-0.000085590	0.000151333	-0.000607185
23	8	0.000311052	-0.000166096	-0.000169466
24	1	0.000095851	0.000168884	0.000093306

Cartesian Forces: Max 0.000942633 RMS 0.000234601

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000633132 RMS 0.000125430
Search for a local minimum.
Step number 9 out of a maximum of 140
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 5 4 6 7 8
9
DE= -3.27D-05 DEPred=-1.81D-05 R= 1.81D+00
TightC=F SS= 1.41D+00 RLast= 6.39D-02 DXNew= 1.2000D+00 1.9164D-01
Trust test= 1.81D+00 RLast= 6.39D-02 DXMaxT set to 7.14D-01
ITU= 1 1 1 0 -1 1 1 1 0

Eigenvalues ---	0.00217	0.00378	0.00394	0.00828	0.01608
Eigenvalues ---	0.01769	0.01978	0.02032	0.02146	0.02215
Eigenvalues ---	0.02338	0.02350	0.02424	0.02547	0.03038
Eigenvalues ---	0.03039	0.03151	0.03647	0.04418	0.04934
Eigenvalues ---	0.05303	0.05602	0.06497	0.08207	0.09737

Eigenvalues --- 0.11026 0.12185 0.14492 0.15394 0.15957
Eigenvalues --- 0.15984 0.15996 0.16000 0.16001 0.16051
Eigenvalues --- 0.16708 0.17865 0.20771 0.21951 0.22839
Eigenvalues --- 0.24477 0.24951 0.27412 0.27940 0.34337
Eigenvalues --- 0.34390 0.35157 0.35493 0.35523 0.35579
Eigenvalues --- 0.35843 0.36041 0.36589 0.36649 0.36866
Eigenvalues --- 0.38221 0.41324 0.42790 0.43731 0.47609
Eigenvalues --- 0.52317 0.53400 0.54381 0.54839 0.59902
Eigenvalues --- 0.94015
En-DIIS/RFO-DIIS IScMMF= 0 using points: 9 8 7 6
RFO step: Lambda=-6.60968092D-06.
DidBck=F Rises=F RFO-DIIS coefs: 2.80954 -1.71897 -0.63982 0.54925
Iteration 1 RMS(Cart)= 0.01630739 RMS(Int)= 0.00015104
Iteration 2 RMS(Cart)= 0.00022341 RMS(Int)= 0.00004907
Iteration 3 RMS(Cart)= 0.00000003 RMS(Int)= 0.00004907

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55767	0.00001	0.00045	0.00016	0.00058	2.55825
R2	2.62598	0.00000	-0.00009	0.00005	-0.00006	2.62592
R3	2.03316	0.00001	0.00004	-0.00001	0.00003	2.03319
R4	2.63057	0.00003	-0.00048	-0.00005	-0.00053	2.63004
R5	2.03101	0.00000	0.00002	0.00002	0.00004	2.03105
R6	2.55292	-0.00014	-0.00319	0.00005	-0.00311	2.54980
R7	2.68176	0.00020	0.00263	0.00040	0.00303	2.68479
R8	2.53459	0.00003	-0.00185	-0.00018	-0.00203	2.53256
R9	5.35887	0.00020	0.04753	0.00537	0.05287	5.41174
R10	2.02626	0.00003	0.00021	0.00006	0.00029	2.02656
R11	2.77425	0.00000	-0.00041	0.00042	0.00000	2.77425
R12	2.05800	-0.00012	-0.00064	0.00022	-0.00041	2.05759
R13	2.06181	0.00006	0.00019	-0.00011	0.00009	2.06190
R14	2.89283	-0.00013	0.00194	-0.00118	0.00077	2.89360
R15	5.11489	-0.00014	-0.00909	-0.00538	-0.01446	5.10044
R16	5.12839	-0.00003	0.00070	-0.00202	-0.00131	5.12708
R17	2.50854	-0.00004	-0.00050	-0.00010	-0.00059	2.50795
R18	2.04913	0.00003	0.00038	0.00011	0.00049	2.04961
R19	2.04343	0.00001	0.00011	0.00002	0.00012	2.04355
R20	2.04748	0.00001	0.00011	0.00004	0.00015	2.04763
R21	2.06778	-0.00019	0.00065	-0.00113	-0.00048	2.06729
R22	2.07631	0.00026	0.00096	0.00029	0.00128	2.07759
R23	2.84458	0.00034	0.00238	-0.00105	0.00133	2.84591
R24	2.28376	-0.00063	-0.00108	0.00043	-0.00065	2.28311
R25	2.55074	0.00034	-0.00003	0.00017	0.00015	2.55088
R26	1.83156	0.00012	0.00041	-0.00013	0.00028	1.83184
A1	1.87632	-0.00005	-0.00055	0.00004	-0.00053	1.87578

A2	2.27678	0.00005	0.00065	0.00015	0.00080	2.27758
A3	2.13005	0.00000	-0.00010	-0.00017	-0.00025	2.12980
A4	1.86945	-0.00001	-0.00023	-0.00008	-0.00032	1.86913
A5	2.28469	0.00004	0.00037	0.00035	0.00072	2.28541
A6	2.12836	-0.00002	-0.00001	-0.00034	-0.00035	2.12801
A7	1.89143	0.00005	0.00009	0.00010	0.00023	1.89166
A8	2.22764	-0.00005	-0.00044	-0.00010	-0.00057	2.22707
A9	2.15395	0.00000	0.00015	0.00011	0.00025	2.15419
A10	1.88876	-0.00003	0.00162	0.00012	0.00164	1.89040
A11	1.81219	-0.00004	-0.00652	-0.00069	-0.00715	1.80504
A12	2.18428	0.00004	0.00284	0.00041	0.00293	2.18720
A13	1.88030	0.00018	0.00273	0.00183	0.00454	1.88483
A14	2.18921	0.00001	0.00265	0.00045	0.00280	2.19201
A15	1.89436	0.00004	-0.00020	-0.00009	-0.00023	1.89414
A16	2.20076	-0.00002	0.00035	-0.00023	0.00015	2.20092
A17	2.17458	-0.00003	-0.00001	0.00028	0.00018	2.17476
A18	1.87511	0.00012	0.00113	0.00072	0.00184	1.87694
A19	1.88695	0.00007	-0.00014	-0.00035	-0.00048	1.88647
A20	1.94951	-0.00009	0.00010	-0.00110	-0.00102	1.94849
A21	1.87378	0.00005	0.00115	-0.00007	0.00109	1.87487
A22	1.92516	-0.00014	-0.00070	-0.00029	-0.00098	1.92418
A23	1.95006	0.00001	-0.00139	0.00111	-0.00027	1.94978
A24	1.23737	-0.00024	-0.01038	-0.00316	-0.01350	1.22387
A25	1.37864	-0.00023	-0.01227	-0.00342	-0.01579	1.36284
A26	2.15785	-0.00012	-0.00228	-0.00065	-0.00293	2.15492
A27	1.95824	0.00000	-0.00106	-0.00003	-0.00109	1.95715
A28	2.16624	0.00012	0.00331	0.00067	0.00397	2.17022
A29	2.08532	0.00002	0.00013	0.00015	0.00027	2.08559
A30	2.14644	-0.00003	-0.00030	-0.00026	-0.00057	2.14587
A31	2.05142	0.00001	0.00018	0.00011	0.00029	2.05172
A32	1.95099	-0.00003	-0.00028	0.00074	0.00053	1.95151
A33	1.91837	-0.00022	-0.00073	-0.00106	-0.00175	1.91663
A34	1.93227	0.00011	-0.00214	0.00058	-0.00147	1.93080
A35	1.85730	0.00005	0.00284	-0.00080	0.00197	1.85927
A36	1.89366	0.00019	0.00301	0.00125	0.00428	1.89794
A37	1.90938	-0.00010	-0.00273	-0.00077	-0.00348	1.90590
A38	2.53646	0.00040	0.01488	0.00554	0.02041	2.55686
A39	2.18953	-0.00007	-0.00210	0.00094	-0.00114	2.18838
A40	1.94810	0.00032	0.00226	-0.00096	0.00131	1.94941
A41	2.14556	-0.00025	-0.00021	0.00002	-0.00017	2.14539
A42	1.87541	0.00003	-0.00047	0.00039	-0.00008	1.87533
D1	0.00387	0.00002	-0.00198	0.00446	0.00249	0.00636
D2	3.10549	0.00004	0.00178	0.00221	0.00399	3.10947
D3	-3.12898	0.00001	-0.00213	0.00172	-0.00040	-3.12938

D4	-0.02736	0.00003	0.00162	-0.00052	0.00109	-0.02626
D5	-0.05708	-0.00002	0.00614	-0.00306	0.00308	-0.05400
D6	-3.02870	0.00000	0.00528	-0.00286	0.00243	-3.02628
D7	3.07666	-0.00001	0.00629	-0.00060	0.00568	3.08234
D8	0.10504	0.00001	0.00542	-0.00040	0.00503	0.11006
D9	0.05022	0.00000	-0.00279	-0.00433	-0.00714	0.04308
D10	3.04160	0.00001	-0.00427	-0.00347	-0.00775	3.03385
D11	-3.05576	-0.00003	-0.00615	-0.00235	-0.00850	-3.06427
D12	-0.06439	-0.00001	-0.00762	-0.00148	-0.00911	-0.07350
D13	-0.08621	-0.00001	0.00656	0.00244	0.00902	-0.07719
D14	1.90843	0.00017	0.00726	0.00424	0.01147	1.91989
D15	-3.01859	-0.00006	-0.02909	-0.00247	-0.03157	-3.05016
D16	-3.08534	-0.00002	0.00802	0.00164	0.00968	-3.07566
D17	-1.09071	0.00016	0.00872	0.00344	0.01213	-1.07858
D18	0.26546	-0.00007	-0.02763	-0.00327	-0.03091	0.23456
D19	0.58002	0.00005	0.02043	0.00431	0.02474	0.60476
D20	-2.51870	0.00005	0.02113	0.00454	0.02567	-2.49304
D21	-2.73255	0.00007	0.01874	0.00529	0.02403	-2.70852
D22	0.45191	0.00007	0.01944	0.00552	0.02496	0.47687
D23	0.08865	0.00002	-0.00780	0.00034	-0.00748	0.08117
D24	3.06343	0.00000	-0.00691	0.00009	-0.00684	3.05660
D25	-1.86059	-0.00001	-0.00235	0.00019	-0.00219	-1.86277
D26	1.11420	-0.00003	-0.00146	-0.00006	-0.00154	1.11265
D27	3.02029	0.00007	0.02800	0.00526	0.03327	3.05356
D28	-0.28811	0.00005	0.02890	0.00500	0.03391	-0.25420
D29	-2.24666	0.00001	-0.00214	-0.00095	-0.00298	-2.24965
D30	-0.24600	0.00003	-0.00218	-0.00038	-0.00258	-0.24857
D31	-2.92164	-0.00010	0.00955	0.00233	0.01187	-2.90977
D32	-0.90437	0.00005	0.01140	0.00245	0.01385	-0.89053
D33	1.24809	0.00005	0.00960	0.00289	0.01250	1.26059
D34	0.41602	-0.00008	0.00855	0.00260	0.01115	0.42717
D35	2.43329	0.00007	0.01041	0.00272	0.01312	2.44641
D36	-1.69743	0.00007	0.00861	0.00316	0.01178	-1.68565
D37	-1.05524	0.00006	-0.00699	-0.00141	-0.00843	-1.06366
D38	1.00312	-0.00004	-0.00412	-0.00263	-0.00678	0.99634
D39	3.11452	-0.00024	-0.00929	-0.00392	-0.01322	3.10131
D40	-3.13935	0.00006	-0.00800	-0.00142	-0.00942	3.13441
D41	-1.08100	-0.00004	-0.00513	-0.00263	-0.00777	-1.08877
D42	1.03041	-0.00024	-0.01030	-0.00392	-0.01421	1.01619
D43	1.06102	0.00009	-0.00810	-0.00186	-0.00996	1.05106
D44	3.11938	-0.00001	-0.00523	-0.00307	-0.00831	3.11107
D45	-1.05240	-0.00021	-0.01039	-0.00436	-0.01475	-1.06715
D46	-0.01097	-0.00001	0.00508	0.00054	0.00570	-0.00527
D47	0.36224	0.00000	0.00403	0.00072	0.00468	0.36691

D48	-3.09036	0.00001	0.00058	0.00065	0.00122	-3.08913
D49	0.04808	0.00000	0.00095	-0.00008	0.00087	0.04895
D50	0.00329	0.00001	-0.00033	0.00037	0.00003	0.00332
D51	-3.14146	0.00000	0.00004	-0.00036	-0.00032	3.14140
D52	-0.34428	-0.00003	-0.00298	-0.00011	-0.00315	-0.34744
D53	1.77127	-0.00017	-0.00202	-0.00029	-0.00232	1.76895
D54	-2.46940	0.00004	0.00163	0.00035	0.00200	-2.46740
D55	-0.12142	0.00010	-0.01065	-0.00970	-0.02036	-0.14178
D56	3.02271	0.00012	-0.01071	-0.00920	-0.01993	3.00279
D57	-2.26842	-0.00006	-0.01114	-0.01183	-0.02293	-2.29135
D58	0.87571	-0.00003	-0.01120	-0.01134	-0.02250	0.85321
D59	1.99531	-0.00017	-0.01455	-0.01116	-0.02574	1.96957
D60	-1.14374	-0.00015	-0.01461	-0.01067	-0.02531	-1.16905
D61	3.11084	-0.00016	-0.00535	-0.00194	-0.00729	3.10355
D62	-0.02829	-0.00014	-0.00541	-0.00146	-0.00687	-0.03516

Item	Value	Threshold	Converged?
Maximum Force	0.000633	0.000450	NO
RMS Force	0.000125	0.000300	YES
Maximum Displacement	0.068250	0.001800	NO
RMS Displacement	0.016400	0.001200	NO

Predicted change in Energy=-2.096037D-05

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.314378	-2.194415	-0.394756
2	6	0	-1.569826	-1.761695	-0.657985
3	7	0	-1.811214	-0.674492	0.176702
4	6	0	-0.692262	-0.428526	0.889480
5	7	0	0.207026	-1.380035	0.603169
6	6	0	1.587134	-1.400441	1.103288
7	1	0	0.252307	-2.999795	-0.828146
8	1	0	-2.295924	-2.100547	-1.374311
9	1	0	1.610245	-0.823409	2.026350
10	1	0	1.840671	-2.431174	1.355924
11	35	0	0.258921	2.043824	-0.198592
12	1	0	-0.603098	0.299425	1.671911
13	6	0	-2.944134	0.182811	0.177850
14	6	0	-4.174716	-0.230149	-0.098654
15	1	0	-2.676882	1.213001	0.386804
16	1	0	-4.983335	0.487319	-0.127000

17	1	0	-4.416417	-1.266187	-0.304332
18	6	0	2.565747	-0.809738	0.084445
19	1	0	2.568432	-1.375441	-0.851895
20	1	0	2.263895	0.216148	-0.170800
21	6	0	3.964574	-0.790183	0.642039
22	8	0	4.266918	-1.051168	1.782280
23	8	0	4.870082	-0.436221	-0.294397
24	1	0	5.738208	-0.409687	0.136098

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.353767	0.000000			
3	N	2.208449	1.391755	0.000000		
4	C	2.215947	2.223084	1.349297	0.000000	
5	N	1.389579	2.212097	2.180128	1.340173	0.000000
6	C	2.547602	3.633040	3.596433	2.487163	1.468071
7	H	1.075917	2.209528	3.267243	3.233245	2.162021
8	H	2.212434	1.074785	2.161995	3.239157	3.270218
9	H	3.383133	4.266015	3.892269	2.598066	2.074681
10	H	2.786606	4.016904	4.220517	3.262503	2.083346
11	Br	4.281334	4.247038	3.437375	2.863767	3.516863
12	H	3.251723	3.257482	2.154926	1.072409	2.149208
13	C	3.590918	2.523578	1.420731	2.439483	3.543048
14	C	4.341454	3.073099	2.420621	3.625362	4.584153
15	H	4.219329	3.341552	2.087140	2.624121	3.884273
16	H	5.390969	4.122142	3.391812	4.503922	5.564172
17	H	4.206722	2.910959	2.714513	3.999524	4.713040
18	C	3.231421	4.308176	4.380022	3.377577	2.481507
19	H	3.031549	4.160765	4.553091	3.815909	2.773710
20	H	3.536730	4.341270	4.185750	3.206035	2.716162
21	C	4.621281	5.767450	5.795658	4.677408	3.803762
22	O	5.199497	6.366107	6.297893	5.077228	4.240422
23	O	5.475395	6.584945	6.702121	5.686942	4.841540
24	H	6.332525	7.474347	7.554174	6.474480	5.635043

		6	7	8	9	10
6	C	0.000000				
7	H	2.840798	0.000000			
8	H	4.659054	2.756887	0.000000		
9	H	1.088828	3.837813	5.334205	0.000000	
10	H	1.091108	2.759782	4.967386	1.757122	0.000000
11	Br	3.914333	5.082762	5.008529	3.872656	4.994403
12	H	2.830193	4.226920	4.231429	2.507044	3.678047
13	C	4.888303	4.621498	2.836036	5.017151	5.578094

14	C	6.001097	5.272725	2.942031	6.191396	6.568500
15	H	5.052253	5.272940	3.771771	5.021408	5.884513
16	H	6.946100	6.329575	3.933829	7.059053	7.568601
17	H	6.167823	5.007671	2.517440	6.476789	6.577599
18	C	1.531227	3.313785	5.237366	2.164294	2.184365
19	H	2.187764	2.829050	4.945771	3.083368	2.553169
20	H	2.166718	3.849789	5.254280	2.517023	3.085177
21	C	2.497476	4.563415	6.706456	2.731352	2.777310
22	O	2.786443	5.169968	7.357728	2.677565	2.823627
23	O	3.696079	5.308545	7.435580	4.020239	3.985064
24	H	4.375897	6.142763	8.347912	4.558980	4.556883

		11	12	13	14	15
11	Br	0.000000				
12	H	2.699034	0.000000			
13	C	3.723525	2.779616	0.000000		
14	C	4.983782	4.021418	1.327148	0.000000	
15	H	3.106750	2.605130	1.084609	2.135851	0.000000
16	H	5.468920	4.738972	2.084227	1.081401	2.471909
17	H	5.729410	4.571441	2.121252	1.083557	3.106448
18	C	3.680268	3.713741	5.599345	6.767813	5.627437
19	H	4.177562	4.385587	5.820387	6.881069	5.978940
20	H	2.713133	3.409130	5.219792	6.454463	5.071086
21	C	4.740265	4.807443	6.992312	8.192088	6.941673
22	O	5.437542	5.055031	7.489738	8.687530	7.435736
23	O	5.236660	5.862017	7.852910	9.049263	7.755040
24	H	6.012846	6.563058	8.702636	9.917329	8.573781

		16	17	18	19	20
16	H	0.000000				
17	H	1.851384	0.000000			
18	C	7.662617	7.007861	0.000000		
19	H	7.811820	7.007131	1.093965	0.000000	
20	H	7.252434	6.844101	1.099412	1.757780	0.000000
21	C	9.071301	8.447675	1.505992	2.126870	2.136754
22	O	9.569716	8.933112	2.415557	3.151013	3.071272
23	O	9.898019	9.323520	2.364952	2.547653	2.689438
24	H	10.762218	10.200196	3.198003	3.457788	3.543545

		21	22	23	24
21	C	0.000000			
22	O	1.208170	0.000000		
23	O	1.349870	2.248234	0.000000	
24	H	1.883224	2.299154	0.969367	0.000000

Stoichiometry C8H11BrN2O2

Framework group C1[X(C8H11BrN2O2)]

Deg. of freedom 66

Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.632278	-2.123035	-0.770112
2	6	0	-1.946634	-1.812223	-0.862577
3	7	0	-2.213323	-0.865346	0.121945
4	6	0	-1.058793	-0.575084	0.757093
5	7	0	-0.099002	-1.375162	0.272592
6	6	0	1.319840	-1.292344	0.640372
7	1	0	-0.031985	-2.800701	-1.351502
8	1	0	-2.703208	-2.147797	-1.548250
9	1	0	1.377432	-0.828048	1.623559
10	1	0	1.704866	-2.308770	0.736020
11	35	0	-0.489758	2.101249	-0.088248
12	1	0	-0.966224	0.062159	1.614655
13	6	0	-3.423752	-0.152256	0.333699
14	6	0	-4.626133	-0.671086	0.118253
15	1	0	-3.245955	0.870695	0.647288
16	1	0	-5.504164	-0.054598	0.254020
17	1	0	-4.777706	-1.697201	-0.195133
18	6	0	2.120622	-0.476737	-0.378544
19	1	0	2.085986	-0.925299	-1.375715
20	1	0	1.688047	0.529569	-0.473056
21	6	0	3.559719	-0.359014	0.049420
22	8	0	4.003868	-0.713939	1.115457
23	8	0	4.321546	0.204956	-0.911676
24	1	0	5.221870	0.282378	-0.560828

Rotational constants (GHZ): 0.8137773 0.3319735 0.2545739
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 404 symmetry adapted cartesian basis functions of A symmetry.
There are 389 symmetry adapted basis functions of A symmetry.
389 basis functions, 625 primitive gaussians, 404 cartesian basis functions
62 alpha electrons 62 beta electrons
nuclear repulsion energy 1073.0064174807 Hartrees.
NAtoms= 24 NActive= 24 NUniq= 24 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 389 RedAO= T EigKep= 6.43D-06 NBF= 389
NBsUse= 389 1.00D-06 EigRej= -1.00D+00 NBFU= 389
Initial guess from the checkpoint file: "./cooh.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 0.000608 -0.000104 0.000624 Ang= 0.10 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=2910765817.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3145.73220634 A.U. after 12 cycles
NFock= 12 Conv=0.50D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000069551	-0.000228185	0.000183289
2	6	0.000128299	0.000106368	-0.000163277
3	7	-0.000304743	-0.000198337	0.000096564
4	6	0.000378681	0.000465280	-0.000240379
5	7	-0.000152334	-0.000037316	-0.000086019
6	6	0.000179735	0.000139548	-0.000119012
7	1	0.000007754	0.000006200	-0.000013223
8	1	0.000000129	0.000038372	-0.000017641
9	1	0.000060405	-0.000023572	-0.000022088
10	1	-0.000061996	-0.000046522	0.000002048
11	35	-0.000023509	0.000000458	0.000104826

12	1	0.000027754	-0.000003985	0.000016019
13	6	0.000040123	-0.000001598	-0.000052077
14	6	-0.000044974	0.000004675	0.000004719
15	1	0.000028050	0.000004559	0.000007958
16	1	-0.000003764	-0.000005260	-0.000006385
17	1	0.000006143	-0.000007950	-0.000002722
18	6	0.000492637	-0.000577288	-0.000136453
19	1	-0.000095679	0.000223460	0.000099542
20	1	-0.000523852	0.000024016	0.000302737
21	6	-0.000272009	-0.000057000	0.000210362
22	8	0.000047990	0.000094538	-0.000076128
23	8	0.000179725	-0.000003162	-0.000115217
24	1	-0.000025015	0.000082700	0.000022558

Cartesian Forces: Max 0.000577288 RMS 0.000169032

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000442686 RMS 0.000088236
Search for a local minimum.
Step number 10 out of a maximum of 140
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 5 4 6 7 8
9 10
DE= -4.32D-05 DEPred=-2.10D-05 R= 2.06D+00
TightC=F SS= 1.41D+00 RLast= 1.30D-01 DXNew= 1.2000D+00 3.9058D-01
Trust test= 2.06D+00 RLast= 1.30D-01 DXMaxT set to 7.14D-01
ITU= 1 1 1 1 0 -1 1 1 1 0

Eigenvalues ---	0.00181	0.00324	0.00391	0.00844	0.01606
Eigenvalues ---	0.01788	0.01999	0.02049	0.02173	0.02231
Eigenvalues ---	0.02281	0.02353	0.02418	0.02569	0.03038
Eigenvalues ---	0.03039	0.03105	0.03480	0.04404	0.04891
Eigenvalues ---	0.05082	0.05497	0.06444	0.07928	0.09626
Eigenvalues ---	0.10795	0.12176	0.14193	0.15555	0.15956
Eigenvalues ---	0.15983	0.15995	0.16000	0.16001	0.16051
Eigenvalues ---	0.16689	0.17885	0.20774	0.21982	0.22848
Eigenvalues ---	0.24475	0.25033	0.27535	0.27966	0.34353
Eigenvalues ---	0.34372	0.35132	0.35445	0.35492	0.35579
Eigenvalues ---	0.35843	0.35999	0.36497	0.36601	0.36651

Eigenvalues --- 0.37606 0.41326 0.42887 0.43882 0.47723
Eigenvalues --- 0.52330 0.53375 0.54251 0.54583 0.59916
Eigenvalues --- 0.92108
En-DIIS/RFO-DIIS IScMMF= 0 using points: 10 9 8 7 6
RFO step: Lambda=-3.19920370D-06.
DidBck=F Rises=F RFO-DIIS coefs: 1.12034 0.57001 -0.90161 0.08852 0.12274
Iteration 1 RMS(Cart)= 0.00917715 RMS(Int)= 0.00004871
Iteration 2 RMS(Cart)= 0.00006633 RMS(Int)= 0.00001903
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001903

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55825	0.00002	0.00015	0.00007	0.00022	2.55846
R2	2.62592	0.00000	0.00000	0.00000	-0.00001	2.62591
R3	2.03319	0.00000	0.00001	0.00001	0.00002	2.03321
R4	2.63004	0.00004	-0.00011	-0.00004	-0.00015	2.62989
R5	2.03105	0.00000	0.00000	0.00001	0.00001	2.03106
R6	2.54980	0.00020	-0.00106	0.00020	-0.00084	2.54896
R7	2.68479	-0.00002	0.00102	0.00015	0.00117	2.68596
R8	2.53256	0.00012	-0.00055	-0.00002	-0.00058	2.53198
R9	5.41174	-0.00004	0.01523	0.00176	0.01698	5.42871
R10	2.02656	0.00004	0.00009	0.00010	0.00020	2.02676
R11	2.77425	0.00013	-0.00030	0.00055	0.00024	2.77449
R12	2.05759	-0.00003	-0.00039	0.00019	-0.00020	2.05739
R13	2.06190	0.00003	0.00017	-0.00006	0.00012	2.06201
R14	2.89360	-0.00021	0.00072	-0.00084	-0.00011	2.89349
R15	5.10044	-0.00015	-0.00553	-0.00474	-0.01028	5.09015
R16	5.12708	-0.00006	0.00012	-0.00258	-0.00245	5.12463
R17	2.50795	0.00004	-0.00018	0.00001	-0.00017	2.50778
R18	2.04961	0.00001	0.00015	0.00009	0.00024	2.04985
R19	2.04355	0.00000	0.00005	0.00000	0.00005	2.04360
R20	2.04763	0.00001	0.00005	0.00003	0.00008	2.04770
R21	2.06729	-0.00020	-0.00018	-0.00050	-0.00068	2.06661
R22	2.07759	0.00013	0.00083	0.00013	0.00097	2.07856
R23	2.84591	-0.00006	0.00115	-0.00099	0.00016	2.84607
R24	2.28311	-0.00009	-0.00062	0.00027	-0.00035	2.28276
R25	2.55088	0.00020	0.00035	0.00007	0.00042	2.55130
R26	1.83184	-0.00002	0.00028	-0.00022	0.00006	1.83190
A1	1.87578	-0.00001	-0.00018	-0.00010	-0.00029	1.87549
A2	2.27758	0.00001	0.00026	0.00011	0.00038	2.27796
A3	2.12980	0.00000	-0.00008	-0.00002	-0.00010	2.12971
A4	1.86913	0.00005	-0.00013	0.00013	0.00000	1.86913
A5	2.28541	0.00000	0.00024	0.00017	0.00041	2.28582
A6	2.12801	-0.00005	-0.00005	-0.00025	-0.00030	2.12771

A7	1.89166	-0.00001	0.00011	-0.00011	0.00002	1.89168
A8	2.22707	0.00002	-0.00027	-0.00002	-0.00030	2.22677
A9	2.15419	-0.00001	0.00006	-0.00008	-0.00003	2.15417
A10	1.89040	-0.00009	0.00043	-0.00002	0.00038	1.89078
A11	1.80504	0.00002	-0.00200	-0.00034	-0.00231	1.80274
A12	2.18720	0.00005	0.00090	0.00021	0.00099	2.18820
A13	1.88483	0.00017	0.00144	0.00208	0.00350	1.88834
A14	2.19201	0.00003	0.00083	0.00011	0.00083	2.19284
A15	1.89414	0.00006	-0.00003	0.00016	0.00016	1.89430
A16	2.20092	-0.00002	-0.00016	-0.00001	-0.00015	2.20076
A17	2.17476	-0.00005	0.00027	0.00006	0.00028	2.17504
A18	1.87694	0.00005	0.00053	0.00040	0.00092	1.87786
A19	1.88647	0.00002	-0.00037	-0.00019	-0.00055	1.88591
A20	1.94849	-0.00011	0.00003	-0.00053	-0.00051	1.94798
A21	1.87487	-0.00002	0.00077	-0.00037	0.00039	1.87527
A22	1.92418	-0.00005	-0.00071	-0.00025	-0.00095	1.92323
A23	1.94978	0.00012	-0.00019	0.00094	0.00075	1.95053
A24	1.22387	-0.00022	-0.00393	-0.00245	-0.00636	1.21751
A25	1.36284	-0.00020	-0.00463	-0.00271	-0.00739	1.35545
A26	2.15492	0.00001	-0.00094	-0.00016	-0.00110	2.15382
A27	1.95715	-0.00003	-0.00040	-0.00025	-0.00065	1.95650
A28	2.17022	0.00002	0.00134	0.00040	0.00174	2.17196
A29	2.08559	0.00001	0.00009	0.00011	0.00020	2.08580
A30	2.14587	-0.00002	-0.00018	-0.00014	-0.00032	2.14555
A31	2.05172	0.00000	0.00009	0.00004	0.00012	2.05184
A32	1.95151	0.00004	0.00049	0.00081	0.00132	1.95284
A33	1.91663	-0.00024	-0.00089	-0.00146	-0.00233	1.91429
A34	1.93080	0.00018	-0.00042	0.00056	0.00014	1.93095
A35	1.85927	0.00002	0.00096	-0.00038	0.00055	1.85982
A36	1.89794	0.00003	0.00295	0.00052	0.00349	1.90142
A37	1.90590	-0.00003	-0.00317	-0.00008	-0.00325	1.90264
A38	2.55686	0.00044	0.00610	0.00502	0.01112	2.56798
A39	2.18838	0.00010	-0.00075	0.00060	-0.00014	2.18824
A40	1.94941	-0.00002	0.00115	-0.00081	0.00034	1.94975
A41	2.14539	-0.00009	-0.00042	0.00021	-0.00021	2.14518
A42	1.87533	0.00000	0.00016	-0.00029	-0.00013	1.87520
D1	0.00636	-0.00010	-0.00060	-0.00302	-0.00361	0.00274
D2	3.10947	-0.00002	0.00115	-0.00138	-0.00023	3.10924
D3	-3.12938	-0.00004	-0.00072	-0.00086	-0.00157	-3.13095
D4	-0.02626	0.00004	0.00103	0.00078	0.00181	-0.02446
D5	-0.05400	0.00005	0.00187	0.00280	0.00467	-0.04933
D6	-3.02628	0.00004	0.00133	0.00147	0.00281	-3.02347
D7	3.08234	0.00000	0.00198	0.00086	0.00284	3.08519
D8	0.11006	-0.00001	0.00145	-0.00047	0.00099	0.11105

