Supplementary Information to:

An Indole-Linked C^8-Deoxyguanosine Nucleoside is a Fluorescent Probe for Sensing Watson-Crick Versus Hoogsteen Base Pairing

Katherine M. Schlitt, Andrea L. Millen, Stacey D. Wetmore and Richard A. Manderville

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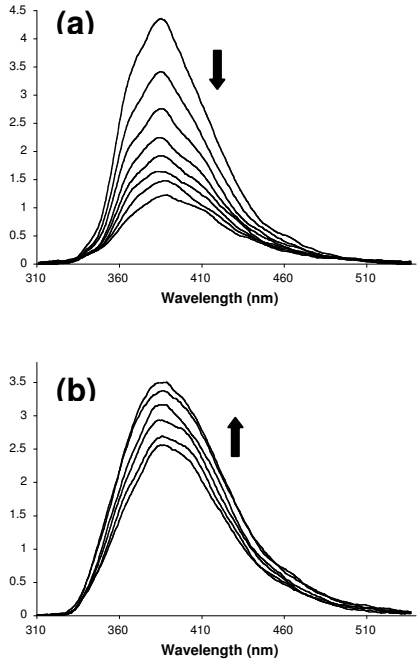

Figure S1. Fluorescence emission titration of bissilyl**1** in $CHCl_3$ with (a) bissilyl dC and (b) $G(TBDMS)_3$.

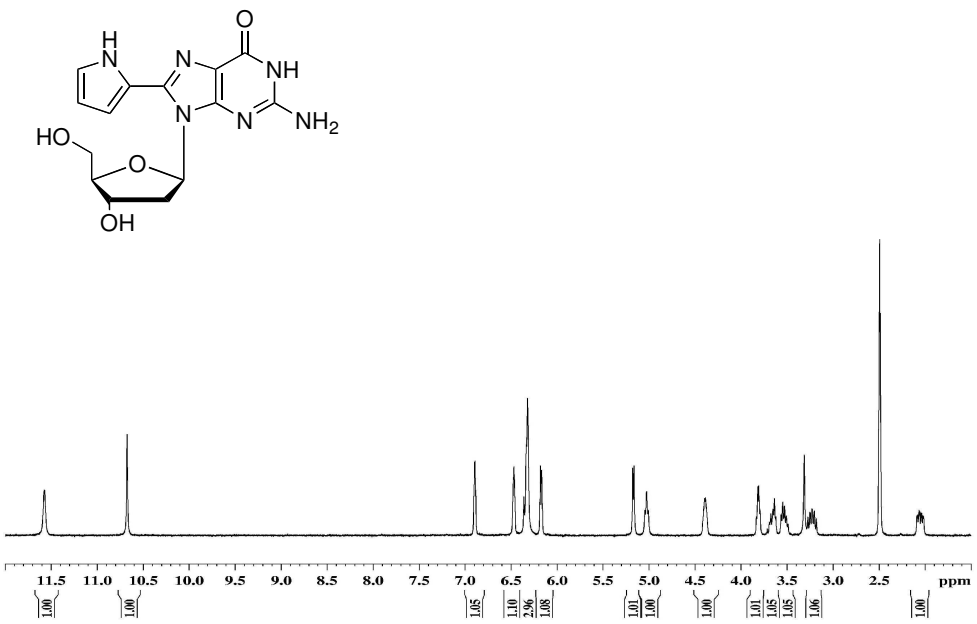

Figure S2. ^{1}H NMR spectrum of 8-(2''-pyrrolyl)-2'-deoxyguanosine (**1**) in DMSO-d_6.

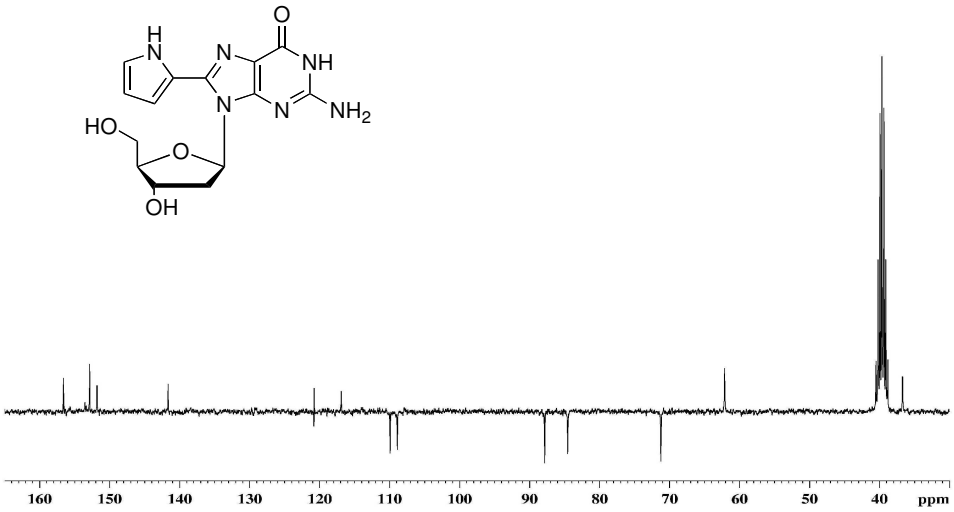

Figure S3. ^{13}C NMR spectrum of 8-(2''-pyrrolyl)-2'-deoxyguanosine (**1**) in DMSO-d_6.

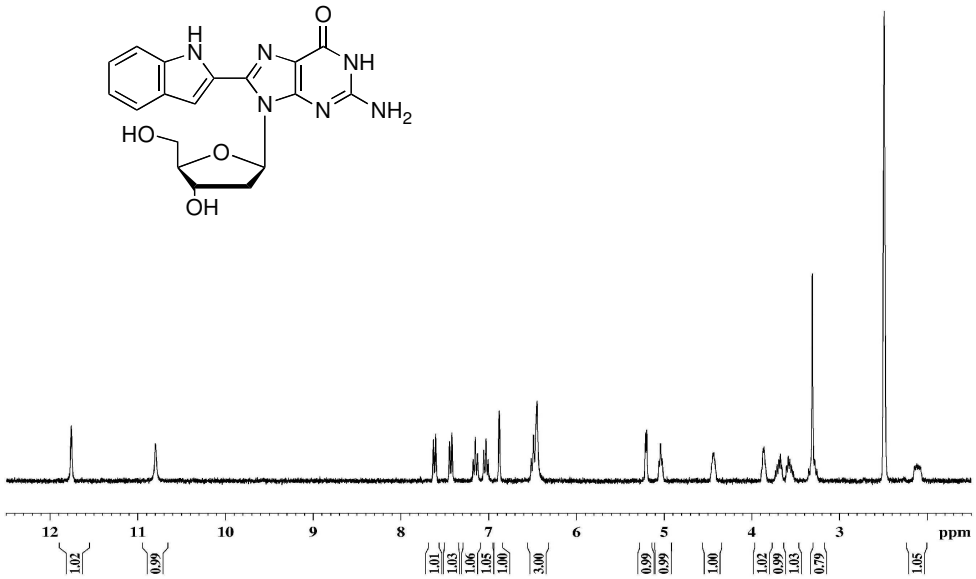

Figure S4. ^{1}H NMR spectrum of 8-(2"-benzopyrrolyl)-2'-deoxyguanosine (**2**) in DMSO-d_6.

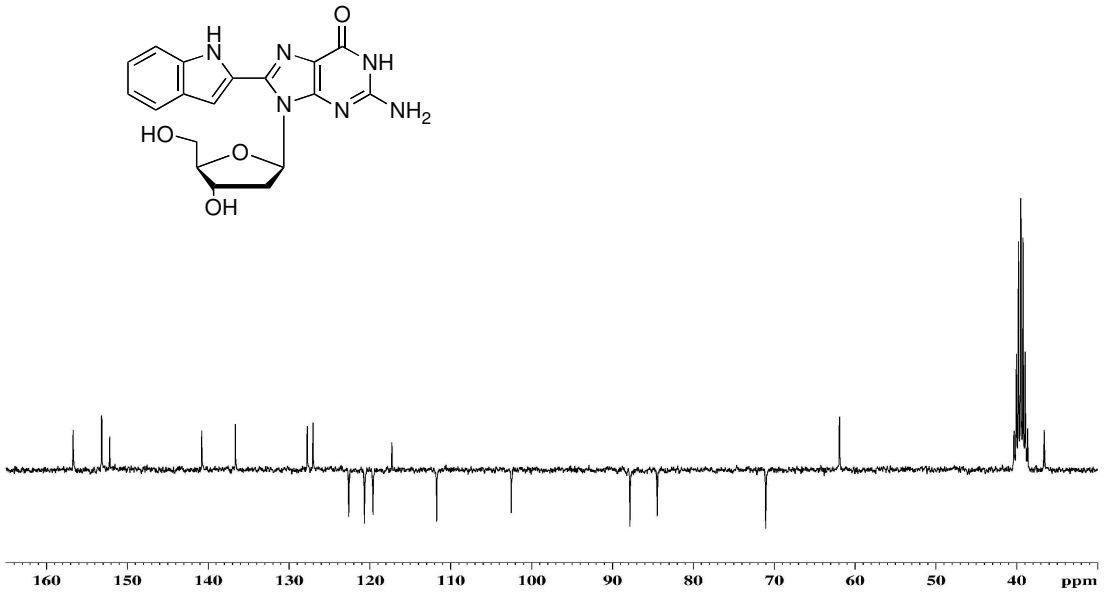

Figure S5. ^{13}C NMR spectrum of 8-(2"-benzopyrrolyl)-2'-deoxyguanosine (**2**) in DMSO-d_6.

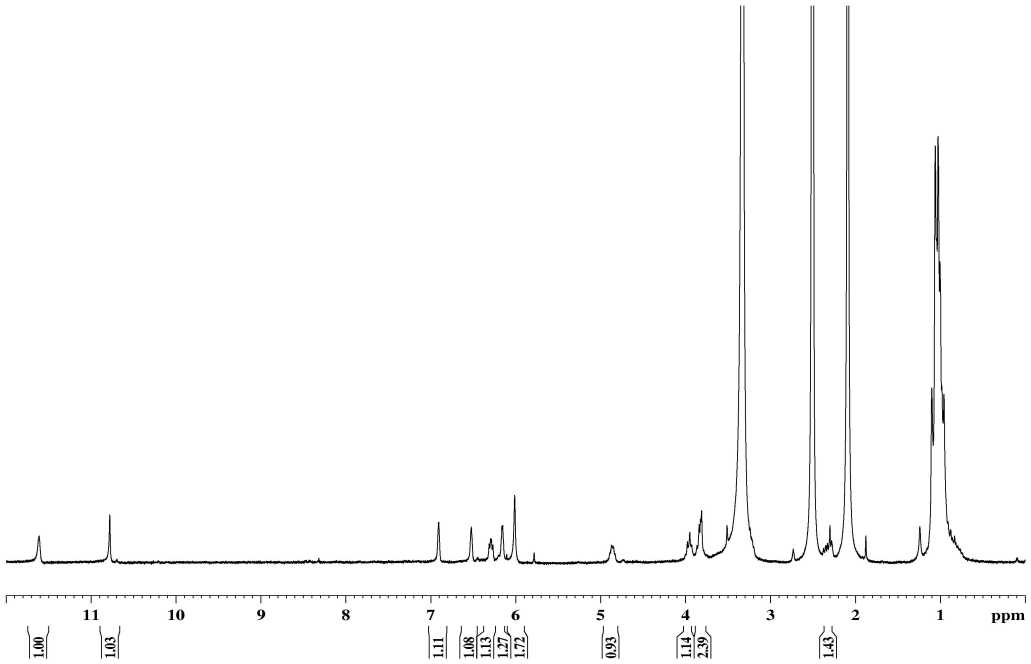

Figure S6. ^{1}H NMR spectrum of 8-(2"-pyrrolyl)-3', 5'-*O*-(1,1,3,3-tetraisopropyldisiloxane-1,3-diyl)-2'-deoxyguanosine (bissilyl**1**) in DMSO-d_6.

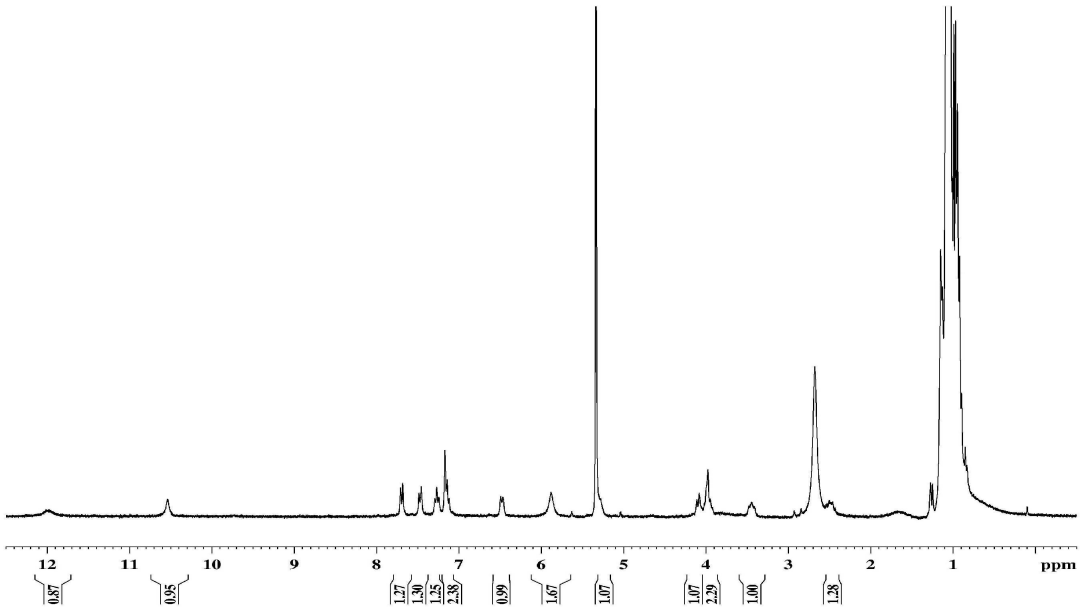

Figure S7. ^{1}H NMR spectrum of 8-(2"-benzopyrrolyl)-3', 5'-*O*-(1,1,3,3-tetraisopropyldisiloxane-1,3-diyl)-2'-deoxyguanosine (bissilyl**2**) in CD_2Cl_2.