D9	0.04308	0.00012	-0.00085	0.00220	0.00134	0.04442
D10	3.03385	0.00008	-0.00153	0.00062	-0.00091	3.03294
D11	-3.06427	0.00005	-0.00242	0.00073	-0.00169	-3.06596
D12	-0.07350	0.00001	-0.00309	-0.00085	-0.00394	-0.07744
D13	-0.07719	-0.00008	0.00201	-0.00046	0.00156	-0.07563
D14	1.91989	0.00008	0.00288	0.00173	0.00459	1.92448
D15	-3.05016	0.00003	-0.01032	-0.00235	-0.01268	-3.06284
D16	-3.07566	-0.00005	0.00268	0.00103	0.00372	-3.07193
D17	-1.07858	0.00012	0.00355	0.00322	0.00675	-1.07182
D18	0.23456	0.00006	-0.00965	-0.00086	-0.01051	0.22404
D19	0.60476	0.00004	0.00849	0.00391	0.01240	0.61716
D20	-2.49304	0.00003	0.00849	0.00394	0.01244	-2.48060
D21	-2.70852	0.00000	0.00773	0.00211	0.00984	-2.69869
D22	0.47687	-0.00001	0.00773	0.00215	0.00987	0.48674
D23	0.08117	0.00002	-0.00238	-0.00142	-0.00381	0.07736
D24	3.05660	0.00003	-0.00191	-0.00013	-0.00204	3.05456
D25	-1.86277	-0.00004	-0.00098	-0.00202	-0.00302	-1.86579
D26	1.11265	-0.00003	-0.00050	-0.00072	-0.00125	1.11141
D27	3.05356	-0.00009	0.00999	0.00050	0.01049	3.06405
D28	-0.25420	-0.00008	0.01047	0.00179	0.01226	-0.24194
D29	-2.24965	0.00004	-0.00096	-0.00103	-0.00195	-2.25160
D30	-0.24857	0.00002	-0.00080	-0.00036	-0.00116	-0.24974
D31	-2.90977	0.00000	0.00373	0.00470	0.00842	-2.90135
D32	-0.89053	0.00001	0.00471	0.00437	0.00907	-0.88146
D33	1.26059	0.00010	0.00423	0.00507	0.00930	1.26990
D34	0.42717	-0.00002	0.00315	0.00315	0.00630	0.43347
D35	2.44641	-0.00001	0.00412	0.00283	0.00695	2.45336
D36	-1.68565	0.00008	0.00365	0.00353	0.00718	-1.67847
D37	-1.06366	0.00004	-0.00315	-0.00153	-0.00469	-1.06835
D38	0.99634	-0.00008	-0.00223	-0.00244	-0.00469	0.99166
D39	3.10131	-0.00016	-0.00702	-0.00313	-0.01016	3.09115
D40	3.13441	0.00008	-0.00336	-0.00151	-0.00488	3.12953
D41	-1.08877	-0.00003	-0.00244	-0.00243	-0.00488	-1.09365
D42	1.01619	-0.00011	-0.00723	-0.00312	-0.01035	1.00584
D43	1.05106	0.00007	-0.00374	-0.00149	-0.00523	1.04583
D44	3.11107	-0.00005	-0.00282	-0.00240	-0.00523	3.10584
D45	-1.06715	-0.00013	-0.00761	-0.00309	-0.01070	-1.07785
D46	-0.00527	-0.00004	0.00201	0.00070	0.00274	-0.00253
D47	0.36691	-0.00002	0.00176	0.00102	0.00274	0.36966
D48	-3.08913	0.00000	0.00005	0.00030	0.00035	-3.08878
D49	0.04895	0.00000	0.00026	0.00016	0.00043	0.04938
D50	0.00332	0.00001	0.00000	0.00024	0.00024	0.00356
D51	3.14140	0.00001	0.00021	0.00010	0.00031	-3.14147
D52	-0.34744	0.00000	-0.00101	-0.00015	-0.00118	-0.34862

D53	1.76895	-0.00008	-0.00034	-0.00023	-0.00057	1.76837
D54	-2.46740	-0.00005	0.00203	0.00013	0.00216	-2.46524
D55	-0.14178	0.00008	-0.00922	-0.00700	-0.01624	-0.15801
D56	3.00279	0.00015	-0.00912	-0.00501	-0.01414	2.98865
D57	-2.29135	-0.00011	-0.01163	-0.00872	-0.02034	-2.31170
D58	0.85321	-0.00003	-0.01152	-0.00673	-0.01824	0.83497
D59	1.96957	-0.00013	-0.01263	-0.00851	-0.02114	1.94843
D60	-1.16905	-0.00005	-0.01252	-0.00652	-0.01904	-1.18809
D61	3.10355	-0.00011	-0.00526	-0.00125	-0.00652	3.09703
D62	-0.03516	-0.00003	-0.00516	0.00068	-0.00448	-0.03964

Item	Value	Threshold	Converged?
Maximum Force	0.000443	0.000450	YES
RMS Force	0.000088	0.000300	YES
Maximum Displacement	0.047898	0.001800	NO
RMS Displacement	0.009194	0.001200	NO

Predicted change in Energy=-9.651970D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.317705	-2.201869	-0.394961
2	6	0	-1.571068	-1.763912	-0.660045
3	7	0	-1.809572	-0.676498	0.175064
4	6	0	-0.690721	-0.434563	0.888538
5	7	0	0.206586	-1.387202	0.601208
6	6	0	1.587254	-1.410382	1.100034
7	1	0	0.246378	-3.009869	-0.826894
8	1	0	-2.298548	-2.100750	-1.375927
9	1	0	1.611974	-0.839475	2.026734
10	1	0	1.841005	-2.442957	1.345087
11	35	0	0.260013	2.049741	-0.196375
12	1	0	-0.595654	0.300013	1.664198
13	6	0	-2.939261	0.186074	0.173949
14	6	0	-4.172370	-0.225336	-0.093011
15	1	0	-2.665846	1.216874	0.372315
16	1	0	-4.978888	0.494398	-0.124579
17	1	0	-4.418123	-1.262603	-0.287602
18	6	0	2.564014	-0.811656	0.084191
19	1	0	2.570373	-1.372364	-0.854710
20	1	0	2.256132	0.214365	-0.165473
21	6	0	3.961334	-0.781819	0.645325

22	8	0	4.260703	-1.025821	1.789908
23	8	0	4.869069	-0.437415	-0.292840
24	1	0	5.734894	-0.397748	0.141339

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.353881	0.000000			
3	N	2.208473	1.391676	0.000000		
4	C	2.215825	2.222676	1.348853	0.000000	
5	N	1.389574	2.211950	2.179815	1.339866	0.000000
6	C	2.547613	3.632885	3.596190	2.487192	1.468199
7	H	1.075928	2.209832	3.267334	3.233120	2.161968
8	H	2.212748	1.074790	2.161750	3.238686	3.270154
9	H	3.382955	4.266746	3.893870	2.600356	2.075391
10	H	2.783149	4.015457	4.220905	3.263697	2.083098
11	Br	4.295275	4.255796	3.442896	2.872751	3.528679
12	H	3.252200	3.257810	2.155155	1.072515	2.149473
13	C	3.591447	2.523875	1.421348	2.439623	3.543177
14	C	4.342383	3.074982	2.420376	3.623408	4.583353
15	H	4.217852	3.339070	2.087335	2.625804	3.883872
16	H	5.391622	4.123096	3.391953	4.503082	5.563840
17	H	4.207989	2.914746	2.713322	3.995307	4.710991
18	C	3.235211	4.308084	4.376618	3.373793	2.481135
19	H	3.039810	4.164461	4.552866	3.814855	2.776222
20	H	3.537724	4.336548	4.176070	3.196247	2.711726
21	C	4.626977	5.768533	5.790993	4.671334	3.803495
22	O	5.207549	6.368407	6.291104	5.067412	4.240221
23	O	5.479631	6.585575	6.699279	5.683918	4.841504
24	H	6.338488	7.475674	7.549690	6.469018	5.634953

		6	7	8	9	10
6	C	0.000000				
7	H	2.840661	0.000000			
8	H	4.659017	2.757641	0.000000		
9	H	1.088724	3.836490	5.334894	0.000000	
10	H	1.091169	2.753493	4.965573	1.757342	0.000000
11	Br	3.926156	5.098764	5.016389	3.888134	5.005994
12	H	2.829986	4.227278	4.231533	2.510675	3.682801
13	C	4.888317	4.622125	2.835876	5.019791	5.579813
14	C	6.000079	5.274234	2.945209	6.191051	6.568610
15	H	5.051822	5.271101	3.768008	5.026471	5.886624
16	H	6.945652	6.330603	3.935084	7.060228	7.569604
17	H	6.165381	5.010124	2.525775	6.472809	6.575377
18	C	1.531166	3.321695	5.238150	2.163476	2.184890

19	H	2.188376	2.843088	4.950617	3.083053	2.552891
20	H	2.165343	3.856459	5.250721	2.516206	3.084717
21	C	2.497621	4.575209	6.709036	2.726006	2.782956
22	O	2.787678	5.186416	7.362185	2.665817	2.839204
23	O	3.695547	5.317142	7.437371	4.018798	3.984240
24	H	4.375779	6.155035	8.350958	4.555031	4.560073

		11	12	13	14	15
11	Br	0.000000				
12	H	2.693594	0.000000			
13	C	3.720988	2.779626	0.000000		
14	C	4.983240	4.019536	1.327058	0.000000	
15	H	3.094790	2.606777	1.084736	2.136846	0.000000
16	H	5.465375	4.738169	2.084288	1.081428	2.473669
17	H	5.732792	4.567555	2.121021	1.083597	3.107052
18	C	3.684390	3.703476	5.593707	6.764173	5.616883
19	H	4.181145	4.377838	5.817468	6.881892	5.968896
20	H	2.711836	3.389354	5.206546	6.443929	5.051743
21	C	4.735607	4.793183	6.984070	8.186083	6.927397
22	O	5.423092	5.035657	7.477935	8.677723	7.417299
23	O	5.238192	5.851238	7.847079	9.046133	7.742999
24	H	6.006545	6.548420	8.693842	9.911535	8.557615

		16	17	18	19	20
16	H	0.000000				
17	H	1.851510	0.000000			
18	C	7.657985	7.006556	0.000000		
19	H	7.810840	7.012327	1.093604	0.000000	
20	H	7.240553	6.836815	1.099928	1.758267	0.000000
21	C	9.063611	8.444928	1.506076	2.129230	2.134828
22	O	9.557529	8.927157	2.415387	3.157739	3.062659
23	O	9.893373	9.323781	2.365478	2.544372	2.696011
24	H	10.754150	10.198810	3.198291	3.457771	3.545504

		21	22	23	24
21	C	0.000000			
22	O	1.207986	0.000000		
23	O	1.350092	2.248148	0.000000	
24	H	1.883355	2.299020	0.969401	0.000000

Stoichiometry C8H11BrN2O2
Framework group C1[X(C8H11BrN2O2)]
Deg. of freedom 66
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.637761	-2.133307	-0.767832
2	6	0	-1.950441	-1.815362	-0.861508
3	7	0	-2.212498	-0.865840	0.121597
4	6	0	-1.056856	-0.579958	0.755764
5	7	0	-0.100307	-1.383381	0.271239
6	6	0	1.319551	-1.304229	0.636407
7	1	0	-0.040810	-2.815864	-1.346957
8	1	0	-2.709354	-2.149452	-1.545328
9	1	0	1.380885	-0.844474	1.621385
10	1	0	1.702945	-2.321892	0.725972
11	35	0	-0.486218	2.105464	-0.090158
12	1	0	-0.958544	0.066741	1.605708
13	6	0	-3.419479	-0.144978	0.330839
14	6	0	-4.624313	-0.662522	0.126864
15	1	0	-3.235262	0.880847	0.631503
16	1	0	-5.499969	-0.041811	0.258890
17	1	0	-4.780106	-1.691970	-0.173383
18	6	0	2.118461	-0.484169	-0.380312
19	1	0	2.085549	-0.928874	-1.378872
20	1	0	1.681722	0.521312	-0.470365
21	6	0	3.555755	-0.357939	0.051565
22	8	0	3.995786	-0.695553	1.124699
23	8	0	4.320783	0.194308	-0.914097
24	1	0	5.218145	0.283493	-0.558393

Rotational constants (GHZ): 0.8103532 0.3324543 0.2545697
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 404 symmetry adapted cartesian basis functions of A symmetry.
There are 389 symmetry adapted basis functions of A symmetry.
389 basis functions, 625 primitive gaussians, 404 cartesian basis functions
62 alpha electrons 62 beta electrons
nuclear repulsion energy 1072.5928609784 Hartrees.
NAtoms= 24 NActive= 24 NUniq= 24 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 389 RedAO= T EigKep= 6.51D-06 NBF= 389
NBsUse= 389 1.00D-06 EigRej= -1.00D+00 NBFU= 389
Initial guess from the checkpoint file: "./cooh.chk"

B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 0.000831 -0.000047 0.000454 Ang= 0.11 deg.
ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00
Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.
HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=2910765817.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3145.73221779 A.U. after 11 cycles
NFock= 11 Conv=0.73D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000033018	0.000022021	-0.000042286
2	6	-0.000035037	-0.000143604	0.000126517
3	7	-0.000337388	-0.000061789	-0.000076780
4	6	0.000515308	0.000645267	-0.000332338
5	7	-0.000206427	-0.000236938	0.000091520
6	6	0.000222355	0.000072138	-0.000149899
7	1	0.000018155	0.000032226	-0.000041746
8	1	-0.000007384	0.000016101	-0.000012575
9	1	-0.000001467	-0.000038765	0.000049994
10	1	-0.000063818	-0.000020318	0.000021242
11	35	0.000006548	-0.000046216	0.000112183
12	1	-0.000033697	-0.000094766	0.000081863
13	6	0.000148579	-0.000051701	-0.000059840
14	6	-0.000039570	0.000015867	-0.000013152
15	1	-0.000009992	0.000005887	0.000022016
16	1	0.000001085	-0.000003685	0.000000548

17	1	0.000004001	-0.000003194	-0.000008102
18	6	0.000431993	-0.000145112	0.000017457
19	1	0.000002646	0.000125285	0.000036800
20	1	-0.000488181	-0.000099397	0.000192296
21	6	-0.000239534	-0.000061825	-0.000103993
22	8	0.000070285	0.000012928	0.000145022
23	8	0.000053513	0.000045893	-0.000052827
24	1	-0.000044988	0.000013697	-0.000003919

Cartesian Forces: Max 0.000645267 RMS 0.000159638

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000407971 RMS 0.000077470
Search for a local minimum.
Step number 11 out of a maximum of 140
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 5 4 6 7 8
9 10 11
DE= -1.15D-05 DEPred=-9.65D-06 R= 1.19D+00
TightC=F SS= 1.41D+00 RLast= 6.98D-02 DXNew= 1.2000D+00 2.0927D-01
Trust test= 1.19D+00 RLast= 6.98D-02 DXMaxT set to 7.14D-01
ITU= 1 1 1 1 1 0 -1 1 1 1 0

Eigenvalues ---	0.00142	0.00287	0.00391	0.00842	0.01597
Eigenvalues ---	0.01787	0.01986	0.02043	0.02124	0.02192
Eigenvalues ---	0.02353	0.02410	0.02485	0.02789	0.03038
Eigenvalues ---	0.03040	0.03086	0.03510	0.04329	0.04452
Eigenvalues ---	0.04948	0.05451	0.06441	0.07722	0.09668
Eigenvalues ---	0.10446	0.12131	0.13469	0.15599	0.15976
Eigenvalues ---	0.15987	0.15996	0.16000	0.16001	0.16062
Eigenvalues ---	0.16693	0.17856	0.20634	0.21983	0.22847
Eigenvalues ---	0.24459	0.25079	0.27391	0.27766	0.34364
Eigenvalues ---	0.34449	0.35160	0.35492	0.35579	0.35585
Eigenvalues ---	0.35843	0.36077	0.36516	0.36604	0.36652
Eigenvalues ---	0.37258	0.41328	0.43007	0.43818	0.47579
Eigenvalues ---	0.52393	0.53214	0.54050	0.54732	0.59910
Eigenvalues ---	0.92914				

En-DIIS/RFO-DIIS IScMMF= 0 using points: 11 10 9 8 7
RFO step: Lambda=-2.31961220D-06.

DidBck=F Rises=F RFO-DIIS coefs: 1.35286 -0.00594 -1.00066 0.72451 -0.07078

Iteration 1 RMS(Cart)= 0.00819367 RMS(Int)= 0.00003575

Iteration 2 RMS(Cart)= 0.00004859 RMS(Int)= 0.00001768

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001768

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55846	0.00001	0.00008	0.00003	0.00012	2.55859
R2	2.62591	0.00000	0.00002	-0.00004	-0.00001	2.62590
R3	2.03321	0.00000	0.00002	-0.00001	0.00001	2.03322
R4	2.62989	0.00002	-0.00003	-0.00003	-0.00006	2.62982
R5	2.03106	0.00000	0.00000	0.00002	0.00002	2.03108
R6	2.54896	0.00026	-0.00026	0.00022	-0.00005	2.54891
R7	2.68596	-0.00010	0.00055	-0.00003	0.00052	2.68648
R8	2.53198	0.00012	-0.00014	0.00000	-0.00015	2.53183
R9	5.42871	-0.00008	0.00552	0.00078	0.00632	5.43503
R10	2.02676	0.00001	0.00012	0.00002	0.00013	2.02690
R11	2.77449	0.00011	0.00026	0.00009	0.00035	2.77485
R12	2.05739	0.00003	-0.00012	0.00005	-0.00007	2.05732
R13	2.06201	0.00001	0.00007	0.00005	0.00012	2.06213
R14	2.89349	-0.00015	-0.00046	0.00017	-0.00029	2.89320
R15	5.09015	-0.00012	-0.00641	-0.00324	-0.00966	5.08050
R16	5.12463	-0.00010	-0.00118	-0.00466	-0.00584	5.11879
R17	2.50778	0.00003	-0.00008	0.00002	-0.00006	2.50771
R18	2.04985	0.00001	0.00012	0.00007	0.00019	2.05004
R19	2.04360	0.00000	0.00002	0.00000	0.00003	2.04363
R20	2.04770	0.00000	0.00004	0.00002	0.00006	2.04776
R21	2.06661	-0.00009	-0.00058	-0.00003	-0.00061	2.06600
R22	2.07856	0.00000	0.00075	0.00000	0.00076	2.07932
R23	2.84607	-0.00017	0.00007	-0.00045	-0.00038	2.84569
R24	2.28276	0.00015	-0.00031	0.00016	-0.00015	2.28261
R25	2.55130	0.00007	0.00039	0.00007	0.00045	2.55176
R26	1.83190	-0.00005	0.00001	-0.00001	0.00000	1.83190
A1	1.87549	0.00002	-0.00011	-0.00005	-0.00015	1.87535
A2	2.27796	-0.00001	0.00020	0.00004	0.00024	2.27820
A3	2.12971	-0.00001	-0.00010	0.00001	-0.00009	2.12962
A4	1.86913	0.00003	-0.00002	0.00003	0.00001	1.86914
A5	2.28582	0.00000	0.00027	0.00002	0.00029	2.28611
A6	2.12771	-0.00003	-0.00023	-0.00008	-0.00031	2.12740
A7	1.89168	-0.00001	0.00008	0.00004	0.00009	1.89177
A8	2.22677	0.00002	-0.00018	0.00000	-0.00017	2.22660
A9	2.15417	-0.00001	0.00004	-0.00011	-0.00006	2.15410
A10	1.89078	-0.00010	0.00006	-0.00015	-0.00005	1.89073
A11	1.80274	0.00005	-0.00068	0.00014	-0.00056	1.80218

A12	2.18820	0.00003	0.00024	0.00004	0.00040	2.18860
A13	1.88834	0.00014	0.00185	0.00229	0.00414	1.89248
A14	2.19284	0.00005	0.00023	0.00007	0.00042	2.19326
A15	1.89430	0.00004	0.00006	0.00012	0.00017	1.89447
A16	2.20076	0.00000	-0.00024	-0.00009	-0.00032	2.20044
A17	2.17504	-0.00005	0.00027	-0.00007	0.00022	2.17526
A18	1.87786	0.00002	0.00123	-0.00080	0.00043	1.87829
A19	1.88591	0.00001	-0.00035	-0.00038	-0.00072	1.88519
A20	1.94798	-0.00011	-0.00023	-0.00033	-0.00057	1.94742
A21	1.87527	-0.00004	0.00026	-0.00022	0.00004	1.87530
A22	1.92323	0.00001	-0.00095	0.00041	-0.00053	1.92270
A23	1.95053	0.00012	0.00011	0.00123	0.00134	1.95188
A24	1.21751	-0.00019	-0.00293	-0.00200	-0.00494	1.21256
A25	1.35545	-0.00016	-0.00339	-0.00236	-0.00574	1.34971
A26	2.15382	0.00002	-0.00062	0.00000	-0.00062	2.15320
A27	1.95650	0.00000	-0.00021	-0.00020	-0.00041	1.95609
A28	2.17196	-0.00002	0.00082	0.00023	0.00105	2.17301
A29	2.08580	0.00000	0.00013	0.00002	0.00015	2.08595
A30	2.14555	-0.00001	-0.00021	-0.00003	-0.00024	2.14530
A31	2.05184	0.00000	0.00008	0.00001	0.00010	2.05193
A32	1.95284	0.00005	0.00096	0.00052	0.00147	1.95431
A33	1.91429	-0.00020	-0.00172	-0.00064	-0.00236	1.91193
A34	1.93095	0.00014	0.00011	0.00085	0.00093	1.93188
A35	1.85982	0.00001	0.00032	-0.00042	-0.00010	1.85973
A36	1.90142	-0.00005	0.00288	-0.00026	0.00262	1.90404
A37	1.90264	0.00004	-0.00260	-0.00011	-0.00271	1.89993
A38	2.56798	0.00041	0.00553	0.00457	0.01011	2.57810
A39	2.18824	0.00011	-0.00002	0.00023	0.00020	2.18844
A40	1.94975	-0.00012	0.00017	-0.00024	-0.00007	1.94968
A41	2.14518	0.00001	-0.00015	0.00002	-0.00014	2.14504
A42	1.87520	-0.00001	-0.00028	0.00024	-0.00005	1.87515
D1	0.00274	0.00006	0.00038	0.00091	0.00129	0.00403
D2	3.10924	0.00003	0.00092	0.00005	0.00097	3.11021
D3	-3.13095	0.00001	0.00019	0.00052	0.00071	-3.13024
D4	-0.02446	-0.00001	0.00073	-0.00034	0.00039	-0.02407
D5	-0.04933	-0.00009	0.00035	-0.00088	-0.00053	-0.04985
D6	-3.02347	-0.00006	-0.00025	-0.00069	-0.00094	-3.02441
D7	3.08519	-0.00005	0.00052	-0.00053	0.00000	3.08518
D8	0.11105	-0.00002	-0.00008	-0.00034	-0.00042	0.11063
D9	0.04442	-0.00001	-0.00098	-0.00063	-0.00161	0.04281
D10	3.03294	-0.00001	-0.00142	-0.00121	-0.00263	3.03030
D11	-3.06596	0.00001	-0.00147	0.00013	-0.00134	-3.06730
D12	-0.07744	0.00001	-0.00191	-0.00045	-0.00236	-0.07980
D13	-0.07563	-0.00004	0.00121	0.00010	0.00130	-0.07433

D14	1.92448	0.00011	0.00300	0.00269	0.00569	1.93017
D15	-3.06284	0.00011	-0.00446	0.00038	-0.00407	-3.06690
D16	-3.07193	-0.00005	0.00165	0.00063	0.00228	-3.06965
D17	-1.07182	0.00010	0.00344	0.00323	0.00667	-1.06515
D18	0.22404	0.00011	-0.00402	0.00092	-0.00309	0.22096
D19	0.61716	0.00000	0.00570	0.00203	0.00773	0.62489
D20	-2.48060	-0.00001	0.00580	0.00157	0.00738	-2.47322
D21	-2.69869	0.00000	0.00519	0.00139	0.00658	-2.69210
D22	0.48674	-0.00001	0.00530	0.00093	0.00623	0.49297
D23	0.07736	0.00008	-0.00097	0.00048	-0.00049	0.07687
D24	3.05456	0.00005	-0.00044	0.00028	-0.00015	3.05441
D25	-1.86579	0.00000	-0.00110	-0.00072	-0.00182	-1.86761
D26	1.11141	-0.00002	-0.00057	-0.00091	-0.00148	1.10992
D27	3.06405	-0.00008	0.00472	0.00018	0.00489	3.06895
D28	-0.24194	-0.00010	0.00525	-0.00001	0.00523	-0.23670
D29	-2.25160	0.00004	-0.00104	-0.00149	-0.00256	-2.25416
D30	-0.24974	0.00001	-0.00054	-0.00066	-0.00118	-0.25092
D31	-2.90135	0.00002	0.00351	0.00449	0.00799	-2.89336
D32	-0.88146	-0.00002	0.00427	0.00362	0.00789	-0.87357
D33	1.26990	0.00006	0.00403	0.00470	0.00871	1.27861
D34	0.43347	0.00004	0.00285	0.00469	0.00753	0.44101
D35	2.45336	0.00001	0.00361	0.00383	0.00743	2.46079
D36	-1.67847	0.00009	0.00336	0.00490	0.00825	-1.67022
D37	-1.06835	0.00001	-0.00231	-0.00257	-0.00488	-1.07323
D38	0.99166	-0.00008	-0.00243	-0.00318	-0.00561	0.98604
D39	3.09115	-0.00006	-0.00672	-0.00319	-0.00991	3.08124
D40	3.12953	0.00006	-0.00307	-0.00163	-0.00470	3.12483
D41	-1.09365	-0.00003	-0.00319	-0.00224	-0.00543	-1.09909
D42	1.00584	-0.00002	-0.00748	-0.00225	-0.00973	0.99611
D43	1.04583	0.00002	-0.00284	-0.00242	-0.00526	1.04057
D44	3.10584	-0.00006	-0.00296	-0.00303	-0.00600	3.09984
D45	-1.07785	-0.00005	-0.00725	-0.00304	-0.01029	-1.08814
D46	-0.00253	-0.00004	0.00144	0.00086	0.00229	-0.00025
D47	0.36966	-0.00003	0.00155	0.00121	0.00279	0.37244
D48	-3.08878	-0.00001	0.00050	-0.00063	-0.00014	-3.08892
D49	0.04938	0.00000	0.00012	0.00008	0.00020	0.04957
D50	0.00356	0.00000	0.00035	-0.00013	0.00022	0.00378
D51	-3.14147	0.00001	-0.00003	0.00058	0.00056	-3.14092
D52	-0.34862	0.00001	-0.00069	0.00026	-0.00041	-0.34903
D53	1.76837	-0.00004	-0.00032	0.00028	-0.00004	1.76833
D54	-2.46524	-0.00007	0.00191	-0.00031	0.00159	-2.46365
D55	-0.15801	0.00006	-0.01229	-0.00039	-0.01268	-0.17070
D56	2.98865	0.00010	-0.00974	-0.00098	-0.01072	2.97793
D57	-2.31170	-0.00007	-0.01549	-0.00143	-0.01693	-2.32863

D58	0.83497	-0.00002	-0.01294	-0.00201	-0.01497	0.82000
D59	1.94843	-0.00007	-0.01605	-0.00072	-0.01676	1.93167
D60	-1.18809	-0.00003	-0.01350	-0.00131	-0.01480	-1.20289
D61	3.09703	-0.00003	-0.00570	0.00060	-0.00509	3.09194
D62	-0.03964	0.00001	-0.00322	0.00004	-0.00319	-0.04282

Item	Value	Threshold	Converged?
Maximum Force	0.000408	0.000450	YES
RMS Force	0.000077	0.000300	YES
Maximum Displacement	0.040215	0.001800	NO
RMS Displacement	0.008203	0.001200	NO

Predicted change in Energy=-6.099434D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.320561	-2.207771	-0.395800
2	6	0	-1.573348	-1.767376	-0.659888
3	7	0	-1.808038	-0.677742	0.173352
4	6	0	-0.688297	-0.438175	0.886177
5	7	0	0.206354	-1.393282	0.599122
6	6	0	1.587460	-1.419891	1.097115
7	1	0	0.241378	-3.017557	-0.827200
8	1	0	-2.302813	-2.103561	-1.374074
9	1	0	1.613235	-0.855005	2.027426
10	1	0	1.840407	-2.454325	1.335343
11	35	0	0.261585	2.052017	-0.194833
12	1	0	-0.589256	0.299800	1.658205
13	6	0	-2.934648	0.189294	0.170059
14	6	0	-4.170080	-0.220209	-0.088807
15	1	0	-2.656092	1.220468	0.359675
16	1	0	-4.974543	0.501732	-0.122804
17	1	0	-4.419699	-1.258297	-0.274040
18	6	0	2.562898	-0.813871	0.084562
19	1	0	2.573154	-1.369744	-0.856799
20	1	0	2.249060	0.211893	-0.160463
21	6	0	3.958649	-0.774252	0.648454
22	8	0	4.256168	-1.004540	1.796271
23	8	0	4.867508	-0.435747	-0.291112
24	1	0	5.731490	-0.384634	0.145533

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.353945	0.000000			
3	N	2.208508	1.391643	0.000000		
4	C	2.215890	2.222703	1.348826	0.000000	
5	N	1.389568	2.211875	2.179691	1.339788	0.000000
6	C	2.547566	3.632976	3.596321	2.487434	1.468386
7	H	1.075935	2.210018	3.267406	3.233137	2.161918
8	H	2.212963	1.074803	2.161548	3.238659	3.270155
9	H	3.382538	4.267129	3.895397	2.602546	2.075839
10	H	2.779825	4.013300	4.221093	3.265112	2.082778
11	Br	4.304077	4.262748	3.445357	2.876094	3.536029
12	H	3.252545	3.258099	2.155413	1.072587	2.149693
13	C	3.591597	2.523986	1.421624	2.439803	3.543238
14	C	4.343207	3.076178	2.420187	3.622281	4.582851
15	H	4.216428	3.337522	2.087370	2.626884	3.883635
16	H	5.392168	4.123764	3.391994	4.502596	5.563627
17	H	4.209425	2.917148	2.712560	3.992752	4.709671
18	C	3.238525	4.309514	4.373957	3.369571	2.480683
19	H	3.047687	4.170176	4.553561	3.813509	2.778849
20	H	3.537387	4.333328	4.166884	3.185296	2.706696
21	C	4.632179	5.770706	5.787030	4.665144	3.803334
22	O	5.215303	6.371647	6.286116	5.059325	4.240905
23	O	5.483346	6.587401	6.696058	5.679171	4.841048
24	H	6.343830	7.478057	7.545274	6.462591	5.634735

		6	7	8	9	10
6	C	0.000000				
7	H	2.840328	0.000000			
8	H	4.659227	2.758146	0.000000		
9	H	1.088687	3.835038	5.335215	0.000000	
10	H	1.091233	2.747858	4.962887	1.757387	0.000000
11	Br	3.934618	5.108902	5.023503	3.900791	5.014104
12	H	2.830239	4.227535	4.231683	2.514134	3.686830
13	C	4.888596	4.622290	2.835621	5.022312	5.581019
14	C	5.999576	5.275542	2.947136	6.190972	6.568518
15	H	5.052034	5.269237	3.765615	5.031514	5.888509
16	H	6.945553	6.331461	3.935908	7.061377	7.570205
17	H	6.163776	5.012646	2.530959	6.469597	6.573396
18	C	1.531014	3.328213	5.240808	2.162931	2.185758
19	H	2.189038	2.855406	4.957935	3.083043	2.553179
20	H	2.163777	3.860657	5.249165	2.515830	3.084339
21	C	2.498136	4.585639	6.712942	2.721957	2.789518
22	O	2.789863	5.201286	7.367439	2.657233	2.854861
23	O	3.695190	5.324868	7.440962	4.017672	3.985392

24	H	4.376099	6.166021	8.355473	4.552229	4.565062
		11	12	13	14	15
11	Br	0.000000				
12	H	2.688484	0.000000			
13	C	3.717363	2.779866	0.000000		
14	C	4.981356	4.018054	1.327025	0.000000	
15	H	3.084120	2.608758	1.084834	2.137485	0.000000
16	H	5.461283	4.737458	2.084360	1.081441	2.474789
17	H	5.734011	4.564376	2.120878	1.083628	3.107439
18	C	3.686112	3.694956	5.588978	6.761323	5.608216
19	H	4.182105	4.371895	5.815576	6.883491	5.961042
20	H	2.708745	3.372139	5.194284	6.434066	5.034708
21	C	4.729399	4.780860	6.976735	8.180877	6.914991
22	O	5.409596	5.019811	7.468443	8.670083	7.402284
23	O	5.235720	5.840988	7.840727	9.042421	7.731179
24	H	5.997748	6.535171	8.685156	9.905707	8.542467
		16	17	18	19	20
16	H	0.000000				
17	H	1.851601	0.000000			
18	C	7.654204	7.005910	0.000000		
19	H	7.810820	7.017979	1.093279	0.000000	
20	H	7.229514	6.829840	1.100329	1.758265	0.000000
21	C	9.056759	8.442868	1.505877	2.130726	2.132961
22	O	9.547655	8.923074	2.415256	3.163019	3.055650
23	O	9.888031	9.323578	2.365446	2.540947	2.700514
24	H	10.746012	10.197351	3.198114	3.456905	3.546377
		21	22	23	24	
21	C	0.000000				
22	O	1.207904	0.000000			
23	O	1.350332	2.248206	0.000000		
24	H	1.883533	2.299085	0.969400	0.000000	

Stoichiometry C8H11BrN2O2

Framework group C1[X(C8H11BrN2O2)]

Deg. of freedom 66

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.643592	-2.140649	-0.766632
2	6	0	-1.955460	-1.818647	-0.858738

3	7	0	-2.212271	-0.864606	0.121325
4	6	0	-1.054809	-0.581639	0.753419
5	7	0	-0.102006	-1.389811	0.269624
6	6	0	1.318870	-1.315380	0.632571
7	1	0	-0.049811	-2.826880	-1.344686
8	1	0	-2.717088	-2.152375	-1.539728
9	1	0	1.383452	-0.860621	1.619618
10	1	0	1.699587	-2.334605	0.716380
11	35	0	-0.481974	2.107119	-0.091779
12	1	0	-0.951898	0.070283	1.598907
13	6	0	-3.415766	-0.136782	0.328421
14	6	0	-4.623087	-0.652226	0.134289
15	1	0	-3.225812	0.891137	0.618533
16	1	0	-5.496248	-0.027436	0.263677
17	1	0	-4.783252	-1.684174	-0.154986
18	6	0	2.116613	-0.491124	-0.381436
19	1	0	2.085607	-0.931629	-1.381563
20	1	0	1.675835	0.513382	-0.467492
21	6	0	3.552067	-0.357148	0.053518
22	8	0	3.989360	-0.680975	1.131917
23	8	0	4.318868	0.187203	-0.915550
24	1	0	5.213824	0.286425	-0.556461

Rotational constants (GHZ): 0.8085345 0.3329069 0.2546721

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 404 symmetry adapted cartesian basis functions of A symmetry.