Cartesian Coordinates and Absolute Energies (Hartrees) for Monomers when dR=H

G Monomer Energy: -542.7434272

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-1.730140	-1.508015	-0.004434
2	6	0	-2.713642	-0.533509	0.001344
3	1	0	-3.764006	-0.790397	-0.000293
4	7	0	-2.226269	0.679981	0.009078
5	6	0	-0.855890	0.502709	0.008377
6	6	0	0.208422	1.473579	0.003091
7	8	0	0.188118	2.691466	-0.004449
8	7	0	1.476486	0.792250	-0.003278
9	1	0	2.267171	1.420794	-0.077048
10	6	0	1.674921	-0.564425	-0.003357
11	7	0	2.978340	-1.003662	-0.068261
12	1	0	3.680994	-0.445022	0.395587
13	1	0	3.064262	-1.996728	0.098969
14	7	0	0.698125	-1.440749	0.006881
15	6	0	-0.526567	-0.853292	-0.000886
16	1	0	-1.852626	-2.509390	-0.012939

Cytosine Monomer Energy: -395.0752911

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.279459	0.896626	0.002873
2	6	0	0.199622	1.715216	0.001612
3	1	0	0.391798	2.783166	0.002686
4	6	0	-1.052113	1.186106	-0.002286
5	1	0	-1.933213	1.814295	-0.014047
6	6	0	-1.131140	-0.253094	-0.003432
7	7	0	-2.358281	-0.845069	-0.041527
8	1	0	-2.378242	-1.844979	0.092567
9	1	0	-3.186583	-0.319159	0.182644
10	7	0	-0.081940	-1.053133	0.002923
11	6	0	1.187476	-0.530054	-0.000074
12	8	0	2.223338	-1.174116	0.000777
13	1	0	2.221799	1.261583	0.005140

1 Monomer Energy: -751.8014893

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	0.259520	-1.215105	-0.002981
2	6	0	1.105109	-0.114815	0.002266
3	6	0	-1.024838	-0.734959	-0.000484
4	7	0	0.435498	1.022833	0.008937
5	6	0	-0.892206	0.654379	0.008020
6	7	0	-2.153050	-1.488307	0.007955
7	6	0	-2.082771	1.463022	0.001706

8	6	0	-3.245708	-0.760632	-0.002898
9	8	0	-2.232634	2.673212	-0.006075
10	7	0	-3.241663	0.610091	-0.004392
11	7	0	-4.473836	-1.381789	-0.068516
12	1	0	-4.113261	1.120253	-0.080195
13	1	0	-5.245242	-0.932817	0.405532
14	1	0	-4.414120	-2.377176	0.097071
15	6	0	2.544935	-0.206770	0.000752
16	6	0	3.439101	-1.270235	-0.002974
17	6	0	4.747337	-0.721633	-0.002671
18	1	0	3.182903	-2.320944	-0.005559
19	6	0	4.618500	0.655299	0.001161
20	7	0	3.284416	0.952760	0.003318
21	1	0	2.852121	1.865238	0.006033
22	1	0	5.366341	1.433834	0.002343
23	1	0	5.678030	-1.270474	-0.005125
24	1	0	0.521352	-2.188937	-0.011009

2 Monomer Energy: -905.4939919

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.001302	-1.237186	-0.001541
2	6	0	0.142293	-0.147412	0.002626
3	6	0	2.278130	-0.741167	0.000124
4	7	0	0.797416	0.998577	0.007996
5	6	0	2.127803	0.647717	0.007350
6	7	0	3.415612	-1.478864	0.008564
7	6	0	3.308482	1.472437	0.000756
8	6	0	4.499177	-0.736442	-0.002517
9	8	0	3.441322	2.683775	-0.007866
10	7	0	4.477883	0.634412	-0.004651
11	7	0	5.732531	-1.342083	-0.066525
12	1	0	5.343071	1.155904	-0.078053
13	1	0	6.506771	-0.877497	0.386586
14	1	0	5.690403	-2.338036	0.099510
15	6	0	-1.297289	-0.254474	0.001546
16	6	0	-2.151547	-1.340005	-0.001786
17	6	0	-3.486400	-0.823864	-0.001517
18	1	0	-1.865019	-2.382673	-0.004119
19	6	0	-3.380715	0.598909	0.002044
20	7	0	-2.041809	0.910030	0.003920
21	1	0	-1.613997	1.823998	0.005705
22	6	0	-4.506996	1.429385	0.003099
23	6	0	-5.754195	0.817521	0.000572
24	6	0	-5.882721	-0.588007	-0.002925
25	6	0	-4.765564	-1.410528	-0.003974
26	1	0	-4.409497	2.510878	0.005695
27	1	0	-6.648496	1.433455	0.001231
28	1	0	-6.875055	-1.028939	-0.004889
29	1	0	-4.873903	-2.491470	-0.006766
30	1	0	0.751874	-2.214436	-0.008710

Cartesian Coordinates and Absolute Energies (Hartrees) for H-bonded Complexes when dR=H

G:C Counterpoise Corrected Energy: -937.857673695388
BSSE energy: 0.001064926403

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-4.667621	0.494244	-0.003690
2	6	0	-4.972871	-0.859244	-0.004977
3	6	0	-3.299205	0.592673	-0.000543
4	7	0	-3.912140	-1.621176	-0.004206
5	6	0	-2.849037	-0.732538	-0.000866
6	7	0	-2.585857	1.737216	0.002044
7	6	0	-1.436470	-0.959032	0.001475
8	6	0	-1.278168	1.514695	0.004782
9	8	0	-0.824455	-2.038309	0.001170
10	7	0	-0.724026	0.255809	0.004201
11	7	0	-0.417929	2.554488	0.010255
12	1	0	0.305995	0.166204	0.004473
13	1	0	0.597657	2.439117	0.002126
14	1	0	-0.824271	3.474740	0.002442
15	1	0	-5.308791	1.272715	-0.004336
16	7	0	4.343221	0.904849	-0.005088
17	6	0	4.941097	-0.317787	-0.002942
18	1	0	6.025459	-0.328628	-0.004370
19	6	0	4.188709	-1.445728	0.000717
20	1	0	4.644641	-2.427177	0.002359
21	6	0	2.753998	-1.277510	0.002094
22	7	0	1.945867	-2.341186	0.005281
23	1	0	0.914006	-2.223457	0.004088
24	1	0	2.336285	-3.269342	0.005882
25	7	0	2.187361	-0.063869	0.000388
26	6	0	2.941940	1.066187	-0.003575
27	8	0	2.487344	2.214372	-0.006014
28	1	0	4.881026	1.760151	-0.008004
29	1	0	-5.997200	-1.205746	-0.007191