There are 389 symmetry adapted basis functions of A symmetry.

389 basis functions, 625 primitive gaussians, 404 cartesian basis functions

62 alpha electrons 62 beta electrons

nuclear repulsion energy 1072.4596187701 Hartrees.

NAtoms= 24 NActive= 24 NUniq= 24 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 389 RedAO= T EigKep= 6.53D-06 NBF= 389

NBsUse= 389 1.00D-06 EigRej= -1.00D+00 NBFU= 389

Initial guess from the checkpoint file: "./cooh.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000682 -0.000072 0.000530 Ang= 0.10 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14
ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000
FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0
NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T
wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid=
0
NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0
NMtDT0= 0
Petite list used in FoFCou.
Keep R1 ints in memory in canonical form, NReq=2910765817.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3145.73222559 A.U. after 10 cycles
NFock= 10 Conv=0.74D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1
NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000045635	-0.000036953	0.000037511
2	6	-0.000008401	-0.000066859	0.000072213
3	7	-0.000278726	-0.000053751	-0.000021873
4	6	0.000436624	0.000592307	-0.000343506
5	7	-0.000104610	-0.000205113	0.000059156
6	6	0.000147407	0.000031453	-0.000142270
7	1	0.000006378	0.000014337	-0.000024137
8	1	0.000012989	0.000022725	-0.000035901
9	1	-0.000011181	-0.000040200	0.000082578
10	1	-0.000027231	0.000009611	-0.000002469
11	35	0.000037037	-0.000032690	0.000076827
12	1	-0.000059972	-0.000158946	0.000103357
13	6	0.000140436	-0.000081694	-0.000020863
14	6	-0.000027605	0.000021701	-0.000015996
15	1	-0.000020303	-0.000002459	0.000026417
16	1	0.000005159	-0.000000858	-0.000007052
17	1	-0.000002233	0.000002223	-0.000013720
18	6	0.000294664	0.000227224	0.000093430
19	1	0.000056538	-0.000009441	-0.000015256
20	1	-0.000421026	-0.000163268	0.000108333
21	6	-0.000088195	-0.000048968	-0.000239403

```
      22        8             0.000049377    -0.000041492     0.000213252
      23        8            -0.000050284     0.000058090     0.000017662
      24        1            -0.000041208    -0.000036978    -0.000008290
 ---------------------------------------------------------------------
 Cartesian Forces:  Max        0.000592307 RMS        0.000141286

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 GSVD:  received Info=                1 from GESDD.
 Internal  Forces:  Max        0.000326055 RMS        0.000063369
 Search for a local minimum.
 Step number  12 out of a maximum of  140
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swapping is turned off.
 Update second derivatives using D2CorX and points      4      6      7      8      9
                                                       10     11     12
 DE= -7.80D-06 DEPred=-6.10D-06 R= 1.28D+00
 TightC=F SS=  1.41D+00  RLast= 5.44D-02 DXNew= 1.2000D+00 1.6315D-01
 Trust test= 1.28D+00 RLast= 5.44D-02 DXMaxT set to 7.14D-01
 ITU=  1  1  1  1  1  1  0 -1  1  1  1  0
      Eigenvalues ---      0.00138     0.00255     0.00390     0.00764     0.01591
      Eigenvalues ---      0.01687     0.01826     0.02004     0.02157     0.02338
      Eigenvalues ---      0.02366     0.02430     0.02500     0.02923     0.03039
      Eigenvalues ---      0.03042     0.03121     0.03723     0.04019     0.04423
      Eigenvalues ---      0.04966     0.05376     0.06420     0.07470     0.09682
      Eigenvalues ---      0.09936     0.11956     0.12715     0.15604     0.15945
      Eigenvalues ---      0.15991     0.15997     0.16000     0.16002     0.16038
      Eigenvalues ---      0.16703     0.17840     0.20494     0.21979     0.22860
      Eigenvalues ---      0.24451     0.25007     0.27261     0.27757     0.34365
      Eigenvalues ---      0.34431     0.35167     0.35493     0.35579     0.35624
      Eigenvalues ---      0.35843     0.36071     0.36589     0.36649     0.36972
      Eigenvalues ---      0.37440     0.41331     0.42887     0.43552     0.47371
      Eigenvalues ---      0.52361     0.53281     0.54079     0.54750     0.59903
      Eigenvalues ---      0.93976
 En-DIIS/RFO-DIIS IScMMF=              0 using points:      12     11     10      9      8
 RFO step:  Lambda=-1.72187117D-06.
 DidBck=F Rises=F RFO-DIIS coefs:         2.53945      -1.50964      -0.55485       1.05383      -
0.52879
 Iteration  1 RMS(Cart)=  0.01002892 RMS(Int)=  0.00003431
 Iteration  2 RMS(Cart)=  0.00005717 RMS(Int)=  0.00000762
 Iteration  3 RMS(Cart)=  0.00000000 RMS(Int)=  0.00000762
```

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55859	-0.00001	0.00008	-0.00003	0.00004	2.55862
R2	2.62590	0.00001	-0.00003	0.00004	0.00000	2.62591
R3	2.03322	0.00000	0.00000	0.00001	0.00002	2.03324
R4	2.62982	0.00001	-0.00003	-0.00004	-0.00007	2.62976
R5	2.03108	0.00000	0.00003	0.00001	0.00004	2.03112
R6	2.54891	0.00018	0.00048	-0.00007	0.00042	2.54933
R7	2.68648	-0.00011	0.00008	0.00004	0.00013	2.68661
R8	2.53183	0.00009	0.00007	0.00001	0.00009	2.53192
R9	5.43503	-0.00007	0.00053	0.00081	0.00133	5.43636
R10	2.02690	-0.00002	0.00011	-0.00017	-0.00006	2.02683
R11	2.77485	0.00006	0.00044	0.00016	0.00060	2.77545
R12	2.05732	0.00005	0.00007	0.00011	0.00018	2.05750
R13	2.06213	-0.00002	0.00011	-0.00011	0.00000	2.06213
R14	2.89320	-0.00009	-0.00026	-0.00048	-0.00074	2.89246
R15	5.08050	-0.00005	-0.00917	-0.00088	-0.01004	5.07046
R16	5.11879	-0.00010	-0.00854	-0.00535	-0.01389	5.10489
R17	2.50771	0.00002	0.00004	-0.00005	-0.00002	2.50770
R18	2.05004	0.00000	0.00016	0.00001	0.00017	2.05021
R19	2.04363	0.00000	0.00001	0.00000	0.00001	2.04364
R20	2.04776	0.00000	0.00005	0.00001	0.00005	2.04781
R21	2.06600	0.00002	-0.00047	0.00015	-0.00032	2.06568
R22	2.07932	-0.00008	0.00042	0.00005	0.00048	2.07980
R23	2.84569	-0.00014	-0.00099	0.00016	-0.00083	2.84487
R24	2.28261	0.00022	0.00014	-0.00002	0.00012	2.28273
R25	2.55176	-0.00005	0.00036	-0.00011	0.00026	2.55201
R26	1.83190	-0.00005	-0.00009	0.00000	-0.00009	1.83181
A1	1.87535	0.00003	-0.00013	0.00004	-0.00009	1.87525
A2	2.27820	-0.00001	0.00014	0.00005	0.00020	2.27840
A3	2.12962	-0.00001	-0.00002	-0.00010	-0.00011	2.12951
A4	1.86914	0.00002	0.00011	-0.00005	0.00006	1.86920
A5	2.28611	-0.00001	0.00018	0.00000	0.00018	2.28630
A6	2.12740	-0.00001	-0.00030	0.00004	-0.00026	2.12714
A7	1.89177	0.00000	0.00001	0.00007	0.00009	1.89186
A8	2.22660	0.00002	-0.00006	-0.00005	-0.00012	2.22648
A9	2.15410	-0.00002	-0.00019	-0.00003	-0.00022	2.15388
A10	1.89073	-0.00007	-0.00029	0.00000	-0.00031	1.89041
A11	1.80218	0.00002	0.00029	0.00000	0.00031	1.80248
A12	2.18860	0.00002	0.00019	-0.00003	0.00012	2.18872
A13	1.89248	0.00011	0.00491	0.00175	0.00664	1.89912
A14	2.19326	0.00003	0.00020	-0.00011	0.00006	2.19332
A15	1.89447	0.00002	0.00029	-0.00004	0.00026	1.89472
A16	2.20044	0.00003	-0.00028	0.00009	-0.00020	2.20024

A17	2.17526	-0.00005	0.00008	-0.00008	-0.00001	2.17525
A18	1.87829	0.00002	-0.00054	0.00127	0.00073	1.87903
A19	1.88519	0.00002	-0.00081	-0.00001	-0.00081	1.88438
A20	1.94742	-0.00009	-0.00067	-0.00027	-0.00096	1.94646
A21	1.87530	-0.00004	-0.00037	-0.00001	-0.00038	1.87492
A22	1.92270	0.00002	0.00005	-0.00030	-0.00024	1.92245
A23	1.95188	0.00008	0.00224	-0.00060	0.00165	1.95352
A24	1.21256	-0.00015	-0.00445	-0.00146	-0.00593	1.20663
A25	1.34971	-0.00013	-0.00515	-0.00168	-0.00685	1.34286
A26	2.15320	0.00004	-0.00016	-0.00012	-0.00028	2.15291
A27	1.95609	0.00000	-0.00045	0.00001	-0.00043	1.95566
A28	2.17301	-0.00004	0.00064	0.00007	0.00071	2.17372
A29	2.08595	-0.00001	0.00012	-0.00006	0.00006	2.08601
A30	2.14530	0.00001	-0.00017	0.00003	-0.00014	2.14517
A31	2.05193	0.00000	0.00005	0.00002	0.00007	2.05201
A32	1.95431	0.00004	0.00160	-0.00071	0.00088	1.95519
A33	1.91193	-0.00014	-0.00237	-0.00023	-0.00258	1.90936
A34	1.93188	0.00007	0.00161	-0.00028	0.00134	1.93322
A35	1.85973	0.00002	-0.00067	0.00044	-0.00024	1.85949
A36	1.90404	-0.00009	0.00123	-0.00006	0.00116	1.90520
A37	1.89993	0.00010	-0.00161	0.00092	-0.00068	1.89925
A38	2.57810	0.00033	0.01020	0.00356	0.01376	2.59186
A39	2.18844	0.00006	0.00055	-0.00015	0.00040	2.18884
A40	1.94968	-0.00012	-0.00055	0.00009	-0.00046	1.94922
A41	2.14504	0.00006	-0.00001	0.00006	0.00005	2.14509
A42	1.87515	-0.00002	0.00009	-0.00022	-0.00013	1.87502
D1	0.00403	0.00000	-0.00004	-0.00014	-0.00018	0.00385
D2	3.11021	0.00000	-0.00033	-0.00017	-0.00051	3.10970
D3	-3.13024	0.00000	0.00049	0.00007	0.00056	-3.12968
D4	-0.02407	0.00000	0.00020	0.00004	0.00023	-0.02383
D5	-0.04985	-0.00003	-0.00011	0.00033	0.00022	-0.04964
D6	-3.02441	-0.00001	-0.00065	0.00055	-0.00010	-3.02451
D7	3.08518	-0.00003	-0.00059	0.00014	-0.00045	3.08474
D8	0.11063	0.00000	-0.00112	0.00035	-0.00076	0.10987
D9	0.04281	0.00003	0.00017	-0.00009	0.00007	0.04288
D10	3.03030	0.00002	-0.00160	-0.00014	-0.00174	3.02857
D11	-3.06730	0.00003	0.00042	-0.00006	0.00035	-3.06694
D12	-0.07980	0.00002	-0.00135	-0.00011	-0.00146	-0.08126
D13	-0.07433	-0.00004	-0.00023	0.00030	0.00008	-0.07425
D14	1.93017	0.00007	0.00534	0.00229	0.00762	1.93779
D15	-3.06690	0.00009	-0.00029	0.00130	0.00100	-3.06590
D16	-3.06965	-0.00004	0.00144	0.00035	0.00179	-3.06786
D17	-1.06515	0.00007	0.00700	0.00233	0.00933	-1.05582
D18	0.22096	0.00010	0.00137	0.00135	0.00271	0.22367

D19	0.62489	-0.00002	0.00579	-0.00044	0.00536	0.63025
D20	-2.47322	-0.00001	0.00505	0.00047	0.00552	-2.46770
D21	-2.69210	-0.00003	0.00380	-0.00048	0.00332	-2.68878
D22	0.49297	-0.00002	0.00306	0.00043	0.00348	0.49645
D23	0.07687	0.00004	0.00021	-0.00039	-0.00019	0.07669
D24	3.05441	0.00003	0.00069	-0.00058	0.00010	3.05451
D25	-1.86761	0.00000	-0.00237	-0.00125	-0.00364	-1.87125
D26	1.10992	-0.00001	-0.00189	-0.00144	-0.00335	1.10658
D27	3.06895	-0.00009	0.00028	-0.00139	-0.00111	3.06784
D28	-0.23670	-0.00010	0.00076	-0.00158	-0.00082	-0.23752
D29	-2.25416	0.00002	-0.00304	-0.00090	-0.00395	-2.25811
D30	-0.25092	0.00000	-0.00122	-0.00017	-0.00139	-0.25231
D31	-2.89336	0.00004	0.00961	0.00427	0.01388	-2.87947
D32	-0.87357	0.00001	0.00849	0.00491	0.01340	-0.86017
D33	1.27861	0.00006	0.01031	0.00398	0.01429	1.29290
D34	0.44101	0.00006	0.00899	0.00451	0.01350	0.45450
D35	2.46079	0.00003	0.00786	0.00515	0.01302	2.47381
D36	-1.67022	0.00008	0.00969	0.00421	0.01390	-1.65631
D37	-1.07323	-0.00001	-0.00518	-0.00216	-0.00733	-1.08056
D38	0.98604	-0.00006	-0.00655	-0.00220	-0.00875	0.97729
D39	3.08124	0.00002	-0.00902	-0.00138	-0.01040	3.07085
D40	3.12483	0.00001	-0.00410	-0.00338	-0.00747	3.11736
D41	-1.09909	-0.00004	-0.00547	-0.00342	-0.00889	-1.10797
D42	0.99611	0.00004	-0.00794	-0.00260	-0.01054	0.98558
D43	1.04057	-0.00001	-0.00511	-0.00278	-0.00790	1.03267
D44	3.09984	-0.00005	-0.00649	-0.00282	-0.00931	3.09053
D45	-1.08814	0.00003	-0.00895	-0.00200	-0.01096	-1.09910
D46	-0.00025	-0.00004	0.00197	0.00039	0.00236	0.00212
D47	0.37244	-0.00003	0.00280	0.00056	0.00337	0.37582
D48	-3.08892	0.00001	-0.00073	0.00145	0.00072	-3.08819
D49	0.04957	0.00000	0.00018	0.00015	0.00033	0.04990
D50	0.00378	0.00000	0.00008	0.00043	0.00051	0.00429
D51	-3.14092	0.00000	0.00099	-0.00087	0.00011	-3.14080
D52	-0.34903	0.00001	0.00021	0.00020	0.00041	-0.34862
D53	1.76833	-0.00001	0.00039	-0.00052	-0.00013	1.76821
D54	-2.46365	-0.00005	0.00063	0.00011	0.00076	-2.46289
D55	-0.17070	0.00004	-0.00853	0.00107	-0.00746	-0.17816
D56	2.97793	0.00004	-0.00724	0.00070	-0.00654	2.97139
D57	-2.32863	0.00000	-0.01248	0.00220	-0.01027	-2.33889
D58	0.82000	0.00000	-0.01118	0.00183	-0.00935	0.81065
D59	1.93167	-0.00003	-0.01144	0.00120	-0.01024	1.92143
D60	-1.20289	-0.00003	-0.01015	0.00083	-0.00933	-1.21221
D61	3.09194	0.00003	-0.00249	0.00055	-0.00194	3.09000
D62	-0.04282	0.00003	-0.00123	0.00018	-0.00105	-0.04387

Item	Value	Threshold	Converged?
Maximum Force	0.000326	0.000450	YES
RMS Force	0.000063	0.000300	YES
Maximum Displacement	0.038628	0.001800	NO
RMS Displacement	0.010034	0.001200	NO

Predicted change in Energy=-3.909131D-06

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.325079	-2.217198	-0.393506
2	6	0	-1.576444	-1.772740	-0.657636
3	7	0	-1.805825	-0.679227	0.171934
4	6	0	-0.684136	-0.441333	0.882670
5	7	0	0.206295	-1.401059	0.597685
6	6	0	1.588231	-1.431570	1.094083
7	1	0	0.233427	-3.030435	-0.822894
8	1	0	-2.308172	-2.108254	-1.369852
9	1	0	1.615467	-0.875446	2.029726
10	1	0	1.840994	-2.468232	1.322631
11	35	0	0.263465	2.052526	-0.193752
12	1	0	-0.581477	0.298415	1.652481
13	6	0	-2.928219	0.193352	0.165444
14	6	0	-4.166300	-0.212347	-0.086613
15	1	0	-2.643527	1.224527	0.346258
16	1	0	-4.967441	0.513096	-0.124422
17	1	0	-4.421201	-1.250747	-0.262854
18	6	0	2.560852	-0.815013	0.085781
19	1	0	2.576000	-1.365503	-0.858474
20	1	0	2.238112	0.209508	-0.153952
21	6	0	3.955237	-0.765164	0.651070
22	8	0	4.253076	-0.988864	1.800174
23	8	0	4.862858	-0.424314	-0.289039
24	1	0	5.725777	-0.364752	0.148531

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.353966	0.000000			
3	N	2.208549	1.391608	0.000000		
4	C	2.216133	2.222926	1.349047	0.000000	

5	N	1.389569	2.211818	2.179664	1.339835	0.000000
6	C	2.547722	3.633192	3.596664	2.487753	1.468703
7	H	1.075945	2.210145	3.267478	3.233314	2.161862
8	H	2.213092	1.074824	2.161383	3.238823	3.270149
9	H	3.382022	4.267944	3.898093	2.606216	2.076722
10	H	2.774890	4.010493	4.221840	3.267747	2.082461
11	Br	4.314723	4.270025	3.446472	2.876797	3.543571
12	H	3.252708	3.258263	2.155651	1.072555	2.149741
13	C	3.591589	2.523940	1.421691	2.439907	3.543184
14	C	4.343799	3.077051	2.420054	3.621796	4.582672
15	H	4.215202	3.336177	2.087202	2.627173	3.883092
16	H	5.392442	4.124102	3.391942	4.502429	5.563539
17	H	4.210619	2.919070	2.712170	3.991620	4.709229
18	C	3.244139	4.311279	4.369637	3.362233	2.479805
19	H	3.059058	4.177196	4.553362	3.809745	2.781576
20	H	3.537829	4.328261	4.153249	3.168234	2.699474
21	C	4.639035	5.772991	5.781591	4.656424	3.802865
22	O	5.223078	6.374841	6.281507	5.051501	4.241736
23	O	5.489994	6.589289	6.689456	5.669421	4.839824
24	H	6.351237	7.480292	7.538201	6.452271	5.633857

		6	7	8	9	10
6	C	0.000000				
7	H	2.840187	0.000000			
8	H	4.659488	2.758497	0.000000		
9	H	1.088781	3.832943	5.335905	0.000000	
10	H	1.091234	2.739274	4.959297	1.757218	0.000000
11	Br	3.943660	5.121837	5.030767	3.917242	5.022477
12	H	2.830598	4.227622	4.231787	2.519290	3.692086
13	C	4.888871	4.622296	2.835310	5.026227	5.582876
14	C	5.999597	5.276488	2.948526	6.192529	6.569822
15	H	5.051917	5.267683	3.763632	5.038152	5.890730
16	H	6.945740	6.331943	3.936278	7.064211	7.572124
17	H	6.163379	5.014628	2.534888	6.468240	6.573516
18	C	1.530623	3.339265	5.243923	2.162481	2.186579
19	H	2.189185	2.874180	4.966721	3.082933	2.552149
20	H	2.161729	3.868265	5.245867	2.516596	3.083552
21	C	2.498615	4.599554	6.717016	2.717973	2.796687
22	O	2.792124	5.215945	7.372386	2.650008	2.869620
23	O	3.694696	5.339335	7.444963	4.015687	3.988326
24	H	4.376237	6.181864	8.360001	4.549104	4.571069

		11	12	13	14	15
11	Br	0.000000				
12	H	2.683172	0.000000			
13	C	3.711118	2.780200	0.000000		

14	C	4.976339	4.016999	1.327015	0.000000	
15	H	3.070472	2.610738	1.084926	2.137948	0.000000
16	H	5.453167	4.737103	2.084391	1.081445	2.475530
17	H	5.732581	4.562005	2.120815	1.083656	3.107752
18	C	3.684957	3.683544	5.581491	6.756293	5.595814
19	H	4.180024	4.363849	5.811614	6.883614	5.950050
20	H	2.701394	3.349803	5.176219	6.418643	5.011075
21	C	4.720412	4.766109	6.966818	8.173686	6.898947
22	O	5.398407	5.005178	7.459288	8.663073	7.387564
23	O	5.224771	5.825171	7.828725	9.033914	7.711556
24	H	5.983079	6.517906	8.671989	9.896044	8.521159

		16	17	18	19	20
16	H	0.000000				
17	H	1.851670	0.000000			
18	C	7.647434	7.004318	0.000000		
19	H	7.808422	7.023443	1.093109	0.000000	
20	H	7.212005	6.818405	1.100580	1.758175	0.000000
21	C	9.047072	8.440128	1.505439	2.131063	2.132268
22	O	9.538233	8.920075	2.415158	3.165889	3.052013
23	O	9.876265	9.320806	2.364819	2.537679	2.703567
24	H	10.732661	10.193889	3.197408	3.454947	3.547545

		21	22	23	24
21	C	0.000000			
22	O	1.207969	0.000000		
23	O	1.350467	2.248414	0.000000	
24	H	1.883530	2.299193	0.969352	0.000000

Stoichiometry C8H11BrN2O2
Framework group C1[X(C8H11BrN2O2)]
Deg. of freedom 66
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.651296	-2.150851	-0.763988
2	6	0	-1.961691	-1.822505	-0.854968
3	7	0	-2.211680	-0.862645	0.121119
4	6	0	-1.051393	-0.582481	0.749743
5	7	0	-0.103814	-1.397801	0.267555
6	6	0	1.318502	-1.329151	0.627268
7	1	0	-0.061946	-2.842427	-1.340223

8	1	0	-2.726489	-2.155138	-1.532970
9	1	0	1.387469	-0.883042	1.618063
10	1	0	1.696585	-2.350096	0.701540
11	35	0	-0.476785	2.107677	-0.092184
12	1	0	-0.943580	0.072143	1.592487
13	6	0	-3.410505	-0.126363	0.325842
14	6	0	-4.621132	-0.637185	0.140337
15	1	0	-3.213446	0.903081	0.605978
16	1	0	-5.490602	-0.006584	0.266386
17	1	0	-4.787511	-1.670939	-0.138912
18	6	0	2.113483	-0.497206	-0.382027
19	1	0	2.084984	-0.932024	-1.384528
20	1	0	1.666211	0.505172	-0.462424
21	6	0	3.547253	-0.355629	0.054557
22	8	0	3.984589	-0.673200	1.134870
23	8	0	4.312735	0.189122	-0.915517
24	1	0	5.206321	0.295146	-0.555090

Rotational constants (GHZ): 0.8070445 0.3336174 0.2548708

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 404 symmetry adapted cartesian basis functions of A symmetry.

There are 389 symmetry adapted basis functions of A symmetry.

389 basis functions, 625 primitive gaussians, 404 cartesian basis functions

62 alpha electrons 62 beta electrons

nuclear repulsion energy 1072.5087004791 Hartrees.

NAtoms= 24 NActive= 24 NUniq= 24 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 389 RedAO= T EigKep= 6.55D-06 NBF= 389

NBsUse= 389 1.00D-06 EigRej= -1.00D+00 NBFU= 389

Initial guess from the checkpoint file: "./cooh.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000290 -0.000182 0.000625 Ang= 0.08 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid=

0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Keep R1 ints in memory in canonical form, NReq=2910765817.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3145.73223531 A.U. after 10 cycles

NFock= 10 Conv=0.75D-08 -V/T= 2.0017

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000020467	-0.000001167	-0.000014396
2	6	-0.000040438	-0.000059842	0.000077635
3	7	-0.000073720	0.000044830	0.000000368
4	6	0.000180088	0.000304747	-0.000263346
5	7	0.000023304	-0.000171222	0.000151638
6	6	-0.000036869	-0.000033791	-0.000021789
7	1	0.000006761	0.000007895	-0.000017428
8	1	0.000020632	0.000008666	-0.000027101
9	1	-0.000048497	-0.000050245	0.000047067
10	1	0.000012675	0.000007880	-0.000035123
11	35	0.000063846	0.000021020	0.000012728
12	1	-0.000057736	-0.000141693	0.000107713
13	6	0.000075972	-0.000048636	-0.000016549
14	6	-0.000009505	0.000009122	-0.000048602
15	1	-0.000022453	-0.000009636	0.000037687
16	1	0.000000288	-0.000001228	0.000014006
17	1	-0.000008267	0.000006522	-0.000009882
18	6	0.000093750	0.000374590	0.000016957
19	1	0.000054862	-0.000084997	-0.000044888
20	1	-0.000226021	-0.000112757	0.000019553
21	6	0.000091094	-0.000011431	-0.000190647
22	8	0.000004257	-0.000046851	0.000101477
23	8	-0.000092511	0.000026893	0.000101908
24	1	0.000008954	-0.000038667	0.000001015

Cartesian Forces: Max 0.000374590 RMS 0.000094090

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.

Internal Forces: Max 0.000147481 RMS 0.000037177

Search for a local minimum.

Step number 13 out of a maximum of 140

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 4 6 7 8 9
10 11 12 13

DE= -9.72D-06 DEPred=-3.91D-06 R= 2.49D+00

TightC=F SS= 1.41D+00 RLast= 5.75D-02 DXNew= 1.2000D+00 1.7239D-01

Trust test= 2.49D+00 RLast= 5.75D-02 DXMaxT set to 7.14D-01

ITU= 1 1 1 1 1 1 1 0 -1 1 1 1 0

Eigenvalues ---	0.00137	0.00247	0.00386	0.00564	0.01343
Eigenvalues ---	0.01617	0.01815	0.02007	0.02169	0.02303
Eigenvalues ---	0.02358	0.02421	0.02619	0.02959	0.03039
Eigenvalues ---	0.03048	0.03140	0.03648	0.04215	0.04628
Eigenvalues ---	0.05017	0.05306	0.06381	0.07192	0.09551
Eigenvalues ---	0.09723	0.11276	0.12664	0.15591	0.15892
Eigenvalues ---	0.15992	0.15994	0.16000	0.16003	0.16014
Eigenvalues ---	0.16705	0.17880	0.20559	0.21930	0.22856
Eigenvalues ---	0.24433	0.25030	0.27497	0.27977	0.34378
Eigenvalues ---	0.34520	0.35169	0.35439	0.35496	0.35579
Eigenvalues ---	0.35843	0.36024	0.36583	0.36648	0.36722
Eigenvalues ---	0.37891	0.41329	0.42567	0.43540	0.47335
Eigenvalues ---	0.52342	0.53553	0.54182	0.54491	0.59901
Eigenvalues ---	0.92940				

En-DIIS/RFO-DIIS IScMMF= 0 using points: 13 12 11 10 9

RFO step: Lambda=-8.21935289D-07.