G:G Counterpoise Corrected Energy: -1085.512409624652
BSSE energy: 0.000750990118

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.593890	-2.363465	-0.053756
2	6	0	-1.255935	-2.028720	-0.131449
3	6	0	-3.306583	-1.190763	-0.007923
4	7	0	-1.081970	-0.730598	-0.141860
5	6	0	-2.343262	-0.188094	-0.064897
6	7	0	-4.653579	-1.054485	0.065092
7	6	0	-2.744195	1.183426	-0.006383
8	6	0	-5.034628	0.201529	0.114447
9	8	0	-2.065051	2.206111	-0.010625
10	7	0	-4.163841	1.268285	0.082705
11	7	0	-6.366749	0.499218	0.258201

12	1	0	-4.515133	2.211715	0.195666
13	1	0	-6.710776	1.355450	-0.152255
14	1	0	-6.970165	-0.301092	0.130349
15	7	0	5.523099	0.775904	0.161713
16	6	0	5.976158	-0.532921	0.207970
17	1	0	7.029482	-0.762894	0.294445
18	7	0	5.008445	-1.408512	0.136562
19	6	0	3.856746	-0.646268	0.037203
20	6	0	2.475945	-1.037184	-0.064865
21	8	0	1.968345	-2.157826	-0.087544
22	7	0	1.645880	0.112120	-0.145085
23	1	0	0.638257	-0.100729	-0.195908
24	6	0	2.056791	1.416616	-0.123147
25	7	0	1.092497	2.369257	-0.248566
26	1	0	0.105455	2.163559	-0.131475
27	1	0	1.395990	3.315908	-0.088105
28	7	0	3.324371	1.784417	-0.020878
29	6	0	4.155944	0.719749	0.051047
30	1	0	6.071008	1.621688	0.197815
31	1	0	-0.446077	-2.745996	-0.169509
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1:C Counterpoise Corrected Energy: -1146.915466179709
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3	6	0	-1.627535	1.269004	-0.003704
4	7	0	-2.581419	-0.816225	-0.000924
5	6	0	-1.393161	-0.111691	-0.003493
6	7	0	-0.741533	2.283251	-0.005869
7	6	0	-0.035518	-0.558650	-0.005077
8	6	0	0.515342	1.856718	-0.008219
9	8	0	0.395112	-1.723817	-0.004561
10	7	0	0.861934	0.526449	-0.007293
11	7	0	1.528549	2.748158	-0.015241
12	1	0	1.864595	0.274114	-0.005759
13	1	0	2.513138	2.474380	0.000621
14	1	0	1.272040	3.720799	-0.001554
15	6	0	-4.937185	-0.179029	0.002885
16	6	0	-6.077515	0.614404	0.005219
17	6	0	-7.198503	-0.256303	0.007081
18	1	0	-6.103360	1.695517	0.005698
19	6	0	-6.716170	-1.551845	0.005819
20	7	0	-5.349645	-1.490761	0.003405
21	1	0	-4.692788	-2.257368	0.001580
22	7	0	5.966775	0.360549	0.010682
23	6	0	6.362316	-0.941590	0.005117
24	1	0	7.431112	-1.124900	0.006593
25	6	0	5.440023	-1.935466	-0.001748
26	1	0	5.734269	-2.976877	-0.006095
27	6	0	4.050407	-1.541173	-0.002822
28	7	0	3.082964	-2.462401	-0.009005

29	1	0	2.083061	-2.181420	-0.007211
30	1	0	3.320549	-3.440835	-0.011855
31	7	0	3.684238	-0.252920	0.002147
32	6	0	4.608969	0.742775	0.009494
33	8	0	4.342692	1.948482	0.015183
34	1	0	6.633827	1.119345	0.015948
35	1	0	-7.235065	-2.498541	0.006595
36	1	0	-8.240071	0.031540	0.009151
37	1	0	-3.501723	2.263669	-0.000544

1:G Counterpoise Corrected Energy: -1294.578037604043
BSSE Energy: 0.001152859721

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-3.152093	1.471542	0.051507
2	6	0	-1.762569	1.524345	0.096899
3	6	0	-3.517874	0.160542	-0.053574
4	7	0	-1.233245	0.309173	0.037873
5	6	0	-2.315460	-0.548649	-0.057749
6	7	0	-4.785032	-0.310617	-0.127646
7	6	0	-2.374226	-1.972224	-0.149433
8	6	0	-4.838663	-1.617258	-0.239736
9	8	0	-1.475603	-2.817495	-0.155829
10	7	0	-3.722168	-2.415886	-0.252858
11	7	0	-6.053075	-2.238851	-0.404627
12	1	0	-3.810354	-3.415487	-0.390459
13	1	0	-6.163975	-3.167978	-0.023940
14	1	0	-6.836845	-1.623503	-0.236210
15	6	0	-1.088150	2.792275	0.199507
16	6	0	-1.595396	4.038325	0.575689
17	6	0	-0.529624	4.961311	0.510140
18	1	0	-2.607361	4.245627	0.898249
19	6	0	0.590400	4.255248	0.094120
20	7	0	0.245891	2.952841	-0.086152
21	1	0	0.892334	2.228387	-0.439092
22	7	0	5.618490	-1.587356	0.196993
23	6	0	6.139728	-0.453389	-0.407702
24	1	0	7.204805	-0.328289	-0.547867
25	7	0	5.219786	0.401378	-0.768002
26	6	0	4.029074	-0.194258	-0.386887
27	6	0	2.678452	0.265993	-0.492935
28	8	0	2.267473	1.331840	-0.967316
29	7	0	1.768488	-0.673075	0.043125
30	1	0	0.780814	-0.387056	0.030363
31	6	0	2.111897	-1.885531	0.599803
32	7	0	1.098179	-2.647566	1.086563
33	1	0	0.173282	-2.587210	0.654728
34	1	0	1.394584	-3.575700	1.350625
35	7	0	3.359922	-2.311186	0.712487
36	6	0	4.255893	-1.432837	0.217556
37	1	0	6.122849	-2.382367	0.558726
38	1	0	1.602156	4.584102	-0.091053
39	1	0	-0.568142	6.015264	0.745066
40	1	0	-3.776008	2.263296	0.016999