DidBck=F Rises=F RFO-DIIS coefs: 2.38058 -2.15848 0.40168 0.54831 -0.17209

Iteration 1 RMS(Cart)= 0.00905450 RMS(Int)= 0.00002757

Iteration 2 RMS(Cart)= 0.00003818 RMS(Int)= 0.00001369

Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00001369

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55862	0.00000	-0.00002	0.00003	0.00000	2.55863
R2	2.62591	0.00000	0.00000	0.00000	0.00000	2.62590
R3	2.03324	0.00000	0.00001	0.00001	0.00003	2.03327

R4	2.62976	0.00001	-0.00008	0.00007	-0.00001	2.62975
R5	2.03112	0.00000	0.00004	-0.00004	0.00000	2.03113
R6	2.54933	0.00004	0.00039	-0.00004	0.00037	2.54970
R7	2.68661	-0.00005	-0.00015	0.00007	-0.00008	2.68653
R8	2.53192	0.00006	0.00011	0.00017	0.00028	2.53220
R9	5.43636	-0.00001	-0.00037	0.00112	0.00074	5.43710
R10	2.02683	-0.00002	-0.00021	0.00010	-0.00012	2.02672
R11	2.77545	-0.00006	0.00046	-0.00033	0.00013	2.77558
R12	2.05750	0.00002	0.00030	-0.00015	0.00016	2.05765
R13	2.06213	-0.00002	-0.00012	0.00004	-0.00008	2.06206
R14	2.89246	0.00008	-0.00062	0.00077	0.00016	2.89262
R15	5.07046	0.00003	-0.00497	0.00123	-0.00374	5.06672
R16	5.10489	-0.00008	-0.01394	-0.00326	-0.01719	5.08771
R17	2.50770	0.00002	-0.00001	0.00007	0.00005	2.50775
R18	2.05021	-0.00001	0.00009	0.00000	0.00009	2.05030
R19	2.04364	0.00000	-0.00001	0.00001	0.00000	2.04364
R20	2.04781	0.00000	0.00003	-0.00001	0.00002	2.04783
R21	2.06568	0.00009	0.00021	0.00001	0.00022	2.06589
R22	2.07980	-0.00008	-0.00008	0.00006	-0.00001	2.07979
R23	2.84487	0.00000	-0.00068	0.00035	-0.00033	2.84454
R24	2.28273	0.00010	0.00031	-0.00007	0.00024	2.28297
R25	2.55201	-0.00012	-0.00013	-0.00011	-0.00024	2.55177
R26	1.83181	0.00000	-0.00010	0.00006	-0.00003	1.83178
A1	1.87525	0.00001	0.00001	-0.00007	-0.00007	1.87519
A2	2.27840	0.00000	0.00008	0.00009	0.00018	2.27857
A3	2.12951	-0.00001	-0.00009	-0.00002	-0.00011	2.12940
A4	1.86920	0.00002	0.00002	0.00011	0.00013	1.86933
A5	2.28630	-0.00002	0.00000	-0.00012	-0.00012	2.28617
A6	2.12714	0.00001	-0.00006	0.00002	-0.00004	2.12710
A7	1.89186	-0.00001	0.00009	-0.00009	0.00001	1.89188
A8	2.22648	0.00001	-0.00002	0.00001	-0.00001	2.22646
A9	2.15388	0.00000	-0.00021	0.00013	-0.00009	2.15379
A10	1.89041	-0.00001	-0.00025	0.00004	-0.00024	1.89017
A11	1.80248	0.00000	0.00050	0.00000	0.00052	1.80301
A12	2.18872	0.00000	-0.00002	-0.00004	-0.00015	2.18857
A13	1.89912	0.00005	0.00542	0.00081	0.00621	1.90533
A14	2.19332	0.00000	-0.00008	-0.00015	-0.00031	2.19301
A15	1.89472	0.00000	0.00013	0.00000	0.00015	1.89487
A16	2.20024	0.00003	0.00006	-0.00022	-0.00015	2.20009
A17	2.17525	-0.00002	-0.00026	0.00011	-0.00018	2.17507
A18	1.87903	-0.00001	0.00065	-0.00060	0.00005	1.87907
A19	1.88438	0.00002	-0.00043	-0.00004	-0.00046	1.88392
A20	1.94646	-0.00005	-0.00087	0.00018	-0.00070	1.94576
A21	1.87492	-0.00002	-0.00052	0.00012	-0.00040	1.87452

A22	1.92245	0.00004	0.00026	0.00042	0.00069	1.92314
A23	1.95352	0.00002	0.00090	-0.00011	0.00079	1.95431
A24	1.20663	-0.00006	-0.00426	-0.00044	-0.00471	1.20193
A25	1.34286	-0.00005	-0.00493	-0.00057	-0.00553	1.33733
A26	2.15291	0.00004	0.00000	0.00011	0.00011	2.15303
A27	1.95566	0.00000	-0.00022	-0.00009	-0.00031	1.95535
A28	2.17372	-0.00003	0.00019	0.00002	0.00021	2.17393
A29	2.08601	-0.00001	-0.00006	-0.00002	-0.00009	2.08592
A30	2.14517	0.00002	0.00003	0.00008	0.00011	2.14527
A31	2.05201	-0.00001	0.00003	-0.00005	-0.00002	2.05199
A32	1.95519	0.00001	-0.00034	-0.00010	-0.00043	1.95476
A33	1.90936	-0.00005	-0.00114	0.00031	-0.00083	1.90853
A34	1.93322	-0.00002	0.00082	-0.00033	0.00050	1.93372
A35	1.85949	0.00002	-0.00012	0.00004	-0.00010	1.85939
A36	1.90520	-0.00005	-0.00101	0.00020	-0.00080	1.90440
A37	1.89925	0.00010	0.00180	-0.00010	0.00170	1.90095
A38	2.59186	0.00015	0.01046	0.00143	0.01190	2.60376
A39	2.18884	-0.00002	0.00026	-0.00019	0.00006	2.18890
A40	1.94922	0.00000	-0.00048	0.00040	-0.00008	1.94914
A41	2.14509	0.00002	0.00023	-0.00021	0.00002	2.14511
A42	1.87502	0.00001	-0.00011	0.00016	0.00005	1.87507
D1	0.00385	0.00002	0.00054	-0.00004	0.00049	0.00435
D2	3.10970	0.00001	-0.00068	0.00011	-0.00058	3.10913
D3	-3.12968	0.00001	0.00075	0.00002	0.00077	-3.12891
D4	-0.02383	-0.00001	-0.00047	0.00017	-0.00030	-0.02413
D5	-0.04964	-0.00003	-0.00052	-0.00001	-0.00052	-0.05016
D6	-3.02451	0.00000	-0.00005	0.00070	0.00066	-3.02385
D7	3.08474	-0.00002	-0.00071	-0.00006	-0.00077	3.08397
D8	0.10987	0.00001	-0.00024	0.00064	0.00041	0.11027
D9	0.04288	0.00000	-0.00038	0.00008	-0.00030	0.04258
D10	3.02857	0.00000	-0.00134	0.00044	-0.00091	3.02766
D11	-3.06694	0.00001	0.00070	-0.00005	0.00065	-3.06629
D12	-0.08126	0.00002	-0.00026	0.00030	0.00004	-0.08122
D13	-0.07425	-0.00001	0.00007	-0.00009	-0.00001	-0.07426
D14	1.93779	0.00004	0.00634	0.00085	0.00718	1.94497
D15	-3.06590	0.00006	0.00389	0.00097	0.00485	-3.06105
D16	-3.06786	-0.00002	0.00096	-0.00041	0.00056	-3.06730
D17	-1.05582	0.00003	0.00723	0.00053	0.00775	-1.04807
D18	0.22367	0.00005	0.00478	0.00064	0.00542	0.22909
D19	0.63025	-0.00003	0.00097	-0.00085	0.00012	0.63037
D20	-2.46770	-0.00003	0.00162	-0.00202	-0.00040	-2.46810
D21	-2.68878	-0.00002	-0.00010	-0.00047	-0.00057	-2.68935
D22	0.49645	-0.00003	0.00055	-0.00163	-0.00109	0.49537
D23	0.07669	0.00003	0.00027	0.00006	0.00033	0.07701

D24	3.05451	0.00001	-0.00015	-0.00067	-0.00083	3.05368
D25	-1.87125	0.00001	-0.00285	-0.00036	-0.00323	-1.87448
D26	1.10658	-0.00001	-0.00327	-0.00109	-0.00438	1.10219
D27	3.06784	-0.00005	-0.00356	-0.00098	-0.00453	3.06331
D28	-0.23752	-0.00007	-0.00398	-0.00171	-0.00569	-0.24321
D29	-2.25811	0.00001	-0.00324	-0.00044	-0.00366	-2.26177
D30	-0.25231	0.00001	-0.00101	-0.00005	-0.00107	-0.25337
D31	-2.87947	0.00004	0.01182	0.00224	0.01406	-2.86542
D32	-0.86017	0.00003	0.01133	0.00205	0.01338	-0.84679
D33	1.29290	0.00003	0.01160	0.00201	0.01360	1.30650
D34	0.45450	0.00007	0.01232	0.00307	0.01539	0.46989
D35	2.47381	0.00005	0.01183	0.00288	0.01471	2.48852
D36	-1.65631	0.00006	0.01210	0.00284	0.01493	-1.64138
D37	-1.08056	-0.00003	-0.00602	-0.00152	-0.00755	-1.08811
D38	0.97729	-0.00003	-0.00711	-0.00134	-0.00846	0.96883
D39	3.07085	0.00005	-0.00510	-0.00147	-0.00657	3.06427
D40	3.11736	-0.00001	-0.00645	-0.00116	-0.00761	3.10975
D41	-1.10797	-0.00001	-0.00754	-0.00098	-0.00853	-1.11650
D42	0.98558	0.00007	-0.00553	-0.00111	-0.00663	0.97894
D43	1.03267	-0.00002	-0.00655	-0.00152	-0.00808	1.02460
D44	3.09053	-0.00003	-0.00765	-0.00134	-0.00900	3.08153
D45	-1.09910	0.00005	-0.00564	-0.00147	-0.00710	-1.10621
D46	0.00212	-0.00001	0.00143	0.00041	0.00186	0.00397
D47	0.37582	-0.00001	0.00226	0.00045	0.00270	0.37852
D48	-3.08819	-0.00002	0.00118	-0.00200	-0.00081	-3.08900
D49	0.04990	0.00000	0.00029	-0.00016	0.00013	0.05003
D50	0.00429	-0.00001	0.00045	-0.00069	-0.00024	0.00405
D51	-3.14080	0.00001	-0.00045	0.00114	0.00070	-3.14011
D52	-0.34862	0.00001	0.00079	0.00017	0.00095	-0.34767
D53	1.76821	0.00001	-0.00033	0.00025	-0.00008	1.76812
D54	-2.46289	0.00000	-0.00066	0.00045	-0.00021	-2.46310
D55	-0.17816	0.00001	0.00217	-0.00072	0.00144	-0.17672
D56	2.97139	-0.00001	0.00120	-0.00029	0.00090	2.97229
D57	-2.33889	0.00004	0.00271	-0.00051	0.00220	-2.33669
D58	0.81065	0.00002	0.00173	-0.00008	0.00165	0.81231
D59	1.92143	0.00000	0.00242	-0.00061	0.00182	1.92324
D60	-1.21221	-0.00002	0.00144	-0.00018	0.00127	-1.21094
D61	3.09000	0.00005	0.00248	-0.00038	0.00210	3.09210
D62	-0.04387	0.00003	0.00153	0.00003	0.00157	-0.04230

Item	Value	Threshold	Converged?
Maximum Force	0.000147	0.000450	YES
RMS Force	0.000037	0.000300	YES
Maximum Displacement	0.036487	0.001800	NO
RMS Displacement	0.009053	0.001200	NO

Predicted change in Energy=-2.378377D-06
GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.329452	-2.226470	-0.389168
2	6	0	-1.579570	-1.778586	-0.653429
3	7	0	-1.803712	-0.680295	0.171239
4	6	0	-0.680061	-0.443285	0.879537
5	7	0	0.206224	-1.407992	0.597770
6	6	0	1.589047	-1.440991	1.091735
7	1	0	0.225716	-3.043396	-0.815908
8	1	0	-2.313274	-2.114274	-1.363529
9	1	0	1.616974	-0.893443	2.032498
10	1	0	1.843021	-2.479357	1.310823
11	35	0	0.266213	2.052173	-0.195389
12	1	0	-0.575003	0.296875	1.648542
13	6	0	-2.922423	0.196903	0.161564
14	6	0	-4.162481	-0.204671	-0.087511
15	1	0	-2.633000	1.227601	0.337798
16	1	0	-4.960597	0.523997	-0.127286
17	1	0	-4.422121	-1.242778	-0.258532
18	6	0	2.558485	-0.814042	0.086653
19	1	0	2.577763	-1.361078	-0.859665
20	1	0	2.227950	0.208818	-0.149508
21	6	0	3.952375	-0.758120	0.652134
22	8	0	4.251875	-0.986457	1.800027
23	8	0	4.857565	-0.406462	-0.286151
24	1	0	5.720458	-0.345444	0.151229

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.353967	0.000000			
3	N	2.208655	1.391603	0.000000		
4	C	2.216368	2.223090	1.349241	0.000000	
5	N	1.389569	2.211763	2.179751	1.339984	0.000000
6	C	2.547684	3.633140	3.596775	2.487831	1.468772
7	H	1.075959	2.210249	3.267612	3.233504	2.161807
8	H	2.213033	1.074826	2.161356	3.238971	3.270076
9	H	3.380829	4.267971	3.900104	2.609278	2.076878

10	H	2.770120	4.007929	4.223025	3.270710	2.082155
11	Br	4.324251	4.276847	3.447519	2.877187	3.550414
12	H	3.252665	3.258184	2.155693	1.072494	2.149654
13	C	3.591593	2.523891	1.421648	2.439982	3.543218
14	C	4.344051	3.077158	2.420116	3.622067	4.582923
15	H	4.214904	3.336076	2.086990	2.626654	3.882671
16	H	5.392694	4.124326	3.391955	4.502479	5.563662
17	H	4.211253	2.919441	2.712408	3.992168	4.709791
18	C	3.249852	4.312953	4.365067	3.354744	2.479344
19	H	3.069556	4.183332	4.552314	3.805337	2.783975
20	H	3.539543	4.324455	4.140978	3.152887	2.694415
21	C	4.644826	5.774795	5.776665	4.648688	3.802491
22	O	5.226735	6.375944	6.278281	5.046417	4.241509
23	O	5.498017	6.591989	6.682575	5.659107	4.839354
24	H	6.358593	7.482765	7.531645	6.442566	5.633399

		6	7	8	9	10
6	C	0.000000				
7	H	2.839978	0.000000			
8	H	4.659372	2.758555	0.000000		
9	H	1.088864	3.830315	5.335755	0.000000	
10	H	1.091194	2.730714	4.955828	1.756996	0.000000
11	Br	3.950794	5.133372	5.037616	3.932517	5.028892
12	H	2.830782	4.227538	4.231761	2.523696	3.697074
13	C	4.888894	4.622312	2.835226	5.029451	5.585035
14	C	5.999933	5.276855	2.948622	6.194429	6.572335
15	H	5.051286	5.267325	3.763624	5.043126	5.892629
16	H	6.945865	6.332325	3.936634	7.066700	7.574795
17	H	6.164143	5.015505	2.535303	6.468503	6.576018
18	C	1.530707	3.350589	5.246681	2.163113	2.187179
19	H	2.189043	2.892099	4.974277	3.083246	2.549786
20	H	2.161192	3.876845	5.243407	2.519805	3.083345
21	C	2.498976	4.611466	6.720149	2.716213	2.801053
22	O	2.792656	5.223415	7.374363	2.646771	2.875873
23	O	3.694865	5.356126	7.449718	4.014313	3.991828
24	H	4.376452	6.197297	8.364455	4.547313	4.575233

		11	12	13	14	15
11	Br	0.000000				
12	H	2.681193	0.000000			
13	C	3.706324	2.780554	0.000000		
14	C	4.971751	4.016893	1.327044	0.000000	
15	H	3.060987	2.611447	1.084971	2.138130	0.000000
16	H	5.446054	4.736939	2.084366	1.081447	2.475696
17	H	5.730721	4.561555	2.120910	1.083664	3.107947
18	C	3.680930	3.673198	5.573865	6.750782	5.584165

19	H	4.175501	4.356587	5.807087	6.882180	5.940306
20	H	2.692299	3.331258	5.159772	6.404094	4.990413
21	C	4.712094	4.754261	6.958130	8.167268	6.885424
22	O	5.394484	4.996863	7.453552	8.658832	7.378460
23	O	5.208996	5.809519	7.816183	9.024490	7.692076
24	H	5.968040	6.502873	8.659887	9.886825	8.502326

		16	17	18	19	20
16	H	0.000000				
17	H	1.851669	0.000000			
18	C	7.640204	7.002273	0.000000		
19	H	7.804919	7.026645	1.093224	0.000000	
20	H	7.195487	6.807530	1.100576	1.758200	0.000000
21	C	9.038384	8.437795	1.505266	2.130411	2.133364
22	O	9.532347	8.918608	2.415149	3.164957	3.053791
23	O	9.863433	9.317337	2.364503	2.537264	2.704093
24	H	10.720002	10.190438	3.197160	3.453976	3.548981

		21	22	23	24
21	C	0.000000			
22	O	1.208096	0.000000		
23	O	1.350337	2.248420	0.000000	
24	H	1.883435	2.299167	0.969334	0.000000

Stoichiometry C8H11BrN2O2
Framework group C1[X(C8H11BrN2O2)]
Deg. of freedom 66
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.658370	-2.159623	-0.762160
2	6	0	-1.967465	-1.825737	-0.851694
3	7	0	-2.211206	-0.860774	0.120930
4	6	0	-1.048317	-0.583390	0.746389
5	7	0	-0.105520	-1.405277	0.265566
6	6	0	1.318005	-1.341182	0.621600
7	1	0	-0.073073	-2.855708	-1.337121
8	1	0	-2.734920	-2.157116	-1.527306
9	1	0	1.390359	-0.905284	1.616779
10	1	0	1.695028	-2.363222	0.684778
11	35	0	-0.471687	2.108153	-0.091049
12	1	0	-0.936737	0.070877	1.588842

13	6	0	-3.405970	-0.117657	0.324397
14	6	0	-4.619513	-0.622996	0.142770
15	1	0	-3.202981	0.911758	0.600555
16	1	0	-5.485514	0.012465	0.268311
17	1	0	-4.791751	-1.657022	-0.131917
18	6	0	2.109672	-0.499697	-0.382508
19	1	0	2.083394	-0.929223	-1.387474
20	1	0	1.656627	0.500506	-0.457414
21	6	0	3.542870	-0.354783	0.054262
22	8	0	3.982449	-0.678480	1.131985
23	8	0	4.305205	0.200159	-0.912328
24	1	0	5.198997	0.305931	-0.552389

Rotational constants (GHZ): 0.8057873 0.3343358 0.2550237

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 404 symmetry adapted cartesian basis functions of A symmetry.

There are 389 symmetry adapted basis functions of A symmetry.

389 basis functions, 625 primitive gaussians, 404 cartesian basis functions

62 alpha electrons 62 beta electrons

nuclear repulsion energy 1072.5851121388 Hartrees.

NAtoms= 24 NActive= 24 NUniq= 24 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 389 RedAO= T EigKep= 6.54D-06 NBF= 389

NBsUse= 389 1.00D-06 EigRej= -1.00D+00 NBFU= 389

Initial guess from the checkpoint file: "./cooh.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000400 -0.000207 0.000589 Ang= -0.08 deg.

ExpMin= 3.50D-02 ExpMax= 4.40D+05 ExpMxC= 1.51D+04 IAcc=3 IRadAn= 5 AccDes= 0.00D+00

Harris functional with IExCor= 402 and IRadAn= 5 diagonalized for initial guess.

HarFok: IExCor= 402 AccDes= 0.00D+00 IRadAn= 5 IDoV= 1 UseB2=F ITyADJ=14

ICtDFT= 3500011 ScaDFX= 1.000000 1.000000 1.000000 1.000000

FoFCou: FMM=F IPFlag= 0 FMFlag= 100000 FMFlg1= 0

NFxFlg= 0 DoJE=T BraDBF=F KetDBF=T FulRan=T

wScrn= 0.000000 ICntrl= 500 IOpCl= 0 I1Cent= 200000004 NGrid= 0

NMat0= 1 NMatS0= 1 NMatT0= 0 NMatD0= 1 NMtDS0= 0 NMtDT0= 0

Petite list used in FoFCou.

Keep R1 ints in memory in canonical form, NReq=2910765817.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3145.73224199 A.U. after 11 cycles
NFock= 11 Conv=0.50D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	-0.000023798	0.000022196	-0.000018940
2	6	-0.000038912	-0.000018423	0.000004029
3	7	0.000068072	0.000060426	-0.000038981
4	6	-0.000037118	0.000009252	-0.000084304
5	7	0.000046269	-0.000079548	0.000093000
6	6	-0.000071617	0.000007594	0.000019813
7	1	0.000003656	0.000006262	-0.000012111
8	1	0.000010250	0.000003048	-0.000020452
9	1	0.000013343	-0.000029424	0.000004249
10	1	0.000026316	0.000002540	-0.000046010
11	35	0.000038838	0.000041930	-0.000016639
12	1	-0.000019356	-0.000057048	0.000060739
13	6	-0.000004322	-0.000028187	0.000045626
14	6	0.000011249	-0.000001151	-0.000000686
15	1	-0.000012748	-0.000015475	0.000019974
16	1	0.000005412	0.000001414	-0.000013730
17	1	-0.000003581	0.000008166	-0.000021545
18	6	-0.000004483	0.000110192	-0.000013227
19	1	-0.000004647	-0.000039648	-0.000014794
20	1	-0.000040996	0.000006254	0.000003567
21	6	0.000095138	0.000030073	-0.000022389
22	8	-0.000023559	-0.000026857	-0.000011043
23	8	-0.000050345	-0.000011771	0.000068341
24	1	0.000016939	-0.000001816	0.000015516

Cartesian Forces: Max 0.000110192 RMS 0.000037274

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000071391 RMS 0.000017440
Search for a local minimum.
Step number 14 out of a maximum of 140
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 4 6 7 8 9
10 11 12 13 14
DE= -6.67D-06 DEPred=-2.38D-06 R= 2.81D+00
TightC=F SS= 1.41D+00 RLast= 5.13D-02 DXNew= 1.2000D+00 1.5401D-01
Trust test= 2.81D+00 RLast= 5.13D-02 DXMaxT set to 7.14D-01
ITU= 1 1 1 1 1 1 1 1 0 -1 1 1 1 0
Eigenvalues --- 0.00135 0.00221 0.00379 0.00459 0.01214
Eigenvalues --- 0.01642 0.01812 0.02012 0.02174 0.02229
Eigenvalues --- 0.02364 0.02414 0.02568 0.02968 0.03042
Eigenvalues --- 0.03053 0.03119 0.03520 0.04279 0.04484
Eigenvalues --- 0.05057 0.05248 0.06337 0.07186 0.09688
Eigenvalues --- 0.09988 0.10923 0.12754 0.15579 0.15854
Eigenvalues --- 0.15981 0.15992 0.15999 0.16001 0.16010
Eigenvalues --- 0.16701 0.17900 0.20636 0.21901 0.22873
Eigenvalues --- 0.24430 0.25134 0.27530 0.27906 0.34372
Eigenvalues --- 0.34487 0.35170 0.35420 0.35506 0.35580
Eigenvalues --- 0.35843 0.36014 0.36549 0.36611 0.36652
Eigenvalues --- 0.37637 0.41327 0.42622 0.43623 0.47373
Eigenvalues --- 0.52367 0.53423 0.54137 0.54407 0.59908
Eigenvalues --- 0.92554
En-DIIS/RFO-DIIS IScMMF= 0 using points: 14 13 12 11 10
RFO step: Lambda=-1.51448551D-07.
DidBck=F Rises=F RFO-DIIS coefs: 1.38761 -0.52806 0.03908 0.13616 -0.03479
Iteration 1 RMS(Cart)= 0.00247359 RMS(Int)= 0.00000233
Iteration 2 RMS(Cart)= 0.00000290 RMS(Int)= 0.00000103
Iteration 3 RMS(Cart)= 0.00000000 RMS(Int)= 0.00000103

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55863	0.00000	-0.00001	0.00001	0.00000	2.55862
R2	2.62590	0.00001	0.00000	0.00004	0.00004	2.62595
R3	2.03327	0.00000	0.00001	-0.00001	0.00000	2.03327
R4	2.62975	0.00000	0.00001	-0.00002	-0.00001	2.62974
R5	2.03113	0.00000	-0.00001	0.00001	0.00001	2.03113
R6	2.54970	-0.00003	0.00006	-0.00005	0.00001	2.54971
R7	2.68653	-0.00002	-0.00006	-0.00001	-0.00007	2.68645
R8	2.53220	0.00001	0.00009	0.00001	0.00010	2.53231

R9	5.43710	0.00003	0.00005	0.00123	0.00129	5.43838
R10	2.02672	0.00000	-0.00004	0.00005	0.00000	2.02672
R11	2.77558	-0.00003	-0.00006	0.00004	-0.00002	2.77555
R12	2.05765	0.00000	0.00004	-0.00002	0.00002	2.05767
R13	2.06206	-0.00001	-0.00004	-0.00002	-0.00006	2.06200
R14	2.89262	0.00003	0.00019	-0.00005	0.00014	2.89276
R15	5.06672	0.00005	0.00058	0.00079	0.00137	5.06809
R16	5.08771	-0.00003	-0.00420	-0.00122	-0.00543	5.08228
R17	2.50775	-0.00001	0.00002	-0.00003	-0.00001	2.50774
R18	2.05030	-0.00001	0.00000	-0.00003	-0.00003	2.05027
R19	2.04364	0.00000	0.00000	-0.00001	-0.00001	2.04363
R20	2.04783	0.00000	0.00000	-0.00001	-0.00001	2.04781
R21	2.06589	0.00004	0.00017	-0.00002	0.00015	2.06604
R22	2.07979	-0.00001	-0.00011	0.00009	-0.00002	2.07976
R23	2.84454	0.00004	0.00003	0.00004	0.00007	2.84461
R24	2.28297	-0.00002	0.00008	-0.00002	0.00005	2.28302
R25	2.55177	-0.00007	-0.00016	-0.00007	-0.00023	2.55154
R26	1.83178	0.00002	0.00000	0.00002	0.00002	1.83179
A1	1.87519	0.00001	-0.00001	0.00012	0.00011	1.87529
A2	2.27857	0.00000	0.00003	-0.00003	0.00000	2.27858
A3	2.12940	-0.00001	-0.00002	-0.00009	-0.00011	2.12928
A4	1.86933	-0.00002	0.00004	-0.00012	-0.00008	1.86926
A5	2.28617	0.00000	-0.00009	0.00003	-0.00006	2.28611
A6	2.12710	0.00002	0.00004	0.00009	0.00013	2.12723
A7	1.89188	0.00001	-0.00002	0.00009	0.00008	1.89195
A8	2.22646	0.00000	0.00002	0.00000	0.00002	2.22648
A9	2.15379	-0.00001	0.00000	-0.00002	-0.00002	2.15377
A10	1.89017	0.00001	-0.00003	0.00003	0.00000	1.89017
A11	1.80301	-0.00001	0.00014	-0.00017	-0.00003	1.80297
A12	2.18857	0.00000	-0.00008	0.00005	-0.00003	2.18853
A13	1.90533	0.00000	0.00118	0.00025	0.00143	1.90676
A14	2.19301	-0.00001	-0.00014	-0.00006	-0.00021	2.19280
A15	1.89487	-0.00002	0.00001	-0.00011	-0.00010	1.89477
A16	2.20009	0.00002	0.00000	-0.00003	-0.00004	2.20005
A17	2.17507	0.00000	-0.00008	0.00004	-0.00003	2.17504
A18	1.87907	0.00002	-0.00010	0.00047	0.00037	1.87945
A19	1.88392	0.00001	-0.00001	-0.00008	-0.00009	1.88383
A20	1.94576	0.00000	-0.00010	0.00006	-0.00003	1.94573
A21	1.87452	0.00001	-0.00009	0.00001	-0.00008	1.87444
A22	1.92314	0.00000	0.00032	-0.00010	0.00022	1.92336
A23	1.95431	-0.00002	-0.00004	-0.00033	-0.00037	1.95394
A24	1.20193	0.00000	-0.00071	-0.00028	-0.00099	1.20094
A25	1.33733	0.00000	-0.00086	-0.00034	-0.00119	1.33614
A26	2.15303	0.00001	0.00011	0.00000	0.00011	2.15314

A27	1.95535	0.00000	-0.00004	-0.00003	-0.00007	1.95528
A28	2.17393	-0.00001	-0.00006	-0.00001	-0.00007	2.17386
A29	2.08592	-0.00001	-0.00005	-0.00004	-0.00009	2.08583
A30	2.14527	0.00001	0.00007	0.00005	0.00012	2.14540
A31	2.05199	0.00000	-0.00002	-0.00001	-0.00003	2.05196
A32	1.95476	-0.00001	-0.00039	-0.00014	-0.00053	1.95423
A33	1.90853	0.00001	0.00020	0.00007	0.00027	1.90879
A34	1.93372	-0.00004	-0.00008	-0.00021	-0.00030	1.93343
A35	1.85939	0.00000	0.00002	0.00005	0.00007	1.85947
A36	1.90440	0.00001	-0.00062	0.00029	-0.00033	1.90407
A37	1.90095	0.00003	0.00092	-0.00004	0.00087	1.90183
A38	2.60376	0.00000	0.00204	0.00065	0.00269	2.60644
A39	2.18890	-0.00004	-0.00006	-0.00011	-0.00016	2.18874
A40	1.94914	0.00004	0.00005	0.00008	0.00013	1.94927
A41	2.14511	0.00000	0.00001	0.00003	0.00004	2.14515
A42	1.87507	0.00001	0.00004	0.00000	0.00004	1.87510
D1	0.00435	0.00001	-0.00004	0.00034	0.00030	0.00464
D2	3.10913	0.00000	-0.00026	0.00025	-0.00001	3.10912
D3	-3.12891	0.00000	0.00009	0.00013	0.00022	-3.12869
D4	-0.02413	0.00000	-0.00013	0.00004	-0.00009	-0.02422
D5	-0.05016	0.00000	-0.00002	-0.00020	-0.00021	-0.05037
D6	-3.02385	0.00001	0.00046	0.00042	0.00088	-3.02297
D7	3.08397	0.00000	-0.00014	-0.00001	-0.00014	3.08382
D8	0.11027	0.00002	0.00034	0.00061	0.00095	0.11123
D9	0.04258	-0.00001	0.00008	-0.00036	-0.00028	0.04231
D10	3.02766	0.00000	0.00013	0.00015	0.00028	3.02793
D11	-3.06629	0.00000	0.00028	-0.00028	0.00000	-3.06629
D12	-0.08122	0.00001	0.00032	0.00023	0.00055	-0.08067
D13	-0.07426	0.00000	-0.00009	0.00023	0.00014	-0.07412
D14	1.94497	0.00001	0.00130	0.00045	0.00174	1.94672
D15	-3.06105	0.00001	0.00171	0.00012	0.00183	-3.05922
D16	-3.06730	-0.00001	-0.00014	-0.00025	-0.00039	-3.06769
D17	-1.04807	0.00000	0.00125	-0.00004	0.00122	-1.04685
D18	0.22909	0.00000	0.00167	-0.00037	0.00130	0.23039
D19	0.63037	-0.00004	-0.00106	-0.00170	-0.00276	0.62761
D20	-2.46810	-0.00002	-0.00124	-0.00085	-0.00209	-2.47019
D21	-2.68935	-0.00002	-0.00101	-0.00111	-0.00213	-2.69147
D22	0.49537	-0.00001	-0.00120	-0.00026	-0.00146	0.49391
D23	0.07701	0.00000	0.00007	-0.00003	0.00004	0.07705
D24	3.05368	-0.00002	-0.00039	-0.00064	-0.00104	3.05265
D25	-1.87448	0.00001	-0.00066	0.00003	-0.00063	-1.87511
D26	1.10219	-0.00001	-0.00112	-0.00058	-0.00170	1.10049
D27	3.06331	-0.00001	-0.00173	0.00010	-0.00164	3.06167
D28	-0.24321	-0.00002	-0.00219	-0.00052	-0.00271	-0.24592

D29	-2.26177	0.00000	-0.00067	-0.00004	-0.00070	-2.26248
D30	-0.25337	0.00001	-0.00014	0.00002	-0.00012	-0.25349
D31	-2.86542	0.00000	0.00298	0.00048	0.00347	-2.86195
D32	-0.84679	0.00002	0.00282	0.00070	0.00352	-0.84327
D33	1.30650	0.00000	0.00271	0.00027	0.00298	1.30947
D34	0.46989	0.00002	0.00352	0.00121	0.00473	0.47462
D35	2.48852	0.00004	0.00336	0.00142	0.00478	2.49331
D36	-1.64138	0.00002	0.00325	0.00099	0.00424	-1.63714
D37	-1.08811	0.00000	-0.00156	-0.00019	-0.00175	-1.08986
D38	0.96883	0.00000	-0.00165	-0.00017	-0.00181	0.96702
D39	3.06427	0.00002	-0.00044	-0.00031	-0.00075	3.06353
D40	3.10975	-0.00002	-0.00159	-0.00075	-0.00234	3.10740
D41	-1.11650	-0.00001	-0.00168	-0.00073	-0.00240	-1.11890
D42	0.97894	0.00001	-0.00047	-0.00087	-0.00134	0.97760
D43	1.02460	0.00000	-0.00167	-0.00048	-0.00215	1.02244
D44	3.08153	0.00000	-0.00175	-0.00046	-0.00221	3.07932
D45	-1.10621	0.00002	-0.00054	-0.00060	-0.00114	-1.10735
D46	0.00397	0.00000	0.00025	0.00047	0.00073	0.00470
D47	0.37852	0.00000	0.00039	0.00044	0.00083	0.37935
D48	-3.08900	0.00002	-0.00039	0.00132	0.00093	-3.08807
D49	0.05003	0.00000	0.00000	0.00010	0.00010	0.05013
D50	0.00405	0.00001	-0.00018	0.00036	0.00018	0.00423
D51	-3.14011	-0.00002	0.00021	-0.00086	-0.00065	-3.14076
D52	-0.34767	0.00000	0.00031	-0.00046	-0.00015	-0.34782
D53	1.76812	-0.00001	-0.00003	-0.00056	-0.00059	1.76753
D54	-2.46310	0.00002	-0.00027	-0.00021	-0.00049	-2.46359
D55	-0.17672	0.00000	0.00233	-0.00056	0.00177	-0.17495
D56	2.97229	-0.00002	0.00186	-0.00059	0.00127	2.97356
D57	-2.33669	0.00003	0.00330	-0.00044	0.00286	-2.33383
D58	0.81231	0.00002	0.00284	-0.00047	0.00237	0.81467
D59	1.92324	0.00000	0.00311	-0.00064	0.00247	1.92571
D60	-1.21094	-0.00001	0.00264	-0.00067	0.00198	-1.20897
D61	3.09210	0.00002	0.00138	-0.00033	0.00105	3.09315
D62	-0.04230	0.00000	0.00092	-0.00036	0.00057	-0.04174

Item	Value	Threshold	Converged?
Maximum Force	0.000071	0.000450	YES
RMS Force	0.000017	0.000300	YES
Maximum Displacement	0.010192	0.001800	NO
RMS Displacement	0.002473	0.001200	NO

Predicted change in Energy=-5.185221D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.330673	-2.228861	-0.387127
2	6	0	-1.580492	-1.780224	-0.651509
3	7	0	-1.803180	-0.680540	0.171685
4	6	0	-0.679120	-0.443735	0.879414
5	7	0	0.206165	-1.409738	0.598676
6	6	0	1.589427	-1.442805	1.091366
7	1	0	0.223635	-3.046808	-0.813031
8	1	0	-2.314676	-2.116173	-1.360995
9	1	0	1.618109	-0.897623	2.033491
10	1	0	1.844370	-2.481500	1.307589
11	35	0	0.267146	2.052204	-0.196222
12	1	0	-0.573602	0.296340	1.648440
13	6	0	-2.921150	0.197532	0.161508
14	6	0	-4.161320	-0.202740	-0.089073
15	1	0	-2.630942	1.227930	0.338097
16	1	0	-4.958531	0.526852	-0.129946
17	1	0	-4.421869	-1.240458	-0.261021
18	6	0	2.557581	-0.813160	0.086620
19	1	0	2.577301	-1.359732	-0.860047
20	1	0	2.225328	0.209300	-0.148798
21	6	0	3.951629	-0.756660	0.651754
22	8	0	4.251787	-0.988216	1.798860
23	8	0	4.855976	-0.401069	-0.285687
24	1	0	5.719073	-0.340891	0.151429

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.353965	0.000000			
3	N	2.208585	1.391597	0.000000		
4	C	2.216352	2.223150	1.349246	0.000000	
5	N	1.389591	2.211869	2.179797	1.340039	0.000000
6	C	2.547667	3.633160	3.596754	2.487845	1.468759
7	H	1.075960	2.210249	3.267548	3.233470	2.161764
8	H	2.213003	1.074829	2.161430	3.239061	3.270167
9	H	3.380730	4.268402	3.901110	2.610588	2.077148
10	H	2.768881	4.007435	4.223547	3.271670	2.082054
11	Br	4.326817	4.278849	3.448114	2.877868	3.552551
12	H	3.252566	3.258176	2.155681	1.072495	2.149591
13	C	3.591512	2.523862	1.421609	2.439940	3.543237
14	C	4.343716	3.076600	2.420148	3.622397	4.583096

15	H	4.215044	3.336429	2.086898	2.626232	3.882572
16	H	5.392325	4.123806	3.391905	4.502689	5.563754
17	H	4.210787	2.918433	2.712614	3.992934	4.710247
18	C	3.251255	4.313200	4.363606	3.352795	2.479368
19	H	3.071701	4.184201	4.551306	3.803821	2.784360
20	H	3.540420	4.323793	4.138043	3.149523	2.693886
21	C	4.645940	5.774992	5.775299	4.646890	3.802345
22	O	5.226536	6.375505	6.277339	5.045363	4.240894
23	O	5.500222	6.592724	6.680692	5.656551	4.839448
24	H	6.360337	7.483317	7.529944	6.440296	5.633349

		6	7	8	9	10
6	C	0.000000				
7	H	2.839885	0.000000			
8	H	4.659347	2.758508	0.000000		
9	H	1.088873	3.829653	5.336121	0.000000	
10	H	1.091163	2.728257	4.955044	1.756927	0.000000
11	Br	3.952391	5.136368	5.039629	3.936775	5.030264
12	H	2.830839	4.227419	4.231814	2.525353	3.698535
13	C	4.888829	4.622245	2.835323	5.030761	5.585776
14	C	6.000191	5.276426	2.947729	6.195962	6.573563
15	H	5.050916	5.267551	3.764301	5.044479	5.893064
16	H	6.946000	6.331864	3.935865	7.068365	7.576025
17	H	6.164866	5.014810	2.533196	6.470212	6.577725
18	C	1.530781	3.353485	5.247125	2.163341	2.186960
19	H	2.188792	2.896236	4.975398	3.083205	2.548372
20	H	2.161442	3.879462	5.242984	2.521186	3.083278
21	C	2.498810	4.613926	6.720566	2.715581	2.801024
22	O	2.792017	5.223580	7.373968	2.645660	2.875222
23	O	3.694839	5.360655	7.450914	4.013594	3.992054
24	H	4.376262	6.200968	8.365415	4.546428	4.575176

		11	12	13	14	15
11	Br	0.000000				
12	H	2.681919	0.000000			
13	C	3.705807	2.780595	0.000000		
14	C	4.970670	4.017431	1.327038	0.000000	
15	H	3.060038	2.611035	1.084954	2.138072	0.000000
16	H	5.444152	4.737446	2.084303	1.081443	2.475530
17	H	5.729981	4.562559	2.120967	1.083656	3.107942
18	C	3.679185	3.670774	5.571679	6.748861	5.581224
19	H	4.173582	4.354684	5.805309	6.880556	5.937789
20	H	2.689427	3.327409	5.155838	6.400205	4.985783
21	C	4.710010	4.751832	6.955998	8.165513	6.882384
22	O	5.394615	4.995707	7.452379	8.658039	7.376794
23	O	5.204221	5.805820	7.812938	9.021620	7.687437

24	H	5.964166	6.499605	8.656989	9.884285	8.498164
		16	17	18	19	20
16	H	0.000000				
17	H	1.851640	0.000000			
18	C	7.637701	7.001154	0.000000		
19	H	7.802629	7.025769	1.093302	0.000000	
20	H	7.190899	6.804382	1.100563	1.758301	0.000000
21	C	9.036006	8.436983	1.505303	2.130262	2.134029
22	O	9.531300	8.918466	2.415107	3.164130	3.055152
23	O	9.859506	9.315771	2.364540	2.537969	2.703997
24	H	10.716500	10.189113	3.197228	3.454251	3.549521
		21	22	23	24	
21	C	0.000000				
22	O	1.208125	0.000000			
23	O	1.350217	2.248360	0.000000		
24	H	1.883361	2.299128	0.969344	0.000000	

Stoichiometry C8H11BrN2O2
Framework group C1[X(C8H11BrN2O2)]
Deg. of freedom 66
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.660086	-2.161751	-0.761469
2	6	0	-1.968873	-1.826584	-0.850701
3	7	0	-2.211039	-0.860449	0.121143
4	6	0	-1.047625	-0.583937	0.746023
5	7	0	-0.105907	-1.407340	0.265524
6	6	0	1.317985	-1.343814	0.620133
7	1	0	-0.075747	-2.858867	-1.336157
8	1	0	-2.736896	-2.157665	-1.525819
9	1	0	1.391717	-0.910977	1.616556
10	1	0	1.695366	-2.365907	0.679664
11	35	0	-0.470325	2.108498	-0.090420
12	1	0	-0.935269	0.069727	1.588844
13	6	0	-3.404941	-0.116062	0.324757
14	6	0	-4.619069	-0.619438	0.141632
15	1	0	-3.200736	0.912862	0.601782
16	1	0	-5.484156	0.017370	0.266616
17	1	0	-4.792714	-1.652843	-0.134471

18	6	0	2.108320	-0.499478	-0.382742
19	1	0	2.082144	-0.927813	-1.388304
20	1	0	1.654016	0.500253	-0.456125
21	6	0	3.541676	-0.354686	0.053676
22	8	0	3.982153	-0.682223	1.129904
23	8	0	4.302956	0.204305	-0.911242
24	1	0	5.197080	0.308776	-0.551720

Rotational constants (GHZ): 0.8053793 0.3345388 0.2550521

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 404 symmetry adapted cartesian basis functions of A symmetry.

There are 389 symmetry adapted basis functions of A symmetry.

389 basis functions, 625 primitive gaussians, 404 cartesian basis functions

62 alpha electrons 62 beta electrons

nuclear repulsion energy 1072.5930464611 Hartrees.

NAtoms= 24 NActive= 24 NUniq= 24 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 389 RedAO= T EigKep= 6.52D-06 NBF= 389

NBsUse= 389 1.00D-06 EigRej= -1.00D+00 NBFU= 389

Initial guess from the checkpoint file: "./cooh.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 -0.000227 -0.000060 0.000148 Ang= -0.03 deg.

Keep R1 ints in memory in canonical form, NReq=2910765817.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3145.73224323 A.U. after 10 cycles

NFock= 10 Conv=0.57D-08 -V/T= 2.0017

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Atomic Forces (Hartrees/Bohr)

Number Number X Y Z

1	6	0.000003168	-0.000003624	-0.000015842
2	6	0.000004280	0.000007313	-0.000001294
3	7	0.000032743	0.000055058	-0.000012934
4	6	-0.000048198	-0.000043808	-0.000006140

5	7	0.000008990	-0.000016522	0.000038578
6	6	-0.000027846	-0.000003306	-0.000005786
7	1	0.000004219	0.000004013	-0.000016088
8	1	0.000011703	0.000009269	-0.000015446
9	1	-0.000007639	-0.000017118	-0.000006219
10	1	0.000007278	-0.000011464	-0.000021103
11	35	0.000013291	0.000023776	-0.000004831
12	1	-0.000006839	-0.000021090	0.000021202
13	6	0.000007681	-0.000022386	0.000009201
14	6	0.000002923	0.000005701	-0.000033071
15	1	-0.000009910	-0.000008969	0.000027841
16	1	-0.000002638	-0.000003422	0.000015699
17	1	-0.000004423	0.000003232	-0.000009098
18	6	-0.000006870	-0.000004003	-0.000019074
19	1	-0.000006795	0.000006045	-0.000002309
20	1	0.000003240	0.000028053	0.000016539
21	6	0.000028257	0.000021020	0.000003580
22	8	-0.000008586	-0.000011953	-0.000008742
23	8	-0.000005843	-0.000005247	0.000031103
24	1	0.000007814	0.000009431	0.000014233

Cartesian Forces: Max 0.000055058 RMS 0.000017743

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000032885 RMS 0.000009040
Search for a local minimum.
Step number 15 out of a maximum of 140
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 4 6 7 8 9
10 11 12 13 14
15
DE= -1.25D-06 DEPred=-5.19D-07 R= 2.40D+00
TightC=F SS= 1.41D+00 RLast= 1.59D-02 DXNew= 1.2000D+00 4.7686D-02
Trust test= 2.40D+00 RLast= 1.59D-02 DXMaxT set to 7.14D-01
ITU= 1 1 1 1 1 1 1 1 1 0 -1 1 1 1 0
Eigenvalues --- 0.00127 0.00217 0.00389 0.00428 0.01116
Eigenvalues --- 0.01617 0.01803 0.01901 0.02123 0.02201
Eigenvalues --- 0.02366 0.02405 0.02430 0.02988 0.03041

Eigenvalues --- 0.03111 0.03148 0.03601 0.04094 0.04358
Eigenvalues --- 0.05097 0.05265 0.06395 0.07180 0.09630
Eigenvalues --- 0.09820 0.10895 0.12704 0.15567 0.15846
Eigenvalues --- 0.15952 0.15992 0.15995 0.16001 0.16003
Eigenvalues --- 0.16702 0.17848 0.20521 0.21881 0.23019
Eigenvalues --- 0.24440 0.24991 0.27349 0.27787 0.34331
Eigenvalues --- 0.34409 0.35160 0.35453 0.35490 0.35578
Eigenvalues --- 0.35843 0.36036 0.36468 0.36602 0.36656
Eigenvalues --- 0.37300 0.41339 0.42671 0.43560 0.47368
Eigenvalues --- 0.52340 0.53036 0.54047 0.54494 0.59917
Eigenvalues --- 0.92599
En-DIIS/RFO-DIIS IScMMF= 0 using points: 15 14 13 12 11
RFO step: Lambda=-3.66488620D-08.
DidBck=F Rises=F RFO-DIIS coefs: 1.19771 -0.09683 -0.26157 0.20091 -0.04021
Iteration 1 RMS(Cart)= 0.00080918 RMS(Int)= 0.00000135
Iteration 2 RMS(Cart)= 0.00000058 RMS(Int)= 0.00000127

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55862	0.00000	0.00000	-0.00001	-0.00001	2.55861
R2	2.62595	-0.00001	0.00001	-0.00001	0.00000	2.62595
R3	2.03327	0.00000	0.00000	0.00001	0.00001	2.03328
R4	2.62974	0.00001	0.00001	0.00001	0.00001	2.62975
R5	2.03113	0.00000	0.00000	-0.00001	-0.00002	2.03112
R6	2.54971	-0.00003	-0.00003	-0.00003	-0.00006	2.54965
R7	2.68645	-0.00001	-0.00002	-0.00004	-0.00006	2.68639
R8	2.53231	0.00000	0.00003	0.00002	0.00005	2.53236
R9	5.43838	0.00002	0.00037	0.00027	0.00064	5.43903
R10	2.02672	0.00000	0.00000	0.00001	0.00001	2.02673
R11	2.77555	-0.00002	-0.00007	0.00000	-0.00007	2.77548
R12	2.05767	-0.00001	-0.00001	-0.00001	-0.00002	2.05765
R13	2.06200	0.00000	-0.00001	0.00001	0.00000	2.06200
R14	2.89276	0.00002	0.00015	-0.00002	0.00013	2.89289
R15	5.06809	0.00002	0.00112	0.00043	0.00155	5.06965
R16	5.08228	-0.00001	-0.00081	-0.00056	-0.00137	5.08091
R17	2.50774	0.00000	0.00000	0.00001	0.00001	2.50775
R18	2.05027	0.00000	-0.00002	-0.00001	-0.00003	2.05024
R19	2.04363	0.00000	0.00000	0.00000	0.00000	2.04363
R20	2.04781	0.00000	-0.00001	0.00000	-0.00001	2.04780
R21	2.06604	0.00000	0.00008	-0.00003	0.00005	2.06609
R22	2.07976	0.00001	-0.00005	0.00006	0.00001	2.07977
R23	2.84461	0.00002	0.00010	0.00001	0.00010	2.84471
R24	2.28302	-0.00001	0.00001	0.00000	0.00000	2.28303
R25	2.55154	-0.00002	-0.00009	0.00000	-0.00010	2.55144

R26	1.83179	0.00001	0.00001	0.00000	0.00002	1.83181
A1	1.87529	-0.00001	0.00002	-0.00002	0.00000	1.87530
A2	2.27858	0.00001	0.00000	0.00002	0.00001	2.27859
A3	2.12928	0.00000	-0.00002	0.00000	-0.00002	2.12927
A4	1.86926	0.00001	-0.00001	0.00003	0.00002	1.86928
A5	2.28611	-0.00001	-0.00004	-0.00004	-0.00008	2.28603
A6	2.12723	0.00000	0.00005	0.00001	0.00006	2.12730
A7	1.89195	-0.00001	0.00001	-0.00002	-0.00002	1.89194
A8	2.22648	0.00001	0.00002	0.00007	0.00009	2.22657
A9	2.15377	0.00000	0.00002	-0.00002	0.00000	2.15378
A10	1.89017	0.00001	0.00002	0.00001	0.00003	1.89020
A11	1.80297	-0.00001	-0.00003	-0.00014	-0.00017	1.80280
A12	2.18853	0.00000	-0.00002	0.00001	-0.00002	2.18851
A13	1.90676	0.00000	0.00001	0.00007	0.00008	1.90684
A14	2.19280	-0.00001	-0.00007	-0.00002	-0.00008	2.19271
A15	1.89477	0.00000	-0.00004	0.00001	-0.00003	1.89474
A16	2.20005	-0.00001	0.00000	-0.00008	-0.00009	2.19996
A17	2.17504	0.00001	-0.00001	0.00004	0.00003	2.17506
A18	1.87945	-0.00001	-0.00002	0.00004	0.00002	1.87946
A19	1.88383	0.00000	0.00004	-0.00004	0.00000	1.88383
A20	1.94573	0.00001	0.00006	0.00006	0.00012	1.94584
A21	1.87444	0.00000	0.00001	0.00002	0.00002	1.87447
A22	1.92336	0.00000	0.00013	-0.00004	0.00008	1.92344
A23	1.95394	-0.00001	-0.00020	-0.00003	-0.00024	1.95371
A24	1.20094	0.00001	0.00008	-0.00006	0.00003	1.20097
A25	1.33614	0.00000	0.00008	-0.00009	-0.00001	1.33614
A26	2.15314	0.00002	0.00005	0.00009	0.00014	2.15328
A27	1.95528	0.00000	0.00001	-0.00001	0.00000	1.95528
A28	2.17386	-0.00001	-0.00006	-0.00007	-0.00014	2.17373
A29	2.08583	0.00000	-0.00003	-0.00002	-0.00005	2.08578
A30	2.14540	0.00001	0.00005	0.00004	0.00009	2.14549
A31	2.05196	0.00000	-0.00002	-0.00002	-0.00004	2.05192
A32	1.95423	-0.00001	-0.00023	0.00003	-0.00019	1.95403
A33	1.90879	0.00001	0.00029	-0.00004	0.00025	1.90904
A34	1.93343	-0.00001	-0.00019	0.00001	-0.00018	1.93325
A35	1.85947	0.00000	0.00004	-0.00001	0.00003	1.85949
A36	1.90407	0.00001	-0.00023	0.00018	-0.00005	1.90402
A37	1.90183	0.00000	0.00034	-0.00017	0.00017	1.90200
A38	2.60644	-0.00001	-0.00007	0.00022	0.00015	2.60659
A39	2.18874	-0.00002	-0.00008	-0.00003	-0.00011	2.18863
A40	1.94927	0.00003	0.00009	0.00003	0.00012	1.94940
A41	2.14515	-0.00001	0.00000	-0.00001	-0.00001	2.14514
A42	1.87510	0.00001	0.00003	0.00000	0.00003	1.87514
D1	0.00464	0.00000	0.00019	-0.00029	-0.00010	0.00454

D2	3.10912	0.00000	0.00006	-0.00008	-0.00002	3.10910
D3	-3.12869	0.00000	0.00006	-0.00010	-0.00004	-3.12873
D4	-0.02422	0.00000	-0.00007	0.00011	0.00004	-0.02417
D5	-0.05037	0.00001	-0.00015	0.00026	0.00011	-0.05026
D6	-3.02297	0.00001	0.00022	0.00048	0.00070	-3.02227
D7	3.08382	0.00000	-0.00003	0.00009	0.00005	3.08388
D8	0.11123	0.00001	0.00034	0.00031	0.00064	0.11187
D9	0.04231	0.00000	-0.00016	0.00022	0.00006	0.04237
D10	3.02793	0.00001	0.00014	0.00045	0.00059	3.02852
D11	-3.06629	0.00000	-0.00005	0.00004	-0.00001	-3.06630
D12	-0.08067	0.00000	0.00025	0.00027	0.00052	-0.08015
D13	-0.07412	0.00000	0.00007	-0.00006	0.00000	-0.07412
D14	1.94672	0.00000	0.00007	-0.00005	0.00003	1.94675
D15	-3.05922	0.00000	0.00053	-0.00003	0.00049	-3.05873
D16	-3.06769	0.00000	-0.00022	-0.00029	-0.00050	-3.06819
D17	-1.04685	-0.00001	-0.00021	-0.00027	-0.00048	-1.04733
D18	0.23039	-0.00001	0.00024	-0.00026	-0.00001	0.23038
D19	0.62761	-0.00001	-0.00108	-0.00096	-0.00204	0.62556
D20	-2.47019	-0.00002	-0.00104	-0.00120	-0.00224	-2.47244
D21	-2.69147	-0.00001	-0.00075	-0.00070	-0.00145	-2.69292
D22	0.49391	-0.00001	-0.00071	-0.00094	-0.00165	0.49227
D23	0.07705	-0.00001	0.00005	-0.00012	-0.00007	0.07698
D24	3.05265	-0.00001	-0.00031	-0.00035	-0.00066	3.05199
D25	-1.87511	0.00001	0.00006	0.00001	0.00007	-1.87503
D26	1.10049	0.00000	-0.00030	-0.00022	-0.00052	1.09997
D27	3.06167	0.00000	-0.00041	-0.00014	-0.00055	3.06112
D28	-0.24592	0.00000	-0.00077	-0.00038	-0.00114	-0.24706
D29	-2.26248	0.00000	0.00002	-0.00002	0.00000	-2.26247
D30	-0.25349	0.00000	0.00005	-0.00005	-0.00001	-0.25350
D31	-2.86195	0.00000	0.00019	0.00013	0.00033	-2.86162
D32	-0.84327	0.00000	0.00021	0.00015	0.00036	-0.84290
D33	1.30947	0.00000	0.00001	0.00013	0.00014	1.30962
D34	0.47462	0.00001	0.00062	0.00039	0.00102	0.47564
D35	2.49331	0.00001	0.00064	0.00041	0.00105	2.49436
D36	-1.63714	0.00001	0.00044	0.00039	0.00083	-1.63631
D37	-1.08986	0.00000	-0.00013	0.00004	-0.00008	-1.08994
D38	0.96702	0.00000	-0.00003	0.00002	-0.00001	0.96701
D39	3.06353	0.00000	0.00046	-0.00021	0.00025	3.06377
D40	3.10740	0.00000	-0.00022	-0.00002	-0.00023	3.10717
D41	-1.11890	0.00000	-0.00013	-0.00004	-0.00016	-1.11907
D42	0.97760	0.00000	0.00037	-0.00027	0.00010	0.97770
D43	1.02244	0.00000	-0.00018	0.00001	-0.00017	1.02228
D44	3.07932	0.00000	-0.00009	-0.00001	-0.00009	3.07923
D45	-1.10735	0.00000	0.00040	-0.00024	0.00016	-1.10719

D46	0.00470	0.00001	0.00004	0.00050	0.00054	0.00524
D47	0.37935	0.00000	0.00001	0.00050	0.00050	0.37985
D48	-3.08807	-0.00002	-0.00002	-0.00047	-0.00049	-3.08856
D49	0.05013	0.00000	-0.00001	-0.00005	-0.00007	0.05006
D50	0.00423	-0.00001	-0.00006	-0.00020	-0.00027	0.00396
D51	-3.14076	0.00001	-0.00005	0.00022	0.00016	-3.14060
D52	-0.34782	0.00000	-0.00002	-0.00051	-0.00052	-0.34834
D53	1.76753	0.00000	-0.00011	-0.00049	-0.00060	1.76693
D54	-2.46359	0.00001	-0.00017	-0.00038	-0.00056	-2.46414
D55	-0.17495	0.00000	0.00118	-0.00071	0.00047	-0.17447
D56	2.97356	-0.00001	0.00096	-0.00068	0.00029	2.97384
D57	-2.33383	0.00000	0.00176	-0.00088	0.00088	-2.33296
D58	0.81467	0.00000	0.00153	-0.00085	0.00069	0.81536
D59	1.92571	0.00000	0.00164	-0.00086	0.00078	1.92649
D60	-1.20897	0.00000	0.00142	-0.00083	0.00059	-1.20837
D61	3.09315	0.00000	0.00052	-0.00029	0.00023	3.09338
D62	-0.04174	0.00000	0.00031	-0.00026	0.00005	-0.04168

Item	Value	Threshold	Converged?
Maximum Force	0.000033	0.000450	YES
RMS Force	0.000009	0.000300	YES
Maximum Displacement	0.005464	0.001800	NO
RMS Displacement	0.000809	0.001200	YES

Predicted change in Energy=-1.302153D-07

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.330836	-2.229295	-0.386309
2	6	0	-1.580512	-1.780440	-0.650966
3	7	0	-1.803090	-0.680508	0.171937
4	6	0	-0.679075	-0.443746	0.879689
5	7	0	0.206103	-1.409981	0.599280
6	6	0	1.589519	-1.442772	1.091447
7	1	0	0.223347	-3.047485	-0.811919
8	1	0	-2.314639	-2.116490	-1.360450
9	1	0	1.618397	-0.897850	2.033702
10	1	0	1.844859	-2.481454	1.307256
11	35	0	0.267435	2.052103	-0.196854
12	1	0	-0.573629	0.296219	1.648839
13	6	0	-2.921108	0.197455	0.161915
14	6	0	-4.161085	-0.202422	-0.090281

15	1	0	-2.631180	1.227604	0.340311
16	1	0	-4.958262	0.527245	-0.130409
17	1	0	-4.421616	-1.239858	-0.263912
18	6	0	2.557337	-0.812802	0.086476
19	1	0	2.576829	-1.359459	-0.860178
20	1	0	2.225039	0.209655	-0.148915
21	6	0	3.951551	-0.756541	0.651368
22	8	0	4.251862	-0.988939	1.798267
23	8	0	4.855766	-0.400380	-0.285911
24	1	0	5.718959	-0.340632	0.151091

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.353959	0.000000			
3	N	2.208599	1.391603	0.000000		
4	C	2.216350	2.223116	1.349214	0.000000	
5	N	1.389592	2.211865	2.179819	1.340067	0.000000
6	C	2.547576	3.633059	3.596712	2.487853	1.468721
7	H	1.075964	2.210253	3.267568	3.233475	2.161759
8	H	2.212950	1.074821	2.161466	3.239038	3.270143
9	H	3.380638	4.268422	3.901280	2.610812	2.077118
10	H	2.768645	4.007396	4.223729	3.271897	2.082019
11	Br	4.327145	4.278961	3.448223	2.878209	3.552973
12	H	3.252537	3.258132	2.155646	1.072501	2.149576
13	C	3.591542	2.523894	1.421578	2.439887	3.543246
14	C	4.343576	3.076339	2.420220	3.622633	4.583233
15	H	4.215413	3.336894	2.086858	2.625843	3.882538
16	H	5.392315	4.123782	3.391930	4.502728	5.563808
17	H	4.210517	2.917861	2.712843	3.993524	4.710608
18	C	3.251388	4.312996	4.363271	3.352574	2.479494
19	H	3.071755	4.183836	4.550816	3.803496	2.784405
20	H	3.540809	4.323743	4.137772	3.149418	2.694275
21	C	4.645925	5.774787	5.775079	4.646791	3.802378
22	O	5.226086	6.375092	6.277143	5.045311	4.240638
23	O	5.500532	6.592686	6.680454	5.656410	4.839651
24	H	6.360493	7.483223	7.529753	6.440212	5.633468

		6	7	8	9	10
6	C	0.000000				
7	H	2.839777	0.000000			
8	H	4.659200	2.758443	0.000000		
9	H	1.088861	3.829446	5.336115	0.000000	
10	H	1.091161	2.727745	4.954924	1.756932	0.000000
11	Br	3.952439	5.136735	5.039665	3.937347	5.030283

12	H	2.830898	4.227394	4.231796	2.525649	3.698815
13	C	4.888776	4.622292	2.835444	5.030943	5.585947
14	C	6.000366	5.276209	2.947261	6.196559	6.574074
15	H	5.050684	5.268050	3.765070	5.044208	5.892964
16	H	6.946030	6.331842	3.935871	7.068714	7.576385
17	H	6.165381	5.014331	2.531844	6.471304	6.578666
18	C	1.530850	3.353868	5.246841	2.163454	2.186854
19	H	2.188736	2.896660	4.974919	3.083216	2.548024
20	H	2.161689	3.880117	5.242846	2.521587	3.083349
21	C	2.498756	4.614016	6.720269	2.715589	2.800655
22	O	2.791707	5.222989	7.373452	2.645537	2.874432
23	O	3.694871	5.361265	7.450797	4.013557	3.991819
24	H	4.376215	6.201306	8.365233	4.546353	4.574767

		11	12	13	14	15
11	Br	0.000000				
12	H	2.682741	0.000000			
13	C	3.706108	2.780531	0.000000		
14	C	4.970516	4.017837	1.327044	0.000000	
15	H	3.061096	2.610218	1.084938	2.137988	0.000000
16	H	5.444035	4.737520	2.084277	1.081441	2.475357
17	H	5.729634	4.563458	2.121019	1.083650	3.107912
18	C	3.678533	3.670676	5.571326	6.748407	5.581075
19	H	4.172776	4.354518	5.804823	6.879750	5.937797
20	H	2.688704	3.327455	5.155540	6.399673	4.985822
21	C	4.709636	4.751896	6.955797	8.165289	6.882292
22	O	5.394822	4.995931	7.452294	8.658112	7.376650
23	O	5.203401	5.805760	7.812664	9.021145	7.687447
24	H	5.963671	6.499654	8.656813	9.883958	8.498235

		16	17	18	19	20
16	H	0.000000				
17	H	1.851611	0.000000			
18	C	7.637211	7.000782	0.000000		
19	H	7.801911	7.024819	1.093328	0.000000	
20	H	7.190342	6.803847	1.100567	1.758343	0.000000
21	C	9.035710	8.436899	1.505358	2.130292	2.134205
22	O	9.531264	8.918788	2.415092	3.163914	3.055512
23	O	9.858997	9.315312	2.364644	2.538340	2.704004
24	H	10.716133	10.188823	3.197339	3.454512	3.549690

		21	22	23	24
21	C	0.000000			
22	O	1.208127	0.000000		
23	O	1.350166	2.248310	0.000000	
24	H	1.883345	2.299100	0.969352	0.000000

Stoichiometry C8H11BrN2O2

Framework group C1[X(C8H11BrN2O2)]
Deg. of freedom 66
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.660249	-2.162022	-0.761203
2	6	0	-1.968932	-1.826519	-0.850591
3	7	0	-2.211013	-0.860385	0.121284
4	6	0	-1.047629	-0.584159	0.746276
5	7	0	-0.105987	-1.407727	0.265831
6	6	0	1.317975	-1.344011	0.619967
7	1	0	-0.076002	-2.859268	-1.335834
8	1	0	-2.736898	-2.157455	-1.525832
9	1	0	1.391953	-0.911736	1.616604
10	1	0	1.695668	-2.366032	0.678738
11	35	0	-0.470074	2.108558	-0.090259
12	1	0	-0.935301	0.069108	1.589415
13	6	0	-3.404909	-0.116149	0.325268
14	6	0	-4.619072	-0.618827	0.140419
15	1	0	-3.200731	0.912195	0.604394
16	1	0	-5.484032	0.017965	0.266341
17	1	0	-4.792942	-1.651665	-0.137634
18	6	0	2.107956	-0.499083	-0.382794
19	1	0	2.081552	-0.927215	-1.388464
20	1	0	1.653648	0.500676	-0.455837
21	6	0	3.541479	-0.354667	0.053391
22	8	0	3.982152	-0.683344	1.129193
23	8	0	4.302612	0.205125	-0.911108
24	1	0	5.196864	0.309052	-0.551726

Rotational constants (GHZ): 0.8053305 0.3345684 0.2550566
Standard basis: 6-311++G(d,p) (5D, 7F)
There are 404 symmetry adapted cartesian basis functions of A symmetry.
There are 389 symmetry adapted basis functions of A symmetry.
389 basis functions, 625 primitive gaussians, 404 cartesian basis functions
62 alpha electrons 62 beta electrons
nuclear repulsion energy 1072.5915901237 Hartrees.
NAtoms= 24 NActive= 24 NUniq= 24 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 389 RedAO= T EigKep= 6.51D-06 NBF= 389
NBsUse= 389 1.00D-06 EigRej= -1.00D+00 NBFU= 389
Initial guess from the checkpoint file: "./cooh.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 -0.000070 -0.000007 0.000023 Ang= -0.01 deg.
Keep R1 ints in memory in canonical form, NReq=2910765817.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3145.73224366 A.U. after 8 cycles
NFock= 8 Conv=0.83D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000007022	0.000013444	-0.000024427
2	6	-0.000003435	-0.000001229	0.000000401
3	7	0.000011071	0.000033535	-0.000036965
4	6	-0.000013354	-0.000037178	0.000019346
5	7	-0.000009424	0.000000091	0.000012756
6	6	0.000004646	-0.000000872	-0.000010817
7	1	0.000003675	0.000008835	-0.000019080
8	1	0.000005103	0.000009676	-0.000015884
9	1	-0.000002438	-0.000012186	-0.000000756
10	1	-0.000002015	-0.000010764	-0.000009992
11	35	0.000001604	0.000008590	0.000008664
12	1	-0.000000124	-0.000008337	0.000004224
13	6	0.000010045	-0.000021645	0.000023469
14	6	0.000000289	0.000003568	-0.000007407
15	1	-0.000009017	-0.000007130	0.000016286
16	1	0.000000443	-0.000001966	0.000000867
17	1	-0.000000880	0.000001840	-0.000014571
18	6	0.000005326	-0.000030703	-0.000011919
19	1	-0.000002635	0.000021753	0.000003518
20	1	-0.000000367	0.000020306	0.000026650
21	6	-0.000011728	0.000001205	0.000008681

```
      22        8                0.000000074     -0.000006484      0.000007058
      23        8                0.000007520      0.000006134      0.000006272
      24        1               -0.000001400      0.000009518      0.000013626
 ---------------------------------------------------------------------
 Cartesian Forces:  Max        0.000037178 RMS        0.000013162

 GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
 Berny optimization.
 Using GEDIIS/GDIIS optimizer.
 FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
 GSVD:  received Info=                1 from GESDD.
 Internal  Forces:  Max        0.000013183 RMS        0.000003985
 Search for a local minimum.
 Step number  16 out of a maximum of  140
 All quantities printed in internal units (Hartrees-Bohrs-Radians)
 Mixed Optimization -- En-DIIS/RFO-DIIS
 Swapping is turned off.
 Update second derivatives using D2CorX and points      4      6      7      8      9
                                                       10     11     12     13     14
                                                       15     16
 DE= -4.27D-07 DEPred=-1.30D-07 R= 3.28D+00
 Trust test= 3.28D+00 RLast= 5.61D-03 DXMaxT set to 7.14D-01
 ITU=  0  1  1  1  1  1  1  1  1  1  0 -1  1  1  1  0
      Eigenvalues ---      0.00136     0.00224     0.00345     0.00399     0.00914
      Eigenvalues ---      0.01346     0.01793     0.01842     0.02144     0.02228
      Eigenvalues ---      0.02361     0.02419     0.02459     0.03026     0.03051
      Eigenvalues ---      0.03149     0.03318     0.03558     0.04163     0.04407
      Eigenvalues ---      0.05158     0.05277     0.06379     0.07161     0.09598
      Eigenvalues ---      0.09756     0.10901     0.12734     0.15560     0.15826
      Eigenvalues ---      0.15916     0.15993     0.15996     0.16001     0.16012
      Eigenvalues ---      0.16714     0.17858     0.20429     0.21800     0.23097
      Eigenvalues ---      0.24416     0.25073     0.27411     0.27818     0.34380
      Eigenvalues ---      0.34454     0.35177     0.35286     0.35499     0.35578
      Eigenvalues ---      0.35843     0.36032     0.36521     0.36607     0.36658
      Eigenvalues ---      0.37493     0.41344     0.42650     0.43468     0.47325
      Eigenvalues ---      0.52422     0.53227     0.54055     0.54455     0.59923
      Eigenvalues ---      0.93015
 En-DIIS/RFO-DIIS IScMMF=              0 using points:      16     15     14     13     12
 RFO step:  Lambda=-1.04367538D-08.
 DidBck=F Rises=F RFO-DIIS coefs:         1.53041      -0.40575      -0.24454       0.18330      -
0.06342
 Iteration  1 RMS(Cart)=  0.00069405 RMS(Int)=  0.00000050
 Iteration  2 RMS(Cart)=  0.00000059 RMS(Int)=  0.00000030
 Variable            Old X       -DE/DX      Delta X      Delta X      Delta X          New X
```