2:C Counterpoise Corrected Energy: -1300.608510612905
BSSE Energy: 0.001053047568

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	1.709164	1.740998	-0.007471
2	6	0	2.329199	0.497343	-0.013959
3	6	0	0.356318	1.517805	-0.027076
4	7	0	1.457800	-0.491913	-0.035482
5	6	0	0.223818	0.122765	-0.044106
6	7	0	-0.602416	2.462437	-0.027795
7	6	0	-1.098542	-0.424598	-0.063238
8	6	0	-1.824272	1.943706	-0.049605
9	8	0	-1.438809	-1.617519	-0.077517
10	7	0	-2.072944	0.591155	-0.064705
11	7	0	-2.899520	2.758131	-0.075891
12	1	0	-3.055404	0.265102	-0.060508
13	1	0	-3.858967	2.411724	-0.002805
14	1	0	-2.713891	3.744090	0.003396
15	6	0	3.760606	0.310120	0.001468
16	6	0	4.819202	1.197335	0.023980
17	6	0	6.020518	0.418868	0.030474
18	1	0	4.751594	2.276412	0.035055
19	6	0	5.626161	-0.952415	0.011182
20	7	0	4.251897	-0.982005	-0.005975
21	1	0	3.643858	-1.787063	-0.022728
22	6	0	6.558537	-1.995414	0.011767
23	6	0	7.905310	-1.652795	0.031871
24	6	0	8.318287	-0.303893	0.051072
25	6	0	7.392459	0.730099	0.050593
26	1	0	6.241471	-3.034013	-0.003054
27	1	0	8.654290	-2.439140	0.032745
28	1	0	9.379752	-0.074872	0.066461
29	1	0	7.720181	1.765845	0.065437
30	1	0	2.151255	2.647134	0.004808
31	7	0	-7.142056	0.057439	0.088786
32	6	0	-7.447106	-1.268690	0.070345
33	1	0	-8.500103	-1.526396	0.096326
34	6	0	-6.458826	-2.195876	0.022329
35	1	0	-6.680449	-3.254966	0.007370
36	6	0	-5.100581	-1.705945	-0.007559
37	7	0	-4.072559	-2.558175	-0.053799
38	1	0	-3.096039	-2.209473	-0.062675
39	1	0	-4.241438	-3.550743	-0.058199
40	7	0	-4.823711	-0.395522	0.007871
41	6	0	-5.815244	0.532991	0.058290
42	8	0	-5.632580	1.754061	0.083451
43	1	0	-7.859656	0.767781	0.125148

2:G Counterpoise Corrected Energy: -1448.268724051841
BSSE Energy: 0.001192454198

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	7	0	-2.938622	1.685616	-0.028152
2	6	0	-1.597958	1.322936	0.022322
3	6	0	-3.677759	0.539977	-0.088409
4	7	0	-1.452571	0.005621	0.007223
5	6	0	-2.739737	-0.494598	-0.060488
6	7	0	-5.027387	0.463167	-0.154415
7	6	0	-3.217997	-1.840562	-0.100593
8	6	0	-5.466286	-0.772545	-0.219913
9	8	0	-2.609520	-2.912110	-0.070173
10	7	0	-4.637076	-1.867163	-0.196621
11	7	0	-6.809465	-1.010468	-0.369639
12	1	0	-5.019091	-2.799853	-0.297600
13	1	0	-7.191685	-1.857224	0.026350
14	1	0	-7.378079	-0.186760	-0.231328
15	6	0	-0.565566	2.330247	0.084692
16	6	0	-0.683105	3.671878	0.424123
17	6	0	0.622388	4.238405	0.334820
18	1	0	-1.585022	4.176947	0.743521
19	6	0	1.492442	3.183012	-0.070515
20	7	0	0.747643	2.040943	-0.208078
21	1	0	1.123831	1.144766	-0.551054
22	6	0	2.866774	3.378586	-0.269867
23	6	0	3.363618	4.653638	-0.048527
24	6	0	2.521430	5.714954	0.361487
25	6	0	1.163539	5.521774	0.554898
26	1	0	3.500587	2.555429	-0.583546
27	1	0	4.423286	4.844172	-0.191273
28	1	0	2.952771	6.698229	0.525362
29	1	0	0.525454	6.343423	0.868575
30	1	0	-3.298436	2.626027	-0.091405
31	7	0	4.550661	-3.853689	0.250072
32	6	0	5.380958	-2.948658	-0.393976
33	1	0	6.434608	-3.149668	-0.531989
34	7	0	4.753234	-1.874395	-0.792322
35	6	0	3.441992	-2.075863	-0.395722
36	6	0	2.287737	-1.241580	-0.529221
37	8	0	2.204079	-0.122588	-1.049784
38	7	0	1.143935	-1.847489	0.039194
39	1	0	0.287527	-1.281477	0.014529
40	6	0	1.115860	-3.084440	0.645287
41	7	0	-0.075302	-3.490973	1.156666
42	1	0	-0.943666	-3.170347	0.724038
43	1	0	-0.068278	-4.454012	1.458920
44	7	0	2.181903	-3.856151	0.779966
45	6	0	3.295258	-3.302080	0.256945
46	1	0	4.799502	-4.747696	0.645237

Cartesian Coordinates and Absolute Energies (Hartrees) for Monomers when dR=2′-deoxyribose

G *syn* (Hoogsteen) Monomer Energy: -963.895387

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.354082	-1.305528	0.092520
2	8	0	1.726065	-0.432724	1.145874
3	1	0	1.747964	-2.314776	0.272231
4	6	0	1.965544	-0.701479	-1.180810
5	6	0	2.878048	0.359455	0.773947
6	6	0	3.265398	-0.086863	-0.649039
7	1	0	1.314942	0.083158	-1.572011
8	1	0	2.132465	-1.450016	-1.960598
9	6	0	2.524198	1.841233	0.904645
10	1	0	3.700843	0.115734	1.457119
11	1	0	3.597397	0.763206	-1.257349
12	1	0	2.141192	2.007950	1.923937
13	1	0	3.441039	2.433423	0.796772
14	8	0	1.615365	2.286006	-0.083226
15	1	0	0.813520	1.715862	-0.030575
16	8	0	4.299610	-1.061361	-0.507743
17	1	0	4.569672	-1.337848	-1.393535
18	7	0	-0.095231	-1.441030	0.079592
19	6	0	-0.817181	-2.618331	0.233463
20	6	0	-1.037481	-0.444360	-0.018643
21	7	0	-2.111923	-2.445155	0.220708
22	6	0	-2.272462	-1.081807	0.066253
23	7	0	-0.787068	0.885372	-0.149929
24	6	0	-3.474523	-0.289094	-0.004063
25	6	0	-1.869268	1.630897	-0.212630
26	8	0	-4.648929	-0.604363	0.033191
27	7	0	-3.129854	1.106283	-0.148083
28	7	0	-1.733623	2.981395	-0.395778
29	1	0	-3.938033	1.707938	-0.252128
30	1	0	-2.456695	3.588896	-0.040024
31	1	0	-0.786248	3.319987	-0.275250
32	1	0	-0.309179	-3.566781	0.347210