			(Linear)	(Quad)	(Total)	
R1	2.55861	0.00000	0.00000	0.00000	-0.00001	2.55860
R2	2.62595	0.00000	0.00001	0.00000	0.00001	2.62595
R3	2.03328	0.00000	0.00000	0.00000	0.00000	2.03328
R4	2.62975	0.00000	0.00000	-0.00001	0.00000	2.62974
R5	2.03112	0.00000	-0.00001	0.00000	-0.00001	2.03111
R6	2.54965	-0.00001	-0.00005	0.00001	-0.00004	2.54961
R7	2.68639	-0.00001	-0.00002	-0.00005	-0.00007	2.68632
R8	2.53236	-0.00001	0.00001	-0.00001	0.00000	2.53236
R9	5.43903	0.00001	0.00050	-0.00008	0.00042	5.43944
R10	2.02673	0.00000	0.00002	-0.00001	0.00001	2.02674
R11	2.77548	0.00000	-0.00002	-0.00001	-0.00002	2.77546
R12	2.05765	0.00000	-0.00002	0.00000	-0.00001	2.05764
R13	2.06200	0.00000	0.00000	0.00001	0.00001	2.06201
R14	2.89289	0.00000	0.00002	0.00001	0.00003	2.89292
R15	5.06965	0.00001	0.00081	0.00016	0.00097	5.07061
R16	5.08091	0.00000	-0.00022	-0.00029	-0.00051	5.08040
R17	2.50775	0.00000	0.00000	0.00001	0.00000	2.50775
R18	2.05024	0.00000	-0.00002	-0.00001	-0.00003	2.05020
R19	2.04363	0.00000	0.00000	0.00000	-0.00001	2.04362
R20	2.04780	0.00000	-0.00001	0.00000	-0.00001	2.04779
R21	2.06609	-0.00001	0.00000	-0.00001	-0.00002	2.06608
R22	2.07977	0.00001	0.00003	0.00001	0.00005	2.07982
R23	2.84471	0.00000	0.00005	-0.00002	0.00003	2.84475
R24	2.28303	0.00000	-0.00001	0.00001	0.00000	2.28302
R25	2.55144	0.00001	-0.00003	0.00002	-0.00002	2.55143
R26	1.83181	0.00000	0.00001	0.00000	0.00001	1.83182
A1	1.87530	0.00000	0.00002	0.00000	0.00002	1.87532
A2	2.27859	0.00000	0.00000	0.00000	0.00000	2.27859
A3	2.12927	0.00000	-0.00002	0.00000	-0.00001	2.12926
A4	1.86928	0.00000	-0.00001	0.00000	-0.00001	1.86926
A5	2.28603	0.00000	-0.00002	-0.00002	-0.00004	2.28599
A6	2.12730	0.00000	0.00004	0.00001	0.00005	2.12735
A7	1.89194	0.00000	0.00000	0.00000	0.00000	1.89194
A8	2.22657	0.00001	0.00004	0.00004	0.00009	2.22666
A9	2.15378	0.00000	0.00000	0.00000	-0.00001	2.15377
A10	1.89020	0.00000	0.00003	0.00000	0.00002	1.89022
A11	1.80280	-0.00001	-0.00014	-0.00007	-0.00021	1.80259
A12	2.18851	0.00000	0.00001	-0.00001	0.00000	2.18852
A13	1.90684	0.00000	-0.00010	-0.00002	-0.00013	1.90672
A14	2.19271	0.00000	-0.00003	0.00001	-0.00002	2.19269
A15	1.89474	0.00000	-0.00003	-0.00001	-0.00004	1.89470
A16	2.19996	0.00000	-0.00005	-0.00004	-0.00008	2.19988
A17	2.17506	0.00000	0.00003	0.00002	0.00005	2.17511

A18	1.87946	0.00000	0.00010	-0.00008	0.00001	1.87948
A19	1.88383	0.00000	-0.00001	-0.00001	-0.00002	1.88381
A20	1.94584	0.00000	0.00008	-0.00001	0.00007	1.94591
A21	1.87447	0.00000	0.00003	0.00000	0.00002	1.87449
A22	1.92344	0.00000	-0.00003	0.00003	0.00000	1.92344
A23	1.95371	0.00000	-0.00016	0.00008	-0.00008	1.95362
A24	1.20097	0.00000	0.00008	0.00001	0.00009	1.20105
A25	1.33614	0.00000	0.00008	-0.00003	0.00004	1.33618
A26	2.15328	0.00001	0.00006	0.00005	0.00011	2.15339
A27	1.95528	0.00000	0.00000	0.00002	0.00002	1.95531
A28	2.17373	-0.00001	-0.00006	-0.00008	-0.00014	2.17358
A29	2.08578	0.00000	-0.00002	-0.00002	-0.00004	2.08574
A30	2.14549	0.00000	0.00004	0.00003	0.00007	2.14556
A31	2.05192	0.00000	-0.00002	-0.00001	-0.00003	2.05188
A32	1.95403	0.00000	-0.00006	0.00007	0.00001	1.95404
A33	1.90904	0.00000	0.00010	-0.00004	0.00006	1.90910
A34	1.93325	0.00000	-0.00011	0.00004	-0.00006	1.93318
A35	1.85949	0.00000	0.00002	-0.00002	0.00000	1.85949
A36	1.90402	0.00000	0.00010	0.00002	0.00012	1.90414
A37	1.90200	0.00000	-0.00005	-0.00008	-0.00013	1.90187
A38	2.60659	0.00000	-0.00014	0.00006	-0.00008	2.60651
A39	2.18863	0.00000	-0.00006	0.00002	-0.00004	2.18859
A40	1.94940	0.00000	0.00006	0.00000	0.00006	1.94945
A41	2.14514	0.00000	0.00000	-0.00002	-0.00002	2.14512
A42	1.87514	0.00000	0.00001	0.00000	0.00001	1.87515
D1	0.00454	0.00000	-0.00009	0.00027	0.00018	0.00472
D2	3.10910	0.00000	0.00002	0.00013	0.00015	3.10925
D3	-3.12873	0.00000	-0.00005	0.00008	0.00003	-3.12870
D4	-0.02417	0.00000	0.00006	-0.00006	0.00000	-0.02417
D5	-0.05026	0.00000	0.00011	-0.00027	-0.00016	-0.05042
D6	-3.02227	0.00000	0.00040	-0.00010	0.00030	-3.02197
D7	3.08388	0.00000	0.00007	-0.00010	-0.00002	3.08385
D8	0.11187	0.00000	0.00036	0.00007	0.00043	0.11230
D9	0.04237	0.00000	0.00004	-0.00018	-0.00014	0.04223
D10	3.02852	0.00000	0.00034	0.00012	0.00046	3.02898
D11	-3.06630	0.00000	-0.00006	-0.00006	-0.00012	-3.06641
D12	-0.08015	0.00000	0.00025	0.00024	0.00049	-0.07966
D13	-0.07412	0.00000	0.00003	0.00002	0.00005	-0.07407
D14	1.94675	0.00000	-0.00014	-0.00004	-0.00019	1.94656
D15	-3.05873	0.00000	-0.00003	0.00005	0.00003	-3.05871
D16	-3.06819	0.00000	-0.00027	-0.00027	-0.00054	-3.06873
D17	-1.04733	-0.00001	-0.00044	-0.00033	-0.00077	-1.04810
D18	0.23038	-0.00001	-0.00032	-0.00023	-0.00056	0.22982
D19	0.62556	-0.00001	-0.00110	-0.00087	-0.00198	0.62359

D20	-2.47244	-0.00001	-0.00105	-0.00080	-0.00185	-2.47429
D21	-2.69292	-0.00001	-0.00075	-0.00053	-0.00129	-2.69421
D22	0.49227	0.00000	-0.00070	-0.00046	-0.00116	0.49110
D23	0.07698	0.00000	-0.00008	0.00015	0.00007	0.07705
D24	3.05199	-0.00001	-0.00037	-0.00002	-0.00040	3.05159
D25	-1.87503	0.00001	0.00012	0.00024	0.00036	-1.87467
D26	1.09997	0.00000	-0.00017	0.00007	-0.00010	1.09987
D27	3.06112	0.00001	-0.00002	0.00011	0.00009	3.06121
D28	-0.24706	0.00000	-0.00031	-0.00006	-0.00037	-0.24743
D29	-2.26247	0.00000	0.00010	-0.00010	0.00000	-2.26247
D30	-0.25350	0.00000	0.00002	-0.00015	-0.00013	-0.25363
D31	-2.86162	-0.00001	-0.00020	-0.00015	-0.00035	-2.86197
D32	-0.84290	-0.00001	-0.00012	-0.00020	-0.00032	-0.84323
D33	1.30962	0.00000	-0.00028	-0.00012	-0.00040	1.30922
D34	0.47564	0.00000	0.00014	0.00005	0.00019	0.47583
D35	2.49436	0.00000	0.00022	0.00000	0.00021	2.49457
D36	-1.63631	0.00000	0.00006	0.00008	0.00014	-1.63617
D37	-1.08994	0.00000	0.00018	0.00006	0.00023	-1.08971
D38	0.96701	0.00000	0.00023	0.00005	0.00027	0.96728
D39	3.06377	-0.00001	0.00017	-0.00005	0.00011	3.06389
D40	3.10717	0.00000	0.00002	0.00015	0.00017	3.10734
D41	-1.11907	0.00000	0.00007	0.00014	0.00021	-1.11885
D42	0.97770	0.00000	0.00001	0.00004	0.00005	0.97775
D43	1.02228	0.00000	0.00011	0.00009	0.00020	1.02247
D44	3.07923	0.00000	0.00016	0.00008	0.00024	3.07947
D45	-1.10719	-0.00001	0.00010	-0.00002	0.00008	-1.10711
D46	0.00524	0.00000	0.00031	0.00050	0.00081	0.00605
D47	0.37985	0.00000	0.00026	0.00052	0.00078	0.38064
D48	-3.08856	0.00000	0.00000	0.00004	0.00004	-3.08852
D49	0.05006	0.00000	-0.00002	-0.00002	-0.00004	0.05002
D50	0.00396	0.00000	-0.00006	-0.00004	-0.00009	0.00387
D51	-3.14060	0.00000	-0.00007	-0.00010	-0.00017	-3.14077
D52	-0.34834	0.00000	-0.00038	-0.00049	-0.00087	-0.34921
D53	1.76693	0.00000	-0.00039	-0.00044	-0.00083	1.76610
D54	-2.46414	0.00000	-0.00028	-0.00047	-0.00075	-2.46490
D55	-0.17447	0.00000	-0.00017	-0.00037	-0.00055	-0.17502
D56	2.97384	0.00000	-0.00021	-0.00028	-0.00049	2.97335
D57	-2.33296	-0.00001	-0.00009	-0.00051	-0.00060	-2.33356
D58	0.81536	0.00000	-0.00013	-0.00042	-0.00055	0.81482
D59	1.92649	0.00000	-0.00015	-0.00045	-0.00059	1.92590
D60	-1.20837	0.00000	-0.00018	-0.00036	-0.00054	-1.20891
D61	3.09338	0.00000	-0.00012	-0.00010	-0.00022	3.09316
D62	-0.04168	0.00000	-0.00016	-0.00001	-0.00017	-0.04185

Item	Value	Threshold	Converged?

Maximum Force	0.000013	0.000450	YES
RMS Force	0.000004	0.000300	YES
Maximum Displacement	0.005002	0.001800	NO
RMS Displacement	0.000694	0.001200	YES

Predicted change in Energy=-5.071642D-08

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.330800	-2.229219	-0.385986
2	6	0	-1.580487	-1.780413	-0.650649
3	7	0	-1.803061	-0.680439	0.172194
4	6	0	-0.679112	-0.443730	0.880031
5	7	0	0.206069	-1.409990	0.599716
6	6	0	1.589577	-1.442625	1.091594
7	1	0	0.223402	-3.047408	-0.811576
8	1	0	-2.314580	-2.116539	-1.360128
9	1	0	1.618618	-0.897636	2.033797
10	1	0	1.845039	-2.481283	1.307402
11	35	0	0.267552	2.051963	-0.197329
12	1	0	-0.573691	0.296243	1.649184
13	6	0	-2.921257	0.197244	0.162582
14	6	0	-4.160989	-0.202427	-0.091152
15	1	0	-2.631736	1.227210	0.342585
16	1	0	-4.958199	0.527224	-0.130839
17	1	0	-4.421313	-1.239612	-0.266559
18	6	0	2.557233	-0.812724	0.086398
19	1	0	2.576438	-1.359340	-0.860275
20	1	0	2.225062	0.209824	-0.148891
21	6	0	3.951544	-0.756528	0.651107
22	8	0	4.251882	-0.988399	1.798102
23	8	0	4.855787	-0.401052	-0.286394
24	1	0	5.718995	-0.341120	0.150560

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.353954	0.000000			
3	N	2.208583	1.391601	0.000000		
4	C	2.216324	2.223102	1.349195	0.000000	
5	N	1.389595	2.211879	2.179822	1.340067	0.000000

6	C	2.547514	3.633018	3.596696	2.487871	1.468709
7	H	1.075964	2.210247	3.267552	3.233451	2.161755
8	H	2.212923	1.074818	2.161492	3.239037	3.270148
9	H	3.380636	4.268469	3.901363	2.610895	2.077111
10	H	2.768641	4.007419	4.223786	3.271943	2.081997
11	Br	4.326908	4.278767	3.448188	2.878430	3.553051
12	H	3.252518	3.258124	2.155634	1.072506	2.149567
13	C	3.591534	2.523913	1.421542	2.439835	3.543227
14	C	4.343404	3.076047	2.420262	3.622829	4.583306
15	H	4.215688	3.337279	2.086830	2.625572	3.882535
16	H	5.392207	4.123630	3.391927	4.502798	5.563827
17	H	4.210211	2.917239	2.713010	3.994016	4.710852
18	C	3.251206	4.312817	4.363144	3.352602	2.479555
19	H	3.071429	4.183452	4.550485	3.803369	2.784383
20	H	3.540844	4.323773	4.137806	3.149610	2.694540
21	C	4.645735	5.774624	5.775000	4.646851	3.802399
22	O	5.225978	6.374966	6.277002	5.045218	4.240574
23	O	5.500254	6.592491	6.680465	5.656631	4.839733
24	H	6.360254	7.483044	7.529737	6.440375	5.633523

		6	7	8	9	10
6	C	0.000000				
7	H	2.839686	0.000000			
8	H	4.659136	2.758401	0.000000		
9	H	1.088854	3.829399	5.336150	0.000000	
10	H	1.091167	2.727685	4.954914	1.756945	0.000000
11	Br	3.952368	5.136421	5.039435	3.937440	5.030208
12	H	2.830954	4.227375	4.231804	2.525766	3.698882
13	C	4.888748	4.622297	2.835541	5.030972	5.585937
14	C	6.000499	5.275965	2.946752	6.196982	6.574306
15	H	5.050596	5.268421	3.765697	5.043876	5.892818
16	H	6.946079	6.331696	3.935651	7.068974	7.576522
17	H	6.165760	5.013836	2.530459	6.472199	6.579230
18	C	1.530866	3.353645	5.246611	2.163463	2.186816
19	H	2.188750	2.896329	4.974460	3.083220	2.548043
20	H	2.161766	3.880123	5.242843	2.521581	3.083386
21	C	2.498729	4.613742	6.720045	2.715564	2.800512
22	O	2.791655	5.222890	7.373299	2.645348	2.874436
23	O	3.694841	5.360783	7.450500	4.013619	3.991510
24	H	4.376180	6.200907	8.364964	4.546359	4.574508

		11	12	13	14	15
11	Br	0.000000				
12	H	2.683253	0.000000			
13	C	3.706483	2.780441	0.000000		
14	C	4.970465	4.018227	1.327047	0.000000	

15	H	3.062286	2.609492	1.084921	2.137897	0.000000
16	H	5.444053	4.737693	2.084254	1.081439	2.475185
17	H	5.729285	4.564331	2.121057	1.083645	3.107869
18	C	3.678256	3.670803	5.571328	6.748221	5.581430
19	H	4.172222	4.354498	5.804640	6.879165	5.938198
20	H	2.688432	3.327696	5.155752	6.399604	4.986493
21	C	4.709486	4.752078	6.955842	8.165241	6.882586
22	O	5.394481	4.995862	7.452154	8.658142	7.376426
23	O	5.203567	5.806196	7.812935	9.021076	7.688293
24	H	5.963732	6.500000	8.657017	9.883913	8.498897

		16	17	18	19	20
16	H	0.000000				
17	H	1.851587	0.000000			
18	C	7.637039	7.000494	0.000000		
19	H	7.801407	7.023913	1.093320	0.000000	
20	H	7.190292	6.803603	1.100592	1.758354	0.000000
21	C	9.035650	8.436837	1.505376	2.130393	2.134145
22	O	9.531186	8.919094	2.415083	3.164124	3.055245
23	O	9.859016	9.314943	2.364698	2.538323	2.704217
24	H	10.716141	10.188578	3.197384	3.454595	3.549758

		21	22	23	24
21	C	0.000000			
22	O	1.208125	0.000000		
23	O	1.350157	2.248288	0.000000	
24	H	1.883346	2.299084	0.969356	0.000000

Stoichiometry C8H11BrN2O2
Framework group C1[X(C8H11BrN2O2)]
Deg. of freedom 66
Full point group C1 NOp 1
Largest Abelian subgroup C1 NOp 1
Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.660216	-2.161829	-0.761128
2	6	0	-1.968900	-1.826345	-0.850504
3	7	0	-2.210999	-0.860318	0.121469
4	6	0	-1.047677	-0.584276	0.746617
5	7	0	-0.106019	-1.407811	0.266148
6	6	0	1.317983	-1.343971	0.620053
7	1	0	-0.075942	-2.858986	-1.335841
8	1	0	-2.736812	-2.157235	-1.525823

9	1	0	1.392091	-0.911769	1.616703
10	1	0	1.695781	-2.365968	0.678656
11	35	0	-0.469992	2.108528	-0.090308
12	1	0	-0.935386	0.068857	1.589870
13	6	0	-3.404997	-0.116446	0.325934
14	6	0	-4.619101	-0.618673	0.139459
15	1	0	-3.201030	0.911439	0.606832
16	1	0	-5.484041	0.018038	0.265901
17	1	0	-4.792982	-1.650987	-0.140508
18	6	0	2.107818	-0.498948	-0.382768
19	1	0	2.081142	-0.926906	-1.388496
20	1	0	1.653649	0.500920	-0.455559
21	6	0	3.541416	-0.354651	0.053274
22	8	0	3.982045	-0.682997	1.129192
23	8	0	4.302648	0.204641	-0.911424
24	1	0	5.196885	0.308690	-0.552030

Rotational constants (GHZ): 0.8053590 0.3345668 0.2550647

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 404 symmetry adapted cartesian basis functions of A symmetry.

There are 389 symmetry adapted basis functions of A symmetry.

389 basis functions, 625 primitive gaussians, 404 cartesian basis functions

62 alpha electrons 62 beta electrons

nuclear repulsion energy 1072.5938979982 Hartrees.

NAtoms= 24 NActive= 24 NUniq= 24 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F

Integral buffers will be 131072 words long.

Raffenetti 2 integral format.

Two-electron integral symmetry is turned on.

One-electron integrals computed using PRISM.

NBasis= 389 RedAO= T EigKep= 6.50D-06 NBF= 389

NBsUse= 389 1.00D-06 EigRej= -1.00D+00 NBFU= 389

Initial guess from the checkpoint file: "./cooh.chk"

B after Tr= 0.000000 0.000000 0.000000

Rot= 1.000000 0.000006 0.000002 0.000006 Ang= 0.00 deg.

Keep R1 ints in memory in canonical form, NReq=2910765817.

Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.

Requested convergence on MAX density matrix=1.00D-06.

Requested convergence on energy=1.00D-06.

No special actions if energy rises.

SCF Done: E(RB3LYP) = -3145.73224388 A.U. after 8 cycles

NFock= 8 Conv=0.45D-08 -V/T= 2.0017

Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.

***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000000958	0.000001879	-0.000012543
2	6	0.000003564	0.000007302	-0.000008647
3	7	-0.000012921	0.000013492	-0.000022880
4	6	0.000005762	-0.000020341	0.000025675
5	7	-0.000006710	0.000011310	-0.000018691
6	6	0.000014678	-0.000003633	-0.000010082
7	1	0.000003080	0.000009227	-0.000019618
8	1	0.000005058	0.000012337	-0.000017749
9	1	-0.000001878	-0.000011282	0.000003255
10	1	-0.000005077	-0.000008159	-0.000006422
11	35	-0.000003273	-0.000001369	0.000018604
12	1	0.000000877	-0.000005690	-0.000000541
13	6	0.000013147	-0.000018584	0.000011991
14	6	-0.000002331	0.000003070	-0.000006529
15	1	-0.000006990	-0.000004856	0.000014472
16	1	-0.000000392	-0.000002196	0.000002933
17	1	0.000000362	0.000000659	-0.000012518
18	6	0.000012966	-0.000013790	-0.000004567
19	1	0.000003421	0.000020177	0.000003000
20	1	-0.000008338	0.000006192	0.000028227
21	6	-0.000021058	-0.000007559	0.000006499
22	8	0.000001986	-0.000007409	0.000015455
23	8	0.000008131	0.000013182	-0.000002203
24	1	-0.000005022	0.000006041	0.000012878

Cartesian Forces: Max 0.000028227 RMS 0.000011162

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Berny optimization.

Using GEDIIS/GDIIS optimizer.

FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.

Internal Forces: Max 0.000013048 RMS 0.000003992

Search for a local minimum.

Step number 17 out of a maximum of 140

All quantities printed in internal units (Hartrees-Bohrs-Radians)

Mixed Optimization -- En-DIIS/RFO-DIIS

Swapping is turned off.

Update second derivatives using D2CorX and points 4 6 7 8 9
10 11 12 13 14

15 16 17

DE= -2.20D-07 DEPred=-5.07D-08 R= 4.34D+00

Trust test= 4.34D+00 RLast= 4.53D-03 DXMaxT set to 7.14D-01

ITU= 0 0 1 1 1 1 1 1 1 1 1 0 -1 1 1 1 0

Eigenvalues --- 0.00133 0.00206 0.00273 0.00385 0.00803

Eigenvalues --- 0.01226 0.01816 0.01847 0.02164 0.02197

Eigenvalues --- 0.02413 0.02433 0.02493 0.03033 0.03067

Eigenvalues --- 0.03146 0.03320 0.03608 0.04185 0.04382

Eigenvalues --- 0.05134 0.05253 0.06321 0.07215 0.09725

Eigenvalues --- 0.10222 0.10990 0.12754 0.15572 0.15771

Eigenvalues --- 0.15906 0.15991 0.15997 0.16001 0.16025

Eigenvalues --- 0.16722 0.17915 0.20457 0.21705 0.23137

Eigenvalues --- 0.24387 0.25224 0.27508 0.27928 0.34368

Eigenvalues --- 0.34537 0.35183 0.35449 0.35577 0.35646

Eigenvalues --- 0.35843 0.36098 0.36584 0.36652 0.36758

Eigenvalues --- 0.37773 0.41346 0.42710 0.43491 0.47341

Eigenvalues --- 0.52596 0.53598 0.54138 0.54490 0.59929

Eigenvalues --- 0.93583

En-DIIS/RFO-DIIS IScMMF= 0 using points: 17 16 15 14 13

RFO step: Lambda=-5.82023818D-09.

DidBck=F Rises=F RFO-DIIS coefs: 1.71507 -0.75936 -0.07679 0.15152 -0.03043

Iteration 1 RMS(Cart)= 0.00049959 RMS(Int)= 0.00000029

Iteration 2 RMS(Cart)= 0.00000031 RMS(Int)= 0.00000019

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55860	0.00000	-0.00001	0.00000	-0.00001	2.55860
R2	2.62595	0.00000	0.00000	0.00001	0.00001	2.62596
R3	2.03328	0.00000	0.00000	0.00000	0.00000	2.03328
R4	2.62974	0.00000	0.00000	-0.00001	-0.00001	2.62973
R5	2.03111	0.00000	0.00000	0.00000	0.00000	2.03111
R6	2.54961	0.00001	-0.00001	0.00002	0.00000	2.54961
R7	2.68632	-0.00001	-0.00004	-0.00003	-0.00007	2.68625
R8	2.53236	-0.00001	-0.00001	-0.00001	-0.00002	2.53234
R9	5.43944	0.00000	0.00014	-0.00002	0.00012	5.43956
R10	2.02674	0.00000	0.00000	0.00000	0.00000	2.02675
R11	2.77546	0.00001	-0.00001	0.00003	0.00002	2.77548
R12	2.05764	0.00000	-0.00001	0.00001	0.00000	2.05764
R13	2.06201	0.00000	0.00001	-0.00001	0.00001	2.06201
R14	2.89292	-0.00001	0.00000	-0.00004	-0.00004	2.89288
R15	5.07061	0.00000	0.00034	-0.00004	0.00031	5.07092
R16	5.08040	0.00000	-0.00017	-0.00019	-0.00036	5.08004
R17	2.50775	0.00000	0.00001	0.00000	0.00001	2.50776
R18	2.05020	0.00000	-0.00002	-0.00001	-0.00002	2.05018

R19	2.04362	0.00000	0.00000	0.00000	0.00000	2.04362
R20	2.04779	0.00000	0.00000	0.00000	-0.00001	2.04779
R21	2.06608	-0.00001	-0.00002	-0.00001	-0.00003	2.06605
R22	2.07982	0.00000	0.00004	0.00000	0.00003	2.07985
R23	2.84475	-0.00001	0.00000	-0.00004	-0.00003	2.84471
R24	2.28302	0.00001	0.00000	0.00001	0.00000	2.28303
R25	2.55143	0.00001	0.00001	0.00001	0.00002	2.55145
R26	1.83182	0.00000	0.00000	0.00000	0.00000	1.83181
A1	1.87532	0.00000	0.00000	0.00001	0.00001	1.87532
A2	2.27859	0.00000	0.00000	-0.00001	-0.00001	2.27858
A3	2.12926	0.00000	0.00000	0.00000	0.00000	2.12925
A4	1.86926	0.00000	0.00000	-0.00001	0.00000	1.86926
A5	2.28599	0.00000	-0.00002	0.00000	-0.00002	2.28597
A6	2.12735	0.00000	0.00002	0.00001	0.00003	2.12738
A7	1.89194	0.00000	0.00000	0.00000	0.00000	1.89194
A8	2.22666	0.00000	0.00005	0.00001	0.00007	2.22673
A9	2.15377	0.00000	0.00000	0.00000	-0.00001	2.15376
A10	1.89022	0.00000	0.00001	0.00000	0.00001	1.89023
A11	1.80259	0.00000	-0.00012	-0.00007	-0.00020	1.80240
A12	2.18852	0.00000	0.00000	0.00001	0.00001	2.18853
A13	1.90672	0.00000	-0.00008	-0.00002	-0.00010	1.90662
A14	2.19269	0.00000	0.00000	0.00001	0.00001	2.19270
A15	1.89470	0.00000	-0.00001	0.00000	-0.00001	1.89469
A16	2.19988	0.00000	-0.00006	0.00003	-0.00003	2.19985
A17	2.17511	0.00000	0.00003	-0.00001	0.00002	2.17513
A18	1.87948	0.00000	-0.00004	0.00005	0.00001	1.87949
A19	1.88381	0.00000	-0.00002	-0.00001	-0.00003	1.88378
A20	1.94591	0.00000	0.00003	-0.00002	0.00000	1.94592
A21	1.87449	0.00000	0.00001	-0.00002	-0.00001	1.87448
A22	1.92344	0.00000	-0.00001	-0.00003	-0.00004	1.92340
A23	1.95362	0.00000	0.00002	0.00003	0.00005	1.95368
A24	1.20105	0.00000	0.00004	-0.00004	0.00000	1.20106
A25	1.33618	0.00000	0.00001	-0.00008	-0.00007	1.33611
A26	2.15339	0.00001	0.00006	0.00003	0.00009	2.15349
A27	1.95531	0.00000	0.00002	0.00001	0.00003	1.95534
A28	2.17358	-0.00001	-0.00008	-0.00004	-0.00012	2.17346
A29	2.08574	0.00000	-0.00002	-0.00001	-0.00002	2.08571
A30	2.14556	0.00000	0.00003	0.00001	0.00005	2.14560
A31	2.05188	0.00000	-0.00002	0.00000	-0.00002	2.05186
A32	1.95404	0.00000	0.00007	0.00002	0.00008	1.95413
A33	1.90910	-0.00001	-0.00002	-0.00008	-0.00010	1.90900
A34	1.93318	0.00001	0.00001	0.00001	0.00003	1.93321
A35	1.85949	0.00000	-0.00002	0.00001	0.00000	1.85949
A36	1.90414	0.00000	0.00011	-0.00001	0.00010	1.90424

A37	1.90187	0.00000	-0.00015	0.00004	-0.00011	1.90175
A38	2.60651	0.00001	-0.00002	0.00013	0.00011	2.60662
A39	2.18859	0.00001	0.00000	0.00002	0.00002	2.18861
A40	1.94945	-0.00001	0.00002	-0.00003	-0.00001	1.94944
A41	2.14512	0.00000	-0.00002	0.00001	0.00000	2.14512
A42	1.87515	0.00000	0.00000	-0.00002	-0.00002	1.87513
D1	0.00472	0.00000	0.00011	-0.00016	-0.00005	0.00468
D2	3.10925	0.00000	0.00009	-0.00009	0.00000	3.10926
D3	-3.12870	0.00000	0.00002	-0.00006	-0.00003	-3.12873
D4	-0.02417	0.00000	0.00000	0.00001	0.00002	-0.02415
D5	-0.05042	0.00000	-0.00011	0.00015	0.00004	-0.05038
D6	-3.02197	0.00000	0.00010	0.00006	0.00015	-3.02182
D7	3.08385	0.00000	-0.00003	0.00006	0.00003	3.08389
D8	0.11230	0.00000	0.00018	-0.00004	0.00014	0.11244
D9	0.04223	0.00000	-0.00008	0.00012	0.00004	0.04226
D10	3.02898	0.00000	0.00024	0.00020	0.00044	3.02942
D11	-3.06641	0.00000	-0.00006	0.00005	-0.00001	-3.06642
D12	-0.07966	0.00000	0.00026	0.00014	0.00040	-0.07926
D13	-0.07407	0.00000	0.00001	-0.00002	-0.00001	-0.07408
D14	1.94656	0.00000	-0.00013	-0.00009	-0.00021	1.94634
D15	-3.05871	0.00000	-0.00008	-0.00015	-0.00023	-3.05893
D16	-3.06873	0.00000	-0.00030	-0.00010	-0.00040	-3.06913
D17	-1.04810	0.00000	-0.00044	-0.00017	-0.00061	-1.04871
D18	0.22982	-0.00001	-0.00039	-0.00023	-0.00062	0.22920
D19	0.62359	0.00000	-0.00099	-0.00035	-0.00134	0.62225
D20	-2.47429	0.00000	-0.00098	-0.00032	-0.00130	-2.47559
D21	-2.69421	0.00000	-0.00062	-0.00026	-0.00087	-2.69508
D22	0.49110	0.00000	-0.00061	-0.00022	-0.00083	0.49027
D23	0.07705	0.00000	0.00006	-0.00008	-0.00002	0.07703
D24	3.05159	0.00000	-0.00015	0.00002	-0.00014	3.05145
D25	-1.87467	0.00000	0.00023	0.00002	0.00025	-1.87442
D26	1.09987	0.00000	0.00002	0.00012	0.00014	1.10001
D27	3.06121	0.00000	0.00015	0.00005	0.00020	3.06141
D28	-0.24743	0.00000	-0.00006	0.00014	0.00008	-0.24735
D29	-2.26247	0.00000	-0.00002	-0.00011	-0.00013	-2.26260
D30	-0.25363	0.00000	-0.00011	-0.00015	-0.00026	-0.25389
D31	-2.86197	0.00000	-0.00025	0.00012	-0.00014	-2.86211
D32	-0.84323	0.00000	-0.00027	0.00011	-0.00015	-0.84338
D33	1.30922	0.00000	-0.00024	0.00013	-0.00010	1.30912
D34	0.47583	0.00000	-0.00001	0.00001	-0.00001	0.47582
D35	2.49457	-0.00001	-0.00003	0.00000	-0.00002	2.49455
D36	-1.63617	0.00000	0.00001	0.00002	0.00003	-1.63614
D37	-1.08971	0.00000	0.00015	0.00003	0.00018	-1.08953
D38	0.96728	0.00000	0.00016	0.00001	0.00017	0.96745