G *anti* (Watson-Crick) Monomer Energy: -963.8875439

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	3.447770	-1.914606	0.270890
2	6	0	3.952324	-1.127529	-0.805723
3	1	0	3.710657	-1.577721	-1.778104
4	1	0	5.046616	-1.021467	-0.738748
5	6	0	3.325082	0.259488	-0.758253
6	1	0	3.839509	0.893542	-1.490583
7	8	0	1.937844	0.182103	-1.116271
8	6	0	1.105705	0.612450	-0.043065
9	1	0	0.691152	1.602371	-0.258326
10	7	0	-0.032138	-0.282312	0.058628

11	6	0	-0.007290	-1.665820	0.184776
12	1	0	0.934664	-2.194208	0.225764
13	7	0	-1.200374	-2.201784	0.217714
14	6	0	-2.065389	-1.129874	0.103809
15	6	0	-3.504164	-1.092294	0.090335
16	8	0	-4.336726	-1.977577	0.183869
17	7	0	-3.946213	0.271420	-0.054043
18	1	0	-4.952483	0.373219	-0.003332
19	6	0	-3.147845	1.380056	-0.161872
20	7	0	-3.783293	2.602042	-0.237919
21	1	0	-4.660756	2.631264	-0.738935
22	1	0	-3.149312	3.349389	-0.486269
23	7	0	-1.837677	1.333131	-0.145621
24	6	0	-1.359622	0.068308	-0.003648
25	6	0	3.382611	0.948845	0.617919
26	1	0	4.198602	0.552824	1.236445
27	6	0	2.005757	0.629068	1.202952
28	1	0	2.021125	-0.360889	1.663669
29	1	0	1.672362	1.360521	1.944853
30	8	0	3.557228	2.342104	0.364333
31	1	0	3.521965	2.804277	1.212303
32	1	0	3.751836	-2.822996	0.154008

1 *anti* Monomer Energy: -1172.9395688

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.544574	-1.136001	0.224789
2	8	0	-1.425260	-1.136998	-0.898707
3	1	0	0.032947	-2.067606	0.228461
4	6	0	-1.462192	-1.080724	1.463620
5	6	0	-2.497440	-2.010726	-0.533376
6	6	0	-2.779022	-1.724590	0.959419
7	1	0	-1.612950	-0.050310	1.789636
8	1	0	-1.040880	-1.655425	2.292066
9	6	0	-3.658967	-1.781063	-1.488786
10	1	0	-2.173009	-3.062456	-0.602207
11	1	0	-3.613877	-1.019182	1.048940
12	1	0	-3.368056	-2.107525	-2.497761
13	1	0	-4.502353	-2.399786	-1.166367
14	8	0	-4.107670	-0.435482	-1.491844
15	1	0	-3.372310	0.102166	-1.818682
16	8	0	-3.106106	-2.968085	1.569552
17	1	0	-3.510713	-2.784695	2.426631
18	7	0	0.450207	-0.093641	0.090338
19	6	0	0.363749	1.307819	0.070039
20	6	0	1.799612	-0.386159	-0.004719
21	7	0	1.557233	1.870261	-0.014980
22	6	0	2.457407	0.835772	-0.059775
23	7	0	2.328818	-1.635321	-0.032829
24	6	0	3.894707	0.855689	-0.141676
25	6	0	3.638890	-1.636761	-0.106593
26	8	0	4.682870	1.785055	-0.183342
27	7	0	4.392148	-0.493143	-0.161495

28	7	0	4.319402	-2.834069	-0.076425
29	1	0	5.403316	-0.549081	-0.151174
30	1	0	5.181452	-2.889541	-0.600918
31	1	0	3.710261	-3.630564	-0.203954
32	6	0	-0.823686	2.138604	0.133820
33	6	0	-2.202166	1.954450	0.068399
34	6	0	-2.808046	3.233641	0.159525
35	1	0	-2.718311	1.018536	-0.060467
36	6	0	-1.793704	4.165834	0.273538
37	7	0	-0.605966	3.494823	0.259151
38	1	0	0.329172	3.876316	0.290731
39	1	0	-1.828172	5.241203	0.364557
40	1	0	-3.867504	3.444951	0.139562

1 *syn* Monomer Energy: -1172.9475542

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.143374	-1.385316	0.074148
2	8	0	-0.650288	-1.744738	-1.048618
3	1	0	1.100512	-1.908114	0.054155
4	6	0	-0.660196	-1.829331	1.306426
5	6	0	-1.577493	-2.797068	-0.696427
6	6	0	-1.328920	-3.109430	0.792553
7	1	0	-1.418616	-1.087561	1.560523
8	1	0	-0.020640	-2.000928	2.177137
9	6	0	-2.997337	-2.333535	-1.023715
10	1	0	-1.335945	-3.688631	-1.288467
11	1	0	-2.267242	-3.324503	1.318396
12	1	0	-3.015443	-2.020350	-2.079700
13	1	0	-3.680964	-3.185017	-0.920718
14	8	0	-3.458314	-1.312773	-0.160037
15	1	0	-2.794327	-0.585516	-0.179711
16	8	0	-0.442383	-4.228790	0.832902
17	1	0	-0.265037	-4.433125	1.760756
18	7	0	0.447017	0.038216	0.002256
19	6	0	1.701165	0.659366	-0.051348
20	6	0	-0.474010	1.063614	0.037816
21	7	0	1.606644	1.976478	-0.012796
22	6	0	0.259599	2.243808	0.040592
23	7	0	-1.825073	0.923372	0.041562
24	6	0	-0.437114	3.504379	0.074292
25	6	0	-2.487078	2.060281	0.066660
26	8	0	-0.021264	4.648975	0.101455
27	7	0	-1.860984	3.275202	0.083143
28	7	0	-3.855915	2.030575	0.125309
29	1	0	-2.403619	4.127364	0.155690
30	1	0	-4.367359	2.802864	-0.275724
31	1	0	-4.254756	1.114805	-0.047524
32	6	0	2.993856	0.002326	-0.119243
33	6	0	3.472020	-1.250051	-0.496844
34	6	0	4.886282	-1.212676	-0.400994
35	1	0	2.886182	-2.084367	-0.851953
36	6	0	5.239925	0.054548	0.022960
37	7	0	4.092904	0.774303	0.192000

38	1	0	4.002673	1.750516	0.435138
39	1	0	6.208447	0.490055	0.217719
40	1	0	5.567534	-2.021389	-0.622914

2 *anti* Monomer Energy: -1326.631703

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.909356	1.558128	0.230761
2	8	0	-0.186135	2.049658	-0.895664
3	1	0	-1.900127	2.026288	0.254923
4	6	0	-0.092198	1.991589	1.464972
5	6	0	0.249381	3.360115	-0.519837
6	6	0	0.657420	3.254138	0.967420
7	1	0	0.598642	1.203867	1.769769
8	1	0	-0.746115	2.233866	2.306261
9	6	0	1.340865	3.807805	-1.480977
10	1	0	-0.592145	4.070817	-0.572215
11	1	0	1.742334	3.114150	1.043608
12	1	0	0.911171	3.931752	-2.485265
13	1	0	1.712237	4.783567	-1.152348
14	8	0	2.452307	2.926153	-1.500875
15	1	0	2.138170	2.087569	-1.867489
16	8	0	0.263022	4.467366	1.598027
17	1	0	0.720981	4.527670	2.445696
18	7	0	-1.182744	0.142985	0.080715
19	6	0	-0.353124	-0.989458	0.031904
20	6	0	-2.475932	-0.339681	0.003405
21	7	0	-1.054531	-2.106807	-0.053219
22	6	0	-2.369882	-1.723883	-0.069655
23	7	0	-3.598000	0.421823	0.031029
24	6	0	-3.569064	-2.517130	-0.160390
25	6	0	-4.701207	-0.284066	-0.060828
26	8	0	-3.727699	-3.722447	-0.243525
27	7	0	-4.716795	-1.651647	-0.151333
28	7	0	-5.913979	0.360988	-0.122106
29	1	0	-5.592476	-2.143037	-0.283714
30	1	0	-6.716503	-0.107524	0.273898
31	1	0	-5.851027	1.343994	0.103184
32	6	0	1.097165	-1.051763	0.061377
33	6	0	2.129424	-0.134190	-0.018364
34	6	0	3.355738	-0.870143	0.033842
35	1	0	2.034675	0.931250	-0.135377
36	6	0	3.010498	-2.248361	0.142549
37	7	0	1.640510	-2.323636	0.161715
38	1	0	1.056971	-3.147366	0.184286
39	6	0	3.980483	-3.255611	0.212065
40	6	0	5.312499	-2.863884	0.170012
41	6	0	5.677000	-1.504026	0.061317
42	6	0	4.714865	-0.507059	-0.007248
43	1	0	3.702320	-4.302034	0.294120
44	1	0	6.090391	-3.620014	0.220489
45	1	0	6.729652	-1.239114	0.029845
46	1	0	5.000217	0.537404	-0.094928

2 *syn* Monomer Energy: -1326.6396375

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.597015	-1.328301	0.148214
2	8	0	-1.283016	-1.822247	-0.993483
3	1	0	0.420088	-1.720590	0.189328
4	6	0	-1.392482	-1.834329	1.361526
5	6	0	-2.085536	-2.973313	-0.641764
6	6	0	-1.865193	-3.206572	0.865567
7	1	0	-2.252014	-1.191602	1.556521
8	1	0	-0.776387	-1.894903	2.263323
9	6	0	-3.536349	-2.705664	-1.042175
10	1	0	-1.706873	-3.843358	-1.192161
11	1	0	-2.790031	-3.526790	1.360817
12	1	0	-3.547590	-2.429100	-2.108390
13	1	0	-4.110309	-3.634161	-0.936349
14	8	0	-4.161830	-1.727069	-0.234361
15	1	0	-3.596137	-0.921828	-0.250455
16	8	0	-0.843570	-4.197716	0.979742
17	1	0	-0.684009	-4.353336	1.920306
18	7	0	-0.475942	0.121191	0.036389
19	6	0	0.689778	0.896094	0.002130
20	6	0	-1.518408	1.021512	0.028578
21	7	0	0.429873	2.190804	0.018007
22	6	0	-0.939629	2.286162	0.030463
23	7	0	-2.840007	0.711897	-0.001308
24	6	0	-1.790716	3.449579	0.027628
25	6	0	-3.640427	1.757005	-0.012186
26	8	0	-1.522450	4.636866	0.047838
27	7	0	-3.173605	3.041963	0.003306
28	7	0	-4.993801	1.554547	0.006785
29	1	0	-3.821452	3.819426	0.047316
30	1	0	-5.591689	2.255476	-0.405013
31	1	0	-5.272021	0.594274	-0.159303
32	6	0	2.057410	0.407976	-0.046913
33	6	0	2.659307	-0.775974	-0.435654
34	6	0	4.073699	-0.588128	-0.323788
35	1	0	2.165981	-1.657317	-0.816239
36	6	0	4.281593	0.744924	0.134813
37	7	0	3.044220	1.316550	0.300795
38	1	0	2.827868	2.276072	0.527976
39	6	0	5.562235	1.269161	0.346760
40	6	0	6.644106	0.436743	0.091103
41	6	0	6.461756	-0.887511	-0.363480
42	6	0	5.192120	-1.405641	-0.571891
43	1	0	5.703904	2.287694	0.695538
44	1	0	7.651547	0.812517	0.243170
45	1	0	7.333282	-1.507120	-0.552399
46	1	0	5.060111	-2.425039	-0.923260

Cartesian Coordinates and Absolute Energies (Hartrees) for H-bonded Complexes when dR=2′-deoxyribose

G:C Counterpoise Corrected Energy: -1359.001156933865
BSSE energy: 0.001051541185

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-5.891192	-1.766972	-0.139666
2	6	0	-6.325175	-0.907004	0.911692
3	1	0	-6.092954	-1.331937	1.897677
4	1	0	-7.412286	-0.736291	0.858894
5	6	0	-5.614298	0.435369	0.797825
6	1	0	-6.076668	1.128220	1.511889
7	8	0	-4.229687	0.285124	1.135234
8	6	0	-3.390757	0.628788	0.032829
9	1	0	-2.919747	1.601850	0.204235
10	7	0	-2.307450	-0.328159	-0.052566
11	6	0	-2.407290	-1.715827	-0.109320
12	1	0	-3.376654	-2.193661	-0.096620
13	7	0	-1.247528	-2.315779	-0.152332
14	6	0	-0.322841	-1.284087	-0.120720
15	6	0	1.106249	-1.302954	-0.141067
16	8	0	1.869031	-2.280935	-0.197782
17	7	0	1.637477	0.001090	-0.085779
18	1	0	2.669202	0.059877	-0.075045
19	6	0	0.907755	1.164094	-0.021617
20	7	0	1.608769	2.320052	0.001221
21	1	0	2.625676	2.344253	0.098587
22	1	0	1.073754	3.160218	0.144717
23	7	0	-0.417067	1.192791	-0.004037
24	6	0	-0.961104	-0.041763	-0.050512
25	6	0	-5.657896	1.072343	-0.604094
26	1	0	-6.507093	0.700826	-1.192917
27	6	0	-4.312889	0.650140	-1.197209
28	1	0	-4.393890	-0.355065	-1.616628
29	1	0	-3.950604	1.330132	-1.973925
30	8	0	-5.749321	2.482534	-0.404377
31	1	0	-5.671960	2.908992	-1.268110
32	1	0	-6.229719	-2.654014	0.032439
33	7	0	6.558180	1.340451	0.204403
34	6	0	7.323591	0.217293	0.134359
35	1	0	8.397613	0.356742	0.189488
36	6	0	6.740054	-0.999481	0.003178
37	1	0	7.330940	-1.904395	-0.053008
38	6	0	5.296763	-1.032574	-0.055401
39	7	0	4.649732	-2.194593	-0.179752
40	1	0	3.611008	-2.226961	-0.196066
41	1	0	5.169606	-3.055958	-0.220723
42	7	0	4.563961	0.086401	0.010667
43	6	0	5.148822	1.305381	0.145432
44	8	0	4.535847	2.374583	0.219739
45	1	0	6.967928	2.258409	0.304912