D39	3.06389	0.00000	-0.00004	0.00002	-0.00002	3.06387
D40	3.10734	0.00000	0.00019	0.00000	0.00019	3.10753
D41	-1.11885	0.00000	0.00019	-0.00002	0.00017	-1.11868
D42	0.97775	0.00000	-0.00001	-0.00001	-0.00002	0.97774
D43	1.02247	0.00000	0.00016	0.00002	0.00019	1.02266
D44	3.07947	0.00000	0.00017	0.00000	0.00017	3.07964
D45	-1.10711	0.00000	-0.00003	0.00001	-0.00002	-1.10713
D46	0.00605	0.00000	0.00052	0.00040	0.00093	0.00698
D47	0.38064	0.00000	0.00052	0.00043	0.00095	0.38159
D48	-3.08852	0.00000	-0.00009	0.00004	-0.00005	-3.08857
D49	0.05002	0.00000	-0.00003	-0.00001	-0.00004	0.04999
D50	0.00387	0.00000	-0.00008	0.00000	-0.00009	0.00378
D51	-3.14077	0.00000	-0.00003	-0.00005	-0.00008	-3.14085
D52	-0.34921	0.00000	-0.00055	-0.00038	-0.00093	-0.35014
D53	1.76610	0.00000	-0.00050	-0.00039	-0.00089	1.76521
D54	-2.46490	-0.00001	-0.00046	-0.00037	-0.00083	-2.46572
D55	-0.17502	0.00000	-0.00058	-0.00007	-0.00065	-0.17567
D56	2.97335	0.00000	-0.00049	-0.00007	-0.00056	2.97279
D57	-2.33356	-0.00001	-0.00075	-0.00010	-0.00084	-2.33440
D58	0.81482	0.00000	-0.00066	-0.00010	-0.00076	0.81406
D59	1.92590	0.00000	-0.00070	-0.00013	-0.00083	1.92506
D60	-1.20891	0.00000	-0.00061	-0.00013	-0.00075	-1.20966
D61	3.09316	0.00000	-0.00023	0.00003	-0.00020	3.09296
D62	-0.04185	0.00000	-0.00014	0.00003	-0.00011	-0.04196

Item	Value	Threshold	Converged?
Maximum Force	0.000013	0.000450	YES
RMS Force	0.000004	0.000300	YES
Maximum Displacement	0.003399	0.001800	NO
RMS Displacement	0.000500	0.001200	YES

Predicted change in Energy=-2.237803D-08

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.330797	-2.229188	-0.385818
2	6	0	-1.580448	-1.780329	-0.650546
3	7	0	-1.803030	-0.680382	0.172322
4	6	0	-0.679097	-0.443717	0.880205
5	7	0	0.206073	-1.409978	0.599906
6	6	0	1.589627	-1.442591	1.091693
7	1	0	0.223389	-3.047399	-0.811385

8	1	0	-2.314504	-2.116447	-1.360063
9	1	0	1.618753	-0.897541	2.033861
10	1	0	1.845061	-2.481247	1.307560
11	35	0	0.267555	2.051761	-0.197828
12	1	0	-0.573618	0.296360	1.649253
13	6	0	-2.921355	0.197079	0.163077
14	6	0	-4.160929	-0.202440	-0.091681
15	1	0	-2.632143	1.226911	0.344265
16	1	0	-4.958178	0.527190	-0.130924
17	1	0	-4.421114	-1.239441	-0.268358
18	6	0	2.557201	-0.812732	0.086424
19	1	0	2.576268	-1.359206	-0.860317
20	1	0	2.225017	0.209872	-0.148681
21	6	0	3.951541	-0.756470	0.651009
22	8	0	4.251914	-0.987649	1.798138
23	8	0	4.855786	-0.401695	-0.286772
24	1	0	5.718999	-0.341495	0.150133

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.353951	0.000000			
3	N	2.208572	1.391595	0.000000		
4	C	2.216311	2.223097	1.349197	0.000000	
5	N	1.389599	2.211887	2.179824	1.340057	0.000000
6	C	2.547508	3.633020	3.596710	2.487888	1.468721
7	H	1.075964	2.210240	3.267540	3.233437	2.161756
8	H	2.212908	1.074816	2.161503	3.239040	3.270151
9	H	3.380661	4.268517	3.901420	2.610937	2.077133
10	H	2.768650	4.007440	4.223796	3.271932	2.081989
11	Br	4.326649	4.278432	3.448034	2.878493	3.552998
12	H	3.252517	3.258131	2.155644	1.072509	2.149566
13	C	3.591525	2.523917	1.421504	2.439797	3.543198
14	C	4.343287	3.075865	2.420293	3.622973	4.583355
15	H	4.215902	3.337544	2.086806	2.625379	3.882525
16	H	5.392146	4.123555	3.391924	4.502840	5.563831
17	H	4.209999	2.916849	2.713136	3.994378	4.711031
18	C	3.251137	4.312715	4.363085	3.352595	2.479551
19	H	3.071325	4.183256	4.550318	3.803280	2.784359
20	H	3.540824	4.323694	4.137724	3.149551	2.694520
21	C	4.645677	5.774532	5.774947	4.646843	3.802396
22	O	5.226118	6.375016	6.276944	5.045129	4.240631
23	O	5.500016	6.592273	6.680439	5.656725	4.839697
24	H	6.360083	7.482864	7.529691	6.440426	5.633499

		6	7	8	9	10
6	C	0.000000				
7	H	2.839669	0.000000			
8	H	4.659123	2.758373	0.000000		
9	H	1.088857	3.829406	5.336194	0.000000	
10	H	1.091170	2.727687	4.954925	1.756945	0.000000
11	Br	3.952371	5.136130	5.039026	3.937582	5.030198
12	H	2.830981	4.227373	4.231821	2.525829	3.698901
13	C	4.888743	4.622297	2.835600	5.030964	5.585875
14	C	6.000604	5.275794	2.946439	6.197243	6.574402
15	H	5.050567	5.268710	3.766122	5.043624	5.892685
16	H	6.946119	6.331614	3.935557	7.069099	7.576542
17	H	6.166037	5.013481	2.529578	6.472796	6.579555
18	C	1.530846	3.353576	5.246476	2.163421	2.186838
19	H	2.188779	2.896278	4.974214	3.083218	2.548201
20	H	2.161686	3.880143	5.242754	2.521391	3.083363
21	C	2.498720	4.613682	6.719916	2.715525	2.800566
22	O	2.791739	5.223140	7.373348	2.645226	2.874794
23	O	3.694783	5.360417	7.450194	4.013675	3.991352
24	H	4.376147	6.200658	8.364707	4.546387	4.574447

		11	12	13	14	15
11	Br	0.000000				
12	H	2.683415	0.000000			
13	C	3.706648	2.780367	0.000000		
14	C	4.970328	4.018514	1.327050	0.000000	
15	H	3.063085	2.608916	1.084908	2.137822	0.000000
16	H	5.443994	4.737792	2.084240	1.081436	2.475046
17	H	5.728926	4.564990	2.121085	1.083643	3.107831
18	C	3.678125	3.670770	5.571371	6.748145	5.581749
19	H	4.171780	4.354380	5.804585	6.878861	5.938565
20	H	2.688239	3.327523	5.155822	6.399497	4.986920
21	C	4.709399	4.752053	6.955863	8.165213	6.882788
22	O	5.394165	4.995659	7.452032	8.658169	7.376195
23	O	5.203770	5.806368	7.813118	9.021027	7.688930
24	H	5.963807	6.500096	8.657133	9.883865	8.499362

		16	17	18	19	20
16	H	0.000000				
17	H	1.851569	0.000000			
18	C	7.636986	7.000345	0.000000		
19	H	7.801177	7.023397	1.093305	0.000000	
20	H	7.190222	6.803373	1.100609	1.758354	0.000000
21	C	9.035612	8.436814	1.505358	2.130440	2.134058
22	O	9.531096	8.919372	2.415079	3.164368	3.054909
23	O	9.859057	9.314667	2.364681	2.538107	2.704446

24	H	10.716142	10.188392	3.197356	3.454491	3.549817
		21	22	23	24	
21	C	0.000000				
22	O	1.208127	0.000000			
23	O	1.350170	2.248300	0.000000		
24	H	1.883345	2.299081	0.969354	0.000000	

Stoichiometry C8H11BrN2O2

Framework group C1[X(C8H11BrN2O2)]

Deg. of freedom 66

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.660206	-2.161676	-0.761139
2	6	0	-1.968864	-1.826109	-0.850532
3	7	0	-2.210963	-0.860248	0.121599
4	6	0	-1.047649	-0.584353	0.746830
5	7	0	-0.106003	-1.407828	0.266265
6	6	0	1.318032	-1.344010	0.620092
7	1	0	-0.075946	-2.858782	-1.335927
8	1	0	-2.736745	-2.156882	-1.525941
9	1	0	1.392214	-0.911876	1.616769
10	1	0	1.695803	-2.366026	0.678613
11	35	0	-0.470006	2.108432	-0.090402
12	1	0	-0.935320	0.068782	1.590081
13	6	0	-3.405024	-0.116673	0.326511
14	6	0	-4.619098	-0.618580	0.138955
15	1	0	-3.201219	0.910867	0.608738
16	1	0	-5.484023	0.018041	0.265923
17	1	0	-4.792997	-1.650510	-0.142402
18	6	0	2.107791	-0.498893	-0.382677
19	1	0	2.080958	-0.926575	-1.388501
20	1	0	1.653630	0.501021	-0.455137
21	6	0	3.541397	-0.354583	0.053274
22	8	0	3.982002	-0.682412	1.129363
23	8	0	4.302679	0.204182	-0.911707
24	1	0	5.196888	0.308445	-0.552311

Rotational constants (GHZ): 0.8054144 0.3345616 0.2550745

Standard basis: 6-311++G(d,p) (5D, 7F)

There are 404 symmetry adapted cartesian basis functions of A symmetry.
There are 389 symmetry adapted basis functions of A symmetry.
389 basis functions, 625 primitive gaussians, 404 cartesian basis functions
62 alpha electrons 62 beta electrons
nuclear repulsion energy 1072.6014735930 Hartrees.
NAtoms= 24 NActive= 24 NUniq= 24 SFac= 1.00D+00 NAtFMM= 60 NAOKFM=F Big=F
Integral buffers will be 131072 words long.
Raffenetti 2 integral format.
Two-electron integral symmetry is turned on.
One-electron integrals computed using PRISM.
NBasis= 389 RedAO= T EigKep= 6.50D-06 NBF= 389
NBsUse= 389 1.00D-06 EigRej= -1.00D+00 NBFU= 389
Initial guess from the checkpoint file: "./cooh.chk"
B after Tr= 0.000000 0.000000 0.000000
Rot= 1.000000 0.000013 0.000000 -0.000002 Ang= 0.00 deg.
Keep R1 ints in memory in canonical form, NReq=2910765817.
Requested convergence on RMS density matrix=1.00D-08 within 128 cycles.
Requested convergence on MAX density matrix=1.00D-06.
Requested convergence on energy=1.00D-06.
No special actions if energy rises.
SCF Done: E(RB3LYP) = -3145.73224403 A.U. after 8 cycles
NFock= 8 Conv=0.67D-08 -V/T= 2.0017
Calling FoFJK, ICntrl= 2127 FMM=F ISym2X=0 I1Cent= 0 IOpClX= 0 NMat=1 NMatS=1 NMatT=0.
***** Axes restored to original set *****

Center Number	Atomic Number	Forces (Hartrees/Bohr) X	Y	Z
1	6	0.000004133	0.000005417	-0.000015470
2	6	0.000001751	0.000003615	-0.000004386
3	7	-0.000012500	0.000004488	-0.000012666
4	6	0.000006244	-0.000007471	0.000015802
5	7	-0.000000999	0.000005362	-0.000020538
6	6	0.000004998	-0.000009752	-0.000000914
7	1	0.000004279	0.000010081	-0.000021043
8	1	0.000004416	0.000011886	-0.000016672
9	1	-0.000004043	-0.000013107	0.000002854
10	1	-0.000003108	-0.000007670	-0.000008711
11	35	-0.000002719	-0.000002957	0.000023404
12	1	-0.000000992	-0.000008244	0.000001747
13	6	0.000008751	-0.000010043	0.000005314
14	6	-0.000002588	0.000000394	-0.000003049

15	1	-0.000004909	-0.000003293	0.000012341
16	1	-0.000000437	-0.000001856	0.000002141
17	1	0.000001410	-0.000000088	-0.000012115
18	6	0.000008973	0.000004658	-0.000002547
19	1	0.000004538	0.000014273	0.000000371
20	1	-0.000007669	0.000001492	0.000021206
21	6	-0.000011820	-0.000006625	0.000007239
22	8	-0.000000012	-0.000008392	0.000009558
23	8	0.000004773	0.000012977	0.000003652
24	1	-0.000002468	0.000004857	0.000012481

Cartesian Forces: Max 0.000023404 RMS 0.000008937

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad
Berny optimization.
Using GEDIIS/GDIIS optimizer.
FormGI is forming the generalized inverse of G from B-inverse, IUseBI=4.
GSVD: received Info= 1 from GESDD.
Internal Forces: Max 0.000008265 RMS 0.000002353
Search for a local minimum.
Step number 18 out of a maximum of 140
All quantities printed in internal units (Hartrees-Bohrs-Radians)
Mixed Optimization -- En-DIIS/RFO-DIIS
Swapping is turned off.
Update second derivatives using D2CorX and points 4 6 7 8 9
10 11 12 13 14
15 16 17 18
DE= -1.49D-07 DEPred=-2.24D-08 R= 6.64D+00
Trust test= 6.64D+00 RLast= 3.83D-03 DXMaxT set to 7.14D-01
ITU= 0 0 0 1 1 1 1 1 1 1 1 1 0 -1 1 1 1 0

Eigenvalues ---	0.00124	0.00182	0.00249	0.00385	0.00858
Eigenvalues ---	0.01181	0.01819	0.01850	0.02100	0.02197
Eigenvalues ---	0.02394	0.02429	0.02471	0.03032	0.03103
Eigenvalues ---	0.03143	0.03337	0.03717	0.04048	0.04353
Eigenvalues ---	0.05088	0.05260	0.06347	0.07165	0.09718
Eigenvalues ---	0.09899	0.11022	0.12689	0.15573	0.15700
Eigenvalues ---	0.15929	0.15987	0.15996	0.16001	0.16014
Eigenvalues ---	0.16704	0.17833	0.20456	0.21666	0.23165
Eigenvalues ---	0.24405	0.25038	0.27337	0.27836	0.34328
Eigenvalues ---	0.34452	0.35178	0.35458	0.35577	0.35647
Eigenvalues ---	0.35843	0.36110	0.36584	0.36651	0.36767
Eigenvalues ---	0.37183	0.41350	0.42417	0.43574	0.47358
Eigenvalues ---	0.52526	0.53014	0.54093	0.54530	0.59926
Eigenvalues ---	0.93033				

En-DIIS/RFO-DIIS IScMMF= 0 using points: 18 17 16 15 14
RFO step: Lambda=-2.04003476D-09.
DidBck=F Rises=F RFO-DIIS coefs: 1.47846 -0.50958 -0.09727 0.14102 -0.01263
Iteration 1 RMS(Cart)= 0.00018354 RMS(Int)= 0.00000004
Iteration 2 RMS(Cart)= 0.00000005 RMS(Int)= 0.00000002

Variable	Old X	-DE/DX	Delta X (Linear)	Delta X (Quad)	Delta X (Total)	New X
R1	2.55860	0.00000	0.00000	0.00000	0.00000	2.55859
R2	2.62596	0.00000	0.00000	-0.00001	0.00000	2.62596
R3	2.03328	0.00000	0.00000	0.00000	0.00000	2.03328
R4	2.62973	0.00000	-0.00001	0.00000	-0.00001	2.62973
R5	2.03111	0.00000	0.00000	0.00000	0.00000	2.03111
R6	2.54961	0.00001	0.00001	0.00001	0.00002	2.54963
R7	2.68625	-0.00001	-0.00003	-0.00001	-0.00004	2.68621
R8	2.53234	0.00000	-0.00002	0.00001	-0.00001	2.53233
R9	5.43956	0.00000	-0.00002	-0.00010	-0.00012	5.43944
R10	2.02675	0.00000	0.00000	0.00000	0.00000	2.02675
R11	2.77548	0.00000	0.00002	0.00000	0.00002	2.77550
R12	2.05764	0.00000	0.00001	0.00000	0.00001	2.05765
R13	2.06201	0.00000	0.00000	0.00000	0.00000	2.06202
R14	2.89288	0.00000	-0.00003	0.00002	-0.00002	2.89286
R15	5.07092	0.00000	-0.00007	-0.00002	-0.00008	5.07084
R16	5.08004	0.00000	-0.00005	-0.00015	-0.00020	5.07983
R17	2.50776	0.00000	0.00000	0.00000	0.00001	2.50777
R18	2.05018	0.00000	-0.00001	0.00000	-0.00001	2.05017
R19	2.04362	0.00000	0.00000	0.00000	0.00000	2.04362
R20	2.04779	0.00000	0.00000	0.00000	0.00000	2.04779
R21	2.06605	0.00000	-0.00002	0.00000	-0.00002	2.06603
R22	2.07985	0.00000	0.00001	-0.00001	0.00001	2.07986
R23	2.84471	-0.00001	-0.00003	0.00000	-0.00003	2.84468
R24	2.28303	0.00000	0.00000	0.00000	0.00000	2.28303
R25	2.55145	0.00001	0.00002	0.00000	0.00003	2.55148
R26	1.83181	0.00000	0.00000	0.00000	0.00000	1.83181
A1	1.87532	0.00000	0.00000	-0.00001	-0.00001	1.87532
A2	2.27858	0.00000	0.00000	0.00001	0.00000	2.27858
A3	2.12925	0.00000	0.00000	0.00001	0.00001	2.12926
A4	1.86926	0.00000	-0.00001	0.00002	0.00001	1.86927
A5	2.28597	0.00000	0.00000	-0.00002	-0.00002	2.28595
A6	2.12738	0.00000	0.00001	0.00000	0.00000	2.12738
A7	1.89194	0.00000	0.00000	-0.00001	-0.00001	1.89193
A8	2.22673	0.00000	0.00002	0.00001	0.00003	2.22675
A9	2.15376	0.00000	0.00000	0.00001	0.00001	2.15377
A10	1.89023	0.00000	0.00000	0.00000	0.00000	1.89023

A11	1.80240	0.00000	-0.00007	0.00000	-0.00007	1.80233
A12	2.18853	0.00000	0.00001	-0.00001	0.00000	2.18853
A13	1.90662	0.00000	-0.00004	-0.00002	-0.00006	1.90656
A14	2.19270	0.00000	0.00001	0.00001	0.00002	2.19272
A15	1.89469	0.00000	0.00000	0.00001	0.00001	1.89470
A16	2.19985	0.00000	0.00000	0.00000	0.00000	2.19985
A17	2.17513	0.00000	0.00001	0.00000	0.00000	2.17514
A18	1.87949	0.00000	0.00001	-0.00003	-0.00002	1.87947
A19	1.88378	0.00000	-0.00001	0.00000	-0.00001	1.88377
A20	1.94592	0.00000	-0.00002	-0.00001	-0.00002	1.94589
A21	1.87448	0.00000	-0.00001	0.00000	-0.00001	1.87447
A22	1.92340	0.00000	-0.00002	0.00001	-0.00001	1.92339
A23	1.95368	0.00000	0.00005	0.00002	0.00007	1.95375
A24	1.20106	0.00000	-0.00002	0.00000	-0.00002	1.20104
A25	1.33611	0.00000	-0.00005	-0.00003	-0.00008	1.33602
A26	2.15349	0.00000	0.00002	0.00001	0.00004	2.15353
A27	1.95534	0.00000	0.00001	0.00001	0.00002	1.95536
A28	2.17346	0.00000	-0.00004	-0.00002	-0.00006	2.17340
A29	2.08571	0.00000	-0.00001	0.00000	-0.00001	2.08571
A30	2.14560	0.00000	0.00001	0.00000	0.00001	2.14562
A31	2.05186	0.00000	-0.00001	0.00000	-0.00001	2.05186
A32	1.95413	0.00000	0.00006	0.00000	0.00006	1.95418
A33	1.90900	0.00000	-0.00008	-0.00002	-0.00010	1.90890
A34	1.93321	0.00000	0.00003	0.00000	0.00004	1.93324
A35	1.85949	0.00000	0.00000	0.00000	0.00000	1.85949
A36	1.90424	0.00000	0.00005	-0.00002	0.00003	1.90427
A37	1.90175	0.00000	-0.00006	0.00004	-0.00003	1.90173
A38	2.60662	0.00001	0.00007	0.00005	0.00012	2.60674
A39	2.18861	0.00000	0.00002	0.00000	0.00003	2.18863
A40	1.94944	-0.00001	-0.00002	0.00000	-0.00002	1.94942
A41	2.14512	0.00000	0.00000	0.00000	0.00000	2.14511
A42	1.87513	0.00000	-0.00001	0.00000	-0.00001	1.87512
D1	0.00468	0.00000	-0.00001	0.00008	0.00006	0.00474
D2	3.10926	0.00000	0.00000	0.00001	0.00001	3.10926
D3	-3.12873	0.00000	-0.00001	0.00004	0.00003	-3.12871
D4	-0.02415	0.00000	0.00000	-0.00003	-0.00003	-0.02419
D5	-0.05038	0.00000	0.00001	-0.00007	-0.00006	-0.05044
D6	-3.02182	0.00000	-0.00001	-0.00014	-0.00015	-3.02197
D7	3.08389	0.00000	0.00001	-0.00004	-0.00003	3.08386
D8	0.11244	0.00000	-0.00002	-0.00010	-0.00012	0.11233
D9	0.04226	0.00000	0.00001	-0.00006	-0.00005	0.04222
D10	3.02942	0.00000	0.00013	0.00001	0.00013	3.02955
D11	-3.06642	0.00000	0.00000	0.00001	0.00001	-3.06641
D12	-0.07926	0.00000	0.00012	0.00007	0.00019	-0.07908

D13	-0.07408	0.00000	0.00000	0.00001	0.00001	-0.07407
D14	1.94634	0.00000	-0.00008	-0.00002	-0.00010	1.94625
D15	-3.05893	0.00000	-0.00015	0.00003	-0.00012	-3.05906
D16	-3.06913	0.00000	-0.00012	-0.00005	-0.00016	-3.06930
D17	-1.04871	0.00000	-0.00019	-0.00008	-0.00027	-1.04898
D18	0.22920	0.00000	-0.00026	-0.00003	-0.00029	0.22891
D19	0.62225	0.00000	-0.00035	-0.00012	-0.00047	0.62178
D20	-2.47559	0.00000	-0.00030	-0.00017	-0.00048	-2.47606
D21	-2.69508	0.00000	-0.00022	-0.00005	-0.00027	-2.69535
D22	0.49027	0.00000	-0.00017	-0.00010	-0.00027	0.49000
D23	0.07703	0.00000	0.00000	0.00004	0.00003	0.07706
D24	3.05145	0.00000	0.00002	0.00010	0.00012	3.05157
D25	-1.87442	0.00000	0.00009	0.00005	0.00014	-1.87427
D26	1.10001	0.00000	0.00011	0.00012	0.00023	1.10024
D27	3.06141	0.00000	0.00014	0.00002	0.00016	3.06157
D28	-0.24735	0.00000	0.00016	0.00009	0.00025	-0.24710
D29	-2.26260	0.00000	-0.00007	-0.00012	-0.00019	-2.26279
D30	-0.25389	0.00000	-0.00012	-0.00013	-0.00025	-0.25414
D31	-2.86211	0.00000	-0.00005	0.00011	0.00005	-2.86205
D32	-0.84338	0.00000	-0.00007	0.00009	0.00003	-0.84336
D33	1.30912	0.00000	-0.00002	0.00012	0.00010	1.30921
D34	0.47582	0.00000	-0.00008	0.00003	-0.00005	0.47577
D35	2.49455	0.00000	-0.00009	0.00002	-0.00008	2.49447
D36	-1.63614	0.00000	-0.00004	0.00004	-0.00001	-1.63614
D37	-1.08953	0.00000	0.00007	-0.00005	0.00002	-1.08950
D38	0.96745	0.00000	0.00005	-0.00006	-0.00001	0.96744
D39	3.06387	0.00000	-0.00006	-0.00002	-0.00008	3.06379
D40	3.10753	0.00000	0.00009	-0.00002	0.00007	3.10760
D41	-1.11868	0.00000	0.00007	-0.00003	0.00004	-1.11864
D42	0.97774	0.00000	-0.00004	0.00001	-0.00003	0.97771
D43	1.02266	0.00000	0.00008	-0.00004	0.00004	1.02271
D44	3.07964	0.00000	0.00006	-0.00004	0.00001	3.07965
D45	-1.10713	0.00000	-0.00005	-0.00001	-0.00006	-1.10719
D46	0.00698	0.00000	0.00036	0.00025	0.00061	0.00759
D47	0.38159	0.00000	0.00038	0.00027	0.00065	0.38224
D48	-3.08857	0.00000	0.00005	-0.00008	-0.00003	-3.08861
D49	0.04999	0.00000	-0.00001	-0.00001	-0.00002	0.04997
D50	0.00378	0.00000	0.00000	-0.00003	-0.00003	0.00375
D51	-3.14085	0.00000	-0.00006	0.00005	-0.00001	-3.14086
D52	-0.35014	0.00000	-0.00035	-0.00019	-0.00054	-0.35068
D53	1.76521	0.00000	-0.00033	-0.00020	-0.00053	1.76469
D54	-2.46572	0.00000	-0.00031	-0.00020	-0.00051	-2.46623
D55	-0.17567	0.00000	-0.00033	0.00002	-0.00031	-0.17599
D56	2.97279	0.00000	-0.00027	0.00001	-0.00026	2.97252

D57	-2.33440	0.00000	-0.00046	0.00003	-0.00043	-2.33483
D58	0.81406	0.00000	-0.00040	0.00002	-0.00038	0.81368
D59	1.92506	0.00000	-0.00045	0.00002	-0.00043	1.92464
D60	-1.20966	0.00000	-0.00039	0.00001	-0.00038	-1.21004
D61	3.09296	0.00000	-0.00010	0.00005	-0.00005	3.09291
D62	-0.04196	0.00000	-0.00005	0.00004	-0.00001	-0.04197

Item	Value	Threshold	Converged?
Maximum Force	0.000008	0.000450	YES
RMS Force	0.000002	0.000300	YES
Maximum Displacement	0.001050	0.001800	YES
RMS Displacement	0.000184	0.001200	YES

Predicted change in Energy=-6.675148D-09

Optimization completed.

-- Stationary point found.

! Optimized Parameters !

! (Angstroms and Degrees) !

! Name	Definition	Value	Derivative Info.		
! R1	R(1,2)	1.354	-DE/DX =	0.0	!
! R2	R(1,5)	1.3896	-DE/DX =	0.0	!
! R3	R(1,7)	1.076	-DE/DX =	0.0	!
! R4	R(2,3)	1.3916	-DE/DX =	0.0	!
! R5	R(2,8)	1.0748	-DE/DX =	0.0	!
! R6	R(3,4)	1.3492	-DE/DX =	0.0	!
! R7	R(3,13)	1.4215	-DE/DX =	0.0	!
! R8	R(4,5)	1.3401	-DE/DX =	0.0	!
! R9	R(4,11)	2.8785	-DE/DX =	0.0	!
! R10	R(4,12)	1.0725	-DE/DX =	0.0	!
! R11	R(5,6)	1.4687	-DE/DX =	0.0	!
! R12	R(6,9)	1.0889	-DE/DX =	0.0	!
! R13	R(6,10)	1.0912	-DE/DX =	0.0	!
! R14	R(6,18)	1.5308	-DE/DX =	0.0	!
! R15	R(11,12)	2.6834	-DE/DX =	0.0	!
! R16	R(11,20)	2.6882	-DE/DX =	0.0	!
! R17	R(13,14)	1.3271	-DE/DX =	0.0	!
! R18	R(13,15)	1.0849	-DE/DX =	0.0	!
! R19	R(14,16)	1.0814	-DE/DX =	0.0	!
! R20	R(14,17)	1.0836	-DE/DX =	0.0	!
! R21	R(18,19)	1.0933	-DE/DX =	0.0	!
! R22	R(18,20)	1.1006	-DE/DX =	0.0	!
! R23	R(18,21)	1.5054	-DE/DX =	0.0	!
! R24	R(21,22)	1.2081	-DE/DX =	0.0	!

! R25	R(21,23)	1.3502	-DE/DX =	0.0	!
! R26	R(23,24)	0.9694	-DE/DX =	0.0	!
! A1	A(2,1,5)	107.4481	-DE/DX =	0.0	!
! A2	A(2,1,7)	130.5529	-DE/DX =	0.0	!
! A3	A(5,1,7)	121.9973	-DE/DX =	0.0	!
! A4	A(1,2,3)	107.1006	-DE/DX =	0.0	!
! A5	A(1,2,8)	130.9763	-DE/DX =	0.0	!
! A6	A(3,2,8)	121.8898	-DE/DX =	0.0	!
! A7	A(2,3,4)	108.4001	-DE/DX =	0.0	!
! A8	A(2,3,13)	127.582	-DE/DX =	0.0	!
! A9	A(4,3,13)	123.4015	-DE/DX =	0.0	!
! A10	A(3,4,5)	108.3025	-DE/DX =	0.0	!
! A11	A(3,4,11)	103.2698	-DE/DX =	0.0	!
! A12	A(3,4,12)	125.3933	-DE/DX =	0.0	!
! A13	A(5,4,11)	109.2411	-DE/DX =	0.0	!
! A14	A(5,4,12)	125.6325	-DE/DX =	0.0	!
! A15	A(1,5,4)	108.5578	-DE/DX =	0.0	!
! A16	A(1,5,6)	126.0418	-DE/DX =	0.0	!
! A17	A(4,5,6)	124.626	-DE/DX =	0.0	!
! A18	A(5,6,9)	107.6868	-DE/DX =	0.0	!
! A19	A(5,6,10)	107.9325	-DE/DX =	0.0	!
! A20	A(5,6,18)	111.4928	-DE/DX =	0.0	!
! A21	A(9,6,10)	107.3999	-DE/DX =	0.0	!
! A22	A(9,6,18)	110.2029	-DE/DX =	0.0	!
! A23	A(10,6,18)	111.9376	-DE/DX =	0.0	!
! A24	A(4,11,20)	68.8154	-DE/DX =	0.0	!
! A25	A(12,11,20)	76.5533	-DE/DX =	0.0	!
! A26	A(3,13,14)	123.3858	-DE/DX =	0.0	!
! A27	A(3,13,15)	112.0325	-DE/DX =	0.0	!
! A28	A(14,13,15)	124.5302	-DE/DX =	0.0	!
! A29	A(13,14,16)	119.5027	-DE/DX =	0.0	!
! A30	A(13,14,17)	122.9341	-DE/DX =	0.0	!
! A31	A(16,14,17)	117.563	-DE/DX =	0.0	!
! A32	A(6,18,19)	111.9632	-DE/DX =	0.0	!
! A33	A(6,18,20)	109.3777	-DE/DX =	0.0	!
! A34	A(6,18,21)	110.7646	-DE/DX =	0.0	!
! A35	A(19,18,20)	106.5408	-DE/DX =	0.0	!
! A36	A(19,18,21)	109.105	-DE/DX =	0.0	!
! A37	A(20,18,21)	108.9625	-DE/DX =	0.0	!
! A38	A(11,20,18)	149.3482	-DE/DX =	0.0	!
! A39	A(18,21,22)	125.398	-DE/DX =	0.0	!
! A40	A(18,21,23)	111.6946	-DE/DX =	0.0	!
! A41	A(22,21,23)	122.9062	-DE/DX =	0.0	!
! A42	A(21,23,24)	107.4372	-DE/DX =	0.0	!

! D1	D(5,1,2,3)	0.2679	-DE/DX =	0.0	!
! D2	D(5,1,2,8)	178.1473	-DE/DX =	0.0	!
! D3	D(7,1,2,3)	-179.2633	-DE/DX =	0.0	!
! D4	D(7,1,2,8)	-1.3839	-DE/DX =	0.0	!
! D5	D(2,1,5,4)	-2.8863	-DE/DX =	0.0	!
! D6	D(2,1,5,6)	-173.1374	-DE/DX =	0.0	!
! D7	D(7,1,5,4)	176.6936	-DE/DX =	0.0	!
! D8	D(7,1,5,6)	6.4426	-DE/DX =	0.0	!
! D9	D(1,2,3,4)	2.4215	-DE/DX =	0.0	!
! D10	D(1,2,3,13)	173.5731	-DE/DX =	0.0	!
! D11	D(8,2,3,4)	-175.693	-DE/DX =	0.0	!
! D12	D(8,2,3,13)	-4.5414	-DE/DX =	0.0	!
! D13	D(2,3,4,5)	-4.2445	-DE/DX =	0.0	!
! D14	D(2,3,4,11)	111.5173	-DE/DX =	0.0	!
! D15	D(2,3,4,12)	-175.264	-DE/DX =	0.0	!
! D16	D(13,3,4,5)	-175.8483	-DE/DX =	0.0	!
! D17	D(13,3,4,11)	-60.0865	-DE/DX =	0.0	!
! D18	D(13,3,4,12)	13.1322	-DE/DX =	0.0	!
! D19	D(2,3,13,14)	35.6522	-DE/DX =	0.0	!
! D20	D(2,3,13,15)	-141.8407	-DE/DX =	0.0	!
! D21	D(4,3,13,14)	-154.4167	-DE/DX =	0.0	!
! D22	D(4,3,13,15)	28.0904	-DE/DX =	0.0	!
! D23	D(3,4,5,1)	4.4133	-DE/DX =	0.0	!
! D24	D(3,4,5,6)	174.8353	-DE/DX =	0.0	!
! D25	D(11,4,5,1)	-107.3962	-DE/DX =	0.0	!
! D26	D(11,4,5,6)	63.0257	-DE/DX =	0.0	!
! D27	D(12,4,5,1)	175.4058	-DE/DX =	0.0	!
! D28	D(12,4,5,6)	-14.1722	-DE/DX =	0.0	!
! D29	D(3,4,11,20)	-129.6377	-DE/DX =	0.0	!
! D30	D(5,4,11,20)	-14.5469	-DE/DX =	0.0	!
! D31	D(1,5,6,9)	-163.9867	-DE/DX =	0.0	!
! D32	D(1,5,6,10)	-48.3223	-DE/DX =	0.0	!
! D33	D(1,5,6,18)	75.0068	-DE/DX =	0.0	!
! D34	D(4,5,6,9)	27.2626	-DE/DX =	0.0	!
! D35	D(4,5,6,10)	142.9271	-DE/DX =	0.0	!
! D36	D(4,5,6,18)	-93.7439	-DE/DX =	0.0	!
! D37	D(5,6,18,19)	-62.4252	-DE/DX =	0.0	!
! D38	D(5,6,18,20)	55.4308	-DE/DX =	0.0	!
! D39	D(5,6,18,21)	175.5466	-DE/DX =	0.0	!
! D40	D(9,6,18,19)	178.0484	-DE/DX =	0.0	!
! D41	D(9,6,18,20)	-64.0955	-DE/DX =	0.0	!
! D42	D(9,6,18,21)	56.0202	-DE/DX =	0.0	!
! D43	D(10,6,18,19)	58.5943	-DE/DX =	0.0	!
! D44	D(10,6,18,20)	176.4503	-DE/DX =	0.0	!

! D45	D(10,6,18,21)	-63.434	-DE/DX =	0.0 !
! D46	D(4,11,20,18)	0.3999	-DE/DX =	0.0 !
! D47	D(12,11,20,18)	21.8635	-DE/DX =	0.0 !
! D48	D(3,13,14,16)	-176.9621	-DE/DX =	0.0 !
! D49	D(3,13,14,17)	2.864	-DE/DX =	0.0 !
! D50	D(15,13,14,16)	0.2167	-DE/DX =	0.0 !
! D51	D(15,13,14,17)	-179.9572	-DE/DX =	0.0 !
! D52	D(6,18,20,11)	-20.0618	-DE/DX =	0.0 !
! D53	D(19,18,20,11)	101.1392	-DE/DX =	0.0 !
! D54	D(21,18,20,11)	-141.2756	-DE/DX =	0.0 !
! D55	D(6,18,21,22)	-10.0653	-DE/DX =	0.0 !
! D56	D(6,18,21,23)	170.3282	-DE/DX =	0.0 !
! D57	D(19,18,21,22)	-133.7514	-DE/DX =	0.0 !
! D58	D(19,18,21,23)	46.6422	-DE/DX =	0.0 !
! D59	D(20,18,21,22)	110.298	-DE/DX =	0.0 !
! D60	D(20,18,21,23)	-69.3084	-DE/DX =	0.0 !
! D61	D(18,21,23,24)	177.2136	-DE/DX =	0.0 !
! D62	D(22,21,23,24)	-2.4043	-DE/DX =	0.0 !

GradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGradGrad

Input orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.330797	-2.229188	-0.385818
2	6	0	-1.580448	-1.780329	-0.650546
3	7	0	-1.803030	-0.680382	0.172322
4	6	0	-0.679097	-0.443717	0.880205
5	7	0	0.206073	-1.409978	0.599906
6	6	0	1.589627	-1.442591	1.091693
7	1	0	0.223389	-3.047399	-0.811385
8	1	0	-2.314504	-2.116447	-1.360063
9	1	0	1.618753	-0.897541	2.033861
10	1	0	1.845061	-2.481247	1.307560
11	35	0	0.267555	2.051761	-0.197828
12	1	0	-0.573618	0.296360	1.649253
13	6	0	-2.921355	0.197079	0.163077
14	6	0	-4.160929	-0.202440	-0.091681
15	1	0	-2.632143	1.226911	0.344265
16	1	0	-4.958178	0.527190	-0.130924
17	1	0	-4.421114	-1.239441	-0.268358
18	6	0	2.557201	-0.812732	0.086424

19	1	0	2.576268	-1.359206	-0.860317
20	1	0	2.225017	0.209872	-0.148681
21	6	0	3.951541	-0.756470	0.651009
22	8	0	4.251914	-0.987649	1.798138
23	8	0	4.855786	-0.401695	-0.286772
24	1	0	5.718999	-0.341495	0.150133

Distance matrix (angstroms):

		1	2	3	4	5
1	C	0.000000				
2	C	1.353951	0.000000			
3	N	2.208572	1.391595	0.000000		
4	C	2.216311	2.223097	1.349197	0.000000	
5	N	1.389599	2.211887	2.179824	1.340057	0.000000
6	C	2.547508	3.633020	3.596710	2.487888	1.468721
7	H	1.075964	2.210240	3.267540	3.233437	2.161756
8	H	2.212908	1.074816	2.161503	3.239040	3.270151
9	H	3.380661	4.268517	3.901420	2.610937	2.077133
10	H	2.768650	4.007440	4.223796	3.271932	2.081989
11	Br	4.326649	4.278432	3.448034	2.878493	3.552998
12	H	3.252517	3.258131	2.155644	1.072509	2.149566
13	C	3.591525	2.523917	1.421504	2.439797	3.543198
14	C	4.343287	3.075865	2.420293	3.622973	4.583355
15	H	4.215902	3.337544	2.086806	2.625379	3.882525
16	H	5.392146	4.123555	3.391924	4.502840	5.563831
17	H	4.209999	2.916849	2.713136	3.994378	4.711031
18	C	3.251137	4.312715	4.363085	3.352595	2.479551
19	H	3.071325	4.183256	4.550318	3.803280	2.784359
20	H	3.540824	4.323694	4.137724	3.149551	2.694520
21	C	4.645677	5.774532	5.774947	4.646843	3.802396
22	O	5.226118	6.375016	6.276944	5.045129	4.240631
23	O	5.500016	6.592273	6.680439	5.656725	4.839697
24	H	6.360083	7.482864	7.529691	6.440426	5.633499

		6	7	8	9	10
6	C	0.000000				
7	H	2.839669	0.000000			
8	H	4.659123	2.758373	0.000000		
9	H	1.088857	3.829406	5.336194	0.000000	
10	H	1.091170	2.727687	4.954925	1.756945	0.000000
11	Br	3.952371	5.136130	5.039026	3.937582	5.030198
12	H	2.830981	4.227373	4.231821	2.525829	3.698901
13	C	4.888743	4.622297	2.835600	5.030964	5.585875
14	C	6.000604	5.275794	2.946439	6.197243	6.574402
15	H	5.050567	5.268710	3.766122	5.043624	5.892685

16	H	6.946119	6.331614	3.935557	7.069099	7.576542
17	H	6.166037	5.013481	2.529578	6.472796	6.579555
18	C	1.530846	3.353576	5.246476	2.163421	2.186838
19	H	2.188779	2.896278	4.974214	3.083218	2.548201
20	H	2.161686	3.880143	5.242754	2.521391	3.083363
21	C	2.498720	4.613682	6.719916	2.715525	2.800566
22	O	2.791739	5.223140	7.373348	2.645226	2.874794
23	O	3.694783	5.360417	7.450194	4.013675	3.991352
24	H	4.376147	6.200658	8.364707	4.546387	4.574447

		11	12	13	14	15
11	Br	0.000000				
12	H	2.683415	0.000000			
13	C	3.706648	2.780367	0.000000		
14	C	4.970328	4.018514	1.327050	0.000000	
15	H	3.063085	2.608916	1.084908	2.137822	0.000000
16	H	5.443994	4.737792	2.084240	1.081436	2.475046
17	H	5.728926	4.564990	2.121085	1.083643	3.107831
18	C	3.678125	3.670770	5.571371	6.748145	5.581749
19	H	4.171780	4.354380	5.804585	6.878861	5.938565
20	H	2.688239	3.327523	5.155822	6.399497	4.986920
21	C	4.709399	4.752053	6.955863	8.165213	6.882788
22	O	5.394165	4.995659	7.452032	8.658169	7.376195
23	O	5.203770	5.806368	7.813118	9.021027	7.688930
24	H	5.963807	6.500096	8.657133	9.883865	8.499362

		16	17	18	19	20
16	H	0.000000				
17	H	1.851569	0.000000			
18	C	7.636986	7.000345	0.000000		
19	H	7.801177	7.023397	1.093305	0.000000	
20	H	7.190222	6.803373	1.100609	1.758354	0.000000
21	C	9.035612	8.436814	1.505358	2.130440	2.134058
22	O	9.531096	8.919372	2.415079	3.164368	3.054909
23	O	9.859057	9.314667	2.364681	2.538107	2.704446
24	H	10.716142	10.188392	3.197356	3.454491	3.549817

		21	22	23	24
21	C	0.000000			
22	O	1.208127	0.000000		
23	O	1.350170	2.248300	0.000000	
24	H	1.883345	2.299081	0.969354	0.000000

Stoichiometry C8H11BrN2O2

Framework group C1[X(C8H11BrN2O2)]

Deg. of freedom 66

Full point group C1 NOp 1

Largest Abelian subgroup C1 NOp 1

Largest concise Abelian subgroup C1 NOp 1

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.660206	-2.161676	-0.761139
2	6	0	-1.968864	-1.826109	-0.850532
3	7	0	-2.210963	-0.860248	0.121599
4	6	0	-1.047649	-0.584353	0.746830
5	7	0	-0.106003	-1.407828	0.266265
6	6	0	1.318032	-1.344010	0.620092
7	1	0	-0.075946	-2.858782	-1.335927
8	1	0	-2.736745	-2.156882	-1.525941
9	1	0	1.392214	-0.911876	1.616769
10	1	0	1.695803	-2.366026	0.678613
11	35	0	-0.470006	2.108432	-0.090402
12	1	0	-0.935320	0.068782	1.590081
13	6	0	-3.405024	-0.116673	0.326511
14	6	0	-4.619098	-0.618580	0.138955
15	1	0	-3.201219	0.910867	0.608738
16	1	0	-5.484023	0.018041	0.265923
17	1	0	-4.792997	-1.650510	-0.142402
18	6	0	2.107791	-0.498893	-0.382677
19	1	0	2.080958	-0.926575	-1.388501
20	1	0	1.653630	0.501021	-0.455137
21	6	0	3.541397	-0.354583	0.053274
22	8	0	3.982002	-0.682412	1.129363
23	8	0	4.302679	0.204182	-0.911707
24	1	0	5.196888	0.308445	-0.552311

Rotational constants (GHZ): 0.8054144 0.3345616 0.2550745

****

Population analysis using the SCF density.

****

Orbital symmetries:

Occupied (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)

(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A)

Virtual (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A) (A)
(A) (A) (A)

The electronic state is 1-A.

Alpha occ. eigenvalues -- -482.70670 -62.35997 -56.17799 -56.17759 -56.17750
Alpha occ. eigenvalues -- -19.18566 -19.13185 -14.43317 -14.42955 -10.32493
Alpha occ. eigenvalues -- -10.30277 -10.25994 -10.25921 -10.25632 -10.25220
Alpha occ. eigenvalues -- -10.20824 -10.20447 -8.56901 -6.39285 -6.39150
Alpha occ. eigenvalues -- -6.39112 -2.50511 -2.50482 -2.50451 -2.50343
Alpha occ. eigenvalues -- -2.50343 -1.12906 -1.10312 -1.04038 -0.99152
Alpha occ. eigenvalues -- -0.85160 -0.81798 -0.80294 -0.73443 -0.69772
Alpha occ. eigenvalues -- -0.65992 -0.64780 -0.63387 -0.61677 -0.57802
Alpha occ. eigenvalues -- -0.54578 -0.52387 -0.51363 -0.50627 -0.50378
Alpha occ. eigenvalues -- -0.50048 -0.49655 -0.47992 -0.47035 -0.45187
Alpha occ. eigenvalues -- -0.43323 -0.42209 -0.41140 -0.38851 -0.37168
Alpha occ. eigenvalues -- -0.34377 -0.31008 -0.30230 -0.29533 -0.20480
Alpha occ. eigenvalues -- -0.20214 -0.20173

Alpha virt. eigenvalues --	-0.06707	-0.03758	-0.02475	-0.01663	-0.01318
Alpha virt. eigenvalues --	-0.00753	-0.00463	0.00023	0.01075	0.01454
Alpha virt. eigenvalues --	0.02486	0.03071	0.03578	0.04474	0.05291
Alpha virt. eigenvalues --	0.05387	0.06358	0.06516	0.07045	0.07715
Alpha virt. eigenvalues --	0.08180	0.08794	0.09009	0.09096	0.09599
Alpha virt. eigenvalues --	0.09808	0.10018	0.10296	0.10806	0.11123
Alpha virt. eigenvalues --	0.11437	0.12123	0.12439	0.12630	0.12731
Alpha virt. eigenvalues --	0.13087	0.13367	0.13902	0.14388	0.14981
Alpha virt. eigenvalues --	0.15260	0.15390	0.16281	0.16673	0.16813
Alpha virt. eigenvalues --	0.17220	0.17700	0.18114	0.18225	0.19317
Alpha virt. eigenvalues --	0.19723	0.20001	0.20640	0.20761	0.21470
Alpha virt. eigenvalues --	0.22308	0.22547	0.22790	0.23300	0.23815
Alpha virt. eigenvalues --	0.24365	0.24900	0.25089	0.25920	0.26818
Alpha virt. eigenvalues --	0.27020	0.27865	0.28460	0.28717	0.29027
Alpha virt. eigenvalues --	0.29614	0.29976	0.30822	0.31632	0.31804
Alpha virt. eigenvalues --	0.32183	0.33489	0.33814	0.34394	0.34663
Alpha virt. eigenvalues --	0.35116	0.36613	0.37495	0.38082	0.38968
Alpha virt. eigenvalues --	0.40531	0.40946	0.42353	0.43062	0.45910
Alpha virt. eigenvalues --	0.47169	0.47940	0.48461	0.49111	0.50070
Alpha virt. eigenvalues --	0.50341	0.51651	0.52597	0.53613	0.55213
Alpha virt. eigenvalues --	0.55913	0.56633	0.57527	0.59478	0.60278
Alpha virt. eigenvalues --	0.61065	0.62573	0.62659	0.62767	0.64108
Alpha virt. eigenvalues --	0.64309	0.65432	0.66400	0.66896	0.67105
Alpha virt. eigenvalues --	0.68402	0.68644	0.69972	0.71253	0.71424
Alpha virt. eigenvalues --	0.72032	0.72911	0.74001	0.75443	0.76203
Alpha virt. eigenvalues --	0.76710	0.77629	0.78488	0.79376	0.80361
Alpha virt. eigenvalues --	0.81664	0.83521	0.84359	0.85784	0.87051
Alpha virt. eigenvalues --	0.87112	0.90660	0.91815	0.93158	0.94227
Alpha virt. eigenvalues --	0.95950	0.98919	1.00177	1.00773	1.02537
Alpha virt. eigenvalues --	1.04361	1.04715	1.05926	1.06849	1.09495
Alpha virt. eigenvalues --	1.09911	1.11877	1.13205	1.14074	1.14885
Alpha virt. eigenvalues --	1.16059	1.18045	1.20316	1.21393	1.22785
Alpha virt. eigenvalues --	1.23696	1.25455	1.26752	1.29497	1.35024
Alpha virt. eigenvalues --	1.37625	1.39013	1.41195	1.43479	1.45052
Alpha virt. eigenvalues --	1.47709	1.48566	1.50340	1.52143	1.52797
Alpha virt. eigenvalues --	1.53647	1.54326	1.56208	1.56647	1.57654
Alpha virt. eigenvalues --	1.59111	1.60121	1.60892	1.62474	1.64770
Alpha virt. eigenvalues --	1.65576	1.66758	1.68447	1.68974	1.69867
Alpha virt. eigenvalues --	1.73398	1.73519	1.75274	1.75998	1.78785
Alpha virt. eigenvalues --	1.79278	1.80028	1.81640	1.85348	1.88222
Alpha virt. eigenvalues --	1.90443	1.91140	1.95108	1.95801	1.96914
Alpha virt. eigenvalues --	2.01414	2.02138	2.04034	2.05525	2.07092
Alpha virt. eigenvalues --	2.09726	2.10675	2.11189	2.11462	2.12588
Alpha virt. eigenvalues --	2.13972	2.18977	2.19770	2.21225	2.23289

Alpha virt. eigenvalues --	2.25325	2.26371	2.31024	2.32143	2.36539	
Alpha virt. eigenvalues --	2.39364	2.42967	2.46476	2.47683	2.49543	
Alpha virt. eigenvalues --	2.50862	2.52370	2.54863	2.55854	2.56760	
Alpha virt. eigenvalues --	2.58543	2.59370	2.60791	2.62220	2.62779	
Alpha virt. eigenvalues --	2.63686	2.68929	2.69862	2.71479	2.72556	
Alpha virt. eigenvalues --	2.73734	2.75554	2.77129	2.78537	2.80650	
Alpha virt. eigenvalues --	2.81672	2.84221	2.86543	2.87667	2.89368	
Alpha virt. eigenvalues --	2.91500	2.92316	2.93986	2.97046	2.97612	
Alpha virt. eigenvalues --	2.98650	3.05134	3.11163	3.12676	3.15902	
Alpha virt. eigenvalues --	3.16189	3.21197	3.24997	3.35003	3.35847	
Alpha virt. eigenvalues --	3.38708	3.50120	3.54351	3.55989	3.58123	
Alpha virt. eigenvalues --	3.61951	3.65675	3.67559	3.73350	3.76010	
Alpha virt. eigenvalues --	3.78193	3.79189	3.81146	3.85777	3.88994	
Alpha virt. eigenvalues --	3.91532	4.04714	4.05309	4.08528	4.09772	
Alpha virt. eigenvalues --	4.26681	4.27360	4.29449	4.31117	4.35006	
Alpha virt. eigenvalues --	4.46339	4.69357	4.92402	4.95516	5.01509	
Alpha virt. eigenvalues --	5.04947	5.17840	5.22724	5.39031	5.58904	
Alpha virt. eigenvalues --	5.83991	6.77561	7.68166	7.73304	7.76403	
Alpha virt. eigenvalues --	23.71219	23.74714	23.79698	23.83987	23.87781	
Alpha virt. eigenvalues --	23.90762	24.16064	24.23373	35.45389	35.57727	
Alpha virt. eigenvalues --	48.05951	49.85920	49.98654	289.88907	289.94041	
Alpha virt. eigenvalues --	289.96651	1020.85160				

Condensed to atoms (all electrons):

		1	2	3	4	5	6
1	C	7.692146	-2.015096	0.190440	-0.059118	-0.229129	0.200819
2	C	-2.015096	7.826860	0.099039	-0.088445	0.377599	-0.528450
3	N	0.190440	0.099039	6.596981	0.245684	-0.176130	-0.155178
4	C	-0.059118	-0.088445	0.245684	5.853363	0.446992	-0.382003
5	N	-0.229129	0.377599	-0.176130	0.446992	6.751533	-0.156690
6	C	0.200819	-0.528450	-0.155178	-0.382003	-0.156690	8.585312
7	H	0.596537	-0.207204	0.049654	-0.001225	-0.092610	-0.016323
8	H	-0.119174	0.518539	-0.073244	0.003411	0.030724	0.001447
9	H	0.012914	-0.009161	0.011728	0.022745	-0.040997	0.272245
10	H	-0.017016	-0.015696	-0.013438	-0.004765	-0.046794	0.568456
11	Br	0.058807	-0.063579	-0.027723	-0.018658	-0.057346	0.351315
12	H	-0.016396	0.031689	-0.053889	0.443155	-0.027461	-0.009021
13	C	0.347517	-0.381524	0.172534	-0.105704	-0.060332	-0.110155
14	C	-0.169666	0.211829	-0.080308	-0.147202	0.006331	-0.074792
15	H	0.036405	-0.060199	-0.083926	0.024393	-0.006538	-0.025588
16	H	-0.012700	0.018340	0.027311	-0.008531	0.000711	-0.000181
17	H	0.022983	-0.026895	-0.034886	0.010464	-0.000477	-0.001785
18	C	-0.115694	0.183562	0.061796	0.064061	0.045522	-1.853898
19	H	0.017978	-0.015420	-0.000579	-0.010473	-0.012934	-0.081389
20	H	-0.031204	0.025418	0.000398	-0.009328	0.031211	-0.056828

21	C	-0.169969	0.172469	0.005544	0.046589	0.038760	0.119214
22	O	0.011421	-0.002048	0.000074	-0.000460	0.011566	0.020981
23	O	0.002080	0.002257	0.000075	0.001603	0.000217	0.010265
24	H	-0.001115	0.001384	0.000067	0.001129	0.000994	-0.008566
		7	8	9	10	11	12
1	C	0.596537	-0.119174	0.012914	-0.017016	0.058807	-0.016396
2	C	-0.207204	0.518539	-0.009161	-0.015696	-0.063579	0.031689
3	N	0.049654	-0.073244	0.011728	-0.013438	-0.027723	-0.053889
4	C	-0.001225	0.003411	0.022745	-0.004765	-0.018658	0.443155
5	N	-0.092610	0.030724	-0.040997	-0.046794	-0.057346	-0.027461
6	C	-0.016323	0.001447	0.272245	0.568456	0.351315	-0.009021
7	H	0.510472	-0.011471	0.003621	-0.008069	0.001543	-0.002091
8	H	-0.011471	0.492106	0.000198	0.000345	-0.000651	0.000223
9	H	0.003621	0.000198	0.524828	-0.043330	-0.014900	-0.009641
10	H	-0.008069	0.000345	-0.043330	0.527363	0.006182	0.004915
11	Br	0.001543	-0.000651	-0.014900	0.006182	35.601568	-0.035034
12	H	-0.002091	0.000223	-0.009641	0.004915	-0.035034	0.432590
13	C	0.020074	-0.023874	0.004525	-0.008292	-0.060260	-0.018879
14	C	-0.005594	0.009011	0.002324	-0.002224	-0.007207	0.008760
15	H	0.002422	-0.004388	0.005220	-0.001703	0.088645	-0.019682
16	H	-0.000193	0.002360	-0.000182	0.000014	0.000575	-0.000385
17	H	0.000378	-0.006636	0.000141	-0.000065	-0.001021	0.001377
18	C	0.011230	-0.000114	0.131851	-0.145978	-0.294428	-0.016311
19	H	-0.005120	0.000302	0.008788	-0.007811	-0.001501	0.001070
20	H	-0.004046	0.000482	-0.028850	0.012767	0.080271	0.010884
21	C	-0.015946	0.000314	-0.059674	-0.016653	0.008361	0.008700
22	O	0.000945	-0.000042	-0.009075	-0.005322	0.000667	0.001280
23	O	-0.000351	0.000018	-0.003496	-0.000877	0.002740	0.000324
24	H	-0.000164	-0.000003	-0.000881	-0.001369	-0.000559	0.000028
		13	14	15	16	17	18
1	C	0.347517	-0.169666	0.036405	-0.012700	0.022983	-0.115694
2	C	-0.381524	0.211829	-0.060199	0.018340	-0.026895	0.183562
3	N	0.172534	-0.080308	-0.083926	0.027311	-0.034886	0.061796
4	C	-0.105704	-0.147202	0.024393	-0.008531	0.010464	0.064061
5	N	-0.060332	0.006331	-0.006538	0.000711	-0.000477	0.045522
6	C	-0.110155	-0.074792	-0.025588	-0.000181	-0.001785	-1.853898
7	H	0.020074	-0.005594	0.002422	-0.000193	0.000378	0.011230
8	H	-0.023874	0.009011	-0.004388	0.002360	-0.006636	-0.000114
9	H	0.004525	0.002324	0.005220	-0.000182	0.000141	0.131851
10	H	-0.008292	-0.002224	-0.001703	0.000014	-0.000065	-0.145978
11	Br	-0.060260	-0.007207	0.088645	0.000575	-0.001021	-0.294428
12	H	-0.018879	0.008760	-0.019682	-0.000385	0.001377	-0.016311
13	C	5.773766	0.021964	0.371920	-0.070577	0.033705	0.030935
14	C	0.021964	5.800603	-0.015562	0.428942	0.345586	0.029294

15	H	0.371920	-0.015562	0.535276	-0.012846	0.004942	0.023082
16	H	-0.070577	0.428942	-0.012846	0.494477	-0.029124	-0.000152
17	H	0.033705	0.345586	0.004942	-0.029124	0.540702	0.001048
18	C	0.030935	0.029294	0.023082	-0.000152	0.001048	8.616299
19	H	-0.002627	0.000994	-0.000616	-0.000048	0.000088	0.488764
20	H	0.000076	0.001724	-0.014122	0.000484	-0.000142	0.174172
21	C	0.001487	0.003599	-0.003044	0.000205	-0.000248	-1.258033
22	O	-0.000335	-0.000020	-0.000017	0.000000	-0.000001	0.014804
23	O	-0.000054	0.000008	-0.000043	0.000001	-0.000002	-0.155268
24	H	0.000042	0.000014	-0.000014	0.000001	-0.000001	-0.091752

		19	20	21	22	23	24
1	C	0.017978	-0.031204	-0.169969	0.011421	0.002080	-0.001115
2	C	-0.015420	0.025418	0.172469	-0.002048	0.002257	0.001384
3	N	-0.000579	0.000398	0.005544	0.000074	0.000075	0.000067
4	C	-0.010473	-0.009328	0.046589	-0.000460	0.001603	0.001129
5	N	-0.012934	0.031211	0.038760	0.011566	0.000217	0.000994
6	C	-0.081389	-0.056828	0.119214	0.020981	0.010265	-0.008566
7	H	-0.005120	-0.004046	-0.015946	0.000945	-0.000351	-0.000164
8	H	0.000302	0.000482	0.000314	-0.000042	0.000018	-0.000003
9	H	0.008788	-0.028850	-0.059674	-0.009075	-0.003496	-0.000881
10	H	-0.007811	0.012767	-0.016653	-0.005322	-0.000877	-0.001369
11	Br	-0.001501	0.080271	0.008361	0.000667	0.002740	-0.000559
12	H	0.001070	0.010884	0.008700	0.001280	0.000324	0.000028
13	C	-0.002627	0.000076	0.001487	-0.000335	-0.000054	0.000042
14	C	0.000994	0.001724	0.003599	-0.000020	0.000008	0.000014
15	H	-0.000616	-0.014122	-0.003044	-0.000017	-0.000043	-0.000014
16	H	-0.000048	0.000484	0.000205	0.000000	0.000001	0.000001
17	H	0.000088	-0.000142	-0.000248	-0.000001	-0.000002	-0.000001
18	C	0.488764	0.174172	-1.258033	0.014804	-0.155268	-0.091752
19	H	0.564308	-0.027102	-0.094486	0.001057	-0.008838	0.001871
20	H	-0.027102	0.583524	0.049023	-0.015810	-0.023626	0.005402
21	C	-0.094486	0.049023	6.597633	0.309282	0.219890	0.101521
22	O	0.001057	-0.015810	0.309282	8.058538	-0.119930	-0.009301
23	O	-0.008838	-0.023626	0.219890	-0.119930	7.981737	0.234848
24	H	0.001871	0.005402	0.101521	-0.009301	0.234848	0.472588

Mulliken charges:

		1
1	C	-0.233771
2	C	-0.055270
3	N	0.237973
4	C	-0.327677
5	N	0.165277
6	C	-0.669209
7	H	0.173530

8	H	0.180115
9	H	0.219062
10	H	0.219360
11	Br	-0.617807
12	H	0.263795
13	C	0.064068
14	C	-0.368406
15	H	0.155982
16	H	0.161498
17	H	0.139869
18	C	0.055206
19	H	0.183721
20	H	0.235221
21	C	-0.064537
22	O	-0.268255
23	O	-0.143579
24	H	0.293837

Sum of Mulliken charges = 0.00000

Mulliken charges with hydrogens summed into heavy atoms:

		1
1	C	-0.060240
2	C	0.124844
3	N	0.237973
4	C	-0.063882
5	N	0.165277
6	C	-0.230787
11	Br	-0.617807
13	C	0.220050
14	C	-0.067040
18	C	0.474148
21	C	-0.064537
22	O	-0.268255
23	O	0.150257

Electronic spatial extent (au): <R**2>= 4065.5161

Charge= 0.0000 electrons

Dipole moment (field-independent basis, Debye):

X= -2.5110 Y= -9.0557 Z= -0.4936 Tot= 9.4104

Quadrupole moment (field-independent basis, Debye-Ang):

XX= -70.7828 YY= -99.5349 ZZ= -92.8805

XY= 7.6436 XZ= -5.3126 YZ= 7.2187

Traceless Quadrupole moment (field-independent basis, Debye-Ang):

XX= 16.9500 YY= -11.8022 ZZ= -5.1478

XY= 7.6436 XZ= -5.3126 YZ= 7.2187

Octapole moment (field-independent basis, Debye-Ang**2):

XXX= -14.6564 YYY= -1.1499 ZZZ= -1.0982 XYY= 7.8507

XXY= 25.7759 XXZ= -33.0671 XZZ= -9.7458 YZZ= 9.8654

YYZ= -12.7268 XYZ= -3.1392

Hexadecapole moment (field-independent basis, Debye-Ang**3):

XXXX= -2872.9767 YYYY= -1245.4216 ZZZZ= -311.0309 XXXY= 114.9428

XXXZ= -126.7524 YYYX= -13.8260 YYYZ= 24.1618 ZZZX= 0.4426

ZZZY= 6.8513 XXYY= -781.0231 XXZZ= -748.4499 YYZZ= -242.4813

XXYZ= 61.1997 YYXZ= 10.4775 ZZXY= 1.2080

N-N= 1.072601473593D+03 E-N=-9.633210176906D+03 KE= 3.140362840949D+03

1\1\GINC-CN003\FOpt\RB3LYP\6-311++G(d,p)\C8H11Br1N2O2\SYWANG\22-Jul-20
24\0\\# opt b3lyp/6-311++g(d,p)\\cooh\\0,1\C,-0.3307965149,-2.22918751
7,-0.3858182472\C,-1.5804476468,-1.7803288331,-0.6505456\N,-1.80302963
37,-0.6803816202,0.1723221565\C,-0.6790974587,-0.4437172452,0.88020534
05\N,0.2060726151,-1.4099776208,0.5999064931\C,1.589627061,-1.44259126
98,1.0916928601\H,0.2233887755,-3.0473985274,-0.8113850176\H,-2.314504
2817,-2.1164470233,-1.3600631179\H,1.6187527064,-0.8975409873,2.033860
8217\H,1.8450613056,-2.4812474962,1.3075597346\Br,0.2675548825,2.05176
13989,-0.1978281271\H,-0.573618272,0.2963599471,1.6492530543\C,-2.9213
547578,0.1970793561,0.1630770763\C,-4.1609292611,-0.202440088,-0.09168
11051\H,-2.6321425984,1.2269111782,0.3442648651\H,-4.9581775221,0.5271
897216,-0.1309244141\H,-4.4211135019,-1.2394409113,-0.2683575715\C,2.5
572014749,-0.8127324488,0.0864238411\H,2.5762676044,-1.3592062152,-0.8
603169045\H,2.2250174505,0.20987228,-0.148681209\C,3.9515405256,-0.756
4701607,0.6510091616\O,4.2519135813,-0.9876493976,1.7981375257\O,4.855
7861074,-0.4016954602,-0.2867718662\H,5.718999059,-0.34149547,0.150133
4596\\Version=EM64L-G09RevD.01\State=1-A\HF=-3145.732244\RMSD=6.747e-0
9\RMSF=8.937e-06\Dipole=-1.3535622,-3.4440401,0.1169047\Quadrupole=14.
0563106,-8.1579631,-5.8983474,2.404104,-1.9913804,6.535815\PG=C01 [X(C
8H11Br1N2O2)]\\@

BLACK HOLES SUCK.

Job cpu time: 0 days 4 hours 13 minutes 24.6 seconds.

File lengths (MBytes): RWF= 68 Int= 0 D2E= 0 Chk= 12 Scr= 1

Normal termination of Gaussian 09 at Mon Jul 22 20:04:44 2024.