G:G Counterpoise Corrected Energy: -1506.663759671083
BSSE Energy: 0.000779094525

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.525263	-1.670328	0.107910
2	8	0	3.456569	-1.396109	1.138208
3	1	0	1.966437	-2.590207	0.321416
4	6	0	3.356902	-1.816503	-1.174338
5	6	0	4.779627	-1.852028	0.764984
6	6	0	4.641530	-2.463538	-0.643202
7	1	0	3.580916	-0.832003	-1.590848
8	1	0	2.852951	-2.420121	-1.934177
9	6	0	5.751424	-0.676733	0.866321
10	1	0	5.083180	-2.641596	1.462887
11	1	0	5.509987	-2.225501	-1.269501
12	1	0	5.673998	-0.260804	1.883229
13	1	0	6.773997	-1.052013	0.741234
14	8	0	5.538500	0.308999	-0.126223
15	1	0	4.603906	0.603968	-0.053409
16	8	0	4.497059	-3.871269	-0.463940
17	1	0	4.418331	-4.278465	-1.336934
18	7	0	1.532675	-0.599045	0.080851
19	6	0	0.161061	-0.749830	0.205641
20	6	0	1.758427	0.755576	-0.024166
21	7	0	-0.473848	0.394670	0.174512
22	6	0	0.504506	1.350287	0.033651
23	7	0	2.955320	1.383354	-0.145500
24	6	0	0.383294	2.772713	-0.068453
25	6	0	2.871742	2.694028	-0.230276
26	8	0	-0.617872	3.481012	-0.069014
27	7	0	1.676018	3.368825	-0.196177
28	7	0	4.015593	3.419615	-0.406851
29	1	0	1.656212	4.373845	-0.322281
30	1	0	4.045497	4.375244	-0.084917
31	1	0	4.869347	2.887763	-0.286543
32	7	0	-7.174192	-0.615050	-0.147298
33	6	0	-7.118865	-1.999494	-0.169198
34	1	0	-8.015381	-2.599020	-0.250806
35	7	0	-5.899067	-2.460837	-0.082190
36	6	0	-5.105001	-1.329745	0.002909
37	6	0	-3.677449	-1.188866	0.113969
38	8	0	-2.796464	-2.046511	0.158028
39	7	0	-3.324173	0.185393	0.174002
40	1	0	-2.309200	0.355712	0.231075
41	6	0	-4.181974	1.249589	0.125212
42	7	0	-3.631363	2.490745	0.232418
43	1	0	-2.638155	2.654105	0.104009
44	1	0	-4.257512	3.257481	0.047048
45	7	0	-5.495194	1.128478	0.015027
46	6	0	-5.881343	-0.167282	-0.036282
47	1	0	-7.992440	-0.027829	-0.197586
48	1	0	-0.331662	-1.709639	0.299987

1:C Counterpoise Corrected Energy: -1568.053709224956
BSSE Energy: 0.001081686001

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.570392	-1.141129	-0.236408
2	8	0	3.413013	-1.205949	0.917255
3	1	0	1.931732	-2.031625	-0.262162
4	6	0	3.533476	-1.146281	-1.443045
5	6	0	4.432823	-2.149245	0.581534
6	6	0	4.792682	-1.863382	-0.893661
7	1	0	3.754926	-0.128138	-1.767562
8	1	0	3.106799	-1.699978	-2.283111
9	6	0	5.567823	-2.016736	1.585799
10	1	0	4.032629	-3.176304	0.620630
11	1	0	5.665879	-1.201112	-0.937692
12	1	0	5.213435	-2.337788	2.576151
13	1	0	6.378882	-2.687760	1.285698
14	8	0	6.108891	-0.705991	1.632822
15	1	0	5.395183	-0.121873	1.926606
16	8	0	5.083688	-3.115330	-1.505910
17	1	0	5.518372	-2.941287	-2.350080
18	7	0	1.643591	-0.037531	-0.133522
19	6	0	1.819710	1.358025	-0.106958
20	6	0	0.273843	-0.244564	-0.100221
21	7	0	0.666280	1.998219	-0.072911
22	6	0	-0.303850	1.022835	-0.071867
23	7	0	-0.332561	-1.447204	-0.115283
24	6	0	-1.730693	1.116196	-0.044901
25	6	0	-1.656069	-1.356469	-0.089720
26	8	0	-2.436832	2.137213	-0.018030
27	7	0	-2.327691	-0.158239	-0.053922
28	7	0	-2.409150	-2.476031	-0.108766
29	1	0	-3.361788	-0.166800	-0.027544
30	1	0	-3.429337	-2.460465	-0.044568
31	1	0	-1.914295	-3.351797	-0.089712
32	6	0	3.064217	2.104297	-0.117577
33	6	0	4.420722	1.822480	0.012624
34	6	0	5.121053	3.055018	-0.053561
35	1	0	4.858820	0.851530	0.167079
36	6	0	4.183109	4.056654	-0.216591
37	7	0	2.950216	3.471127	-0.257181
38	1	0	2.046342	3.916149	-0.332283
39	7	0	-7.298971	-1.282576	0.144197
40	6	0	-8.010954	-0.123373	0.180593
41	1	0	-9.090160	-0.217126	0.229926
42	6	0	-7.371320	1.071976	0.155392
43	1	0	-7.919383	2.004663	0.184170
44	6	0	-5.928802	1.042943	0.089500
45	7	0	-5.227105	2.179582	0.062659
46	1	0	-4.189911	2.160848	0.027374
47	1	0	-5.703763	3.065800	0.096730
48	7	0	-5.248753	-0.110273	0.052357
49	6	0	-5.890333	-1.307977	0.079508
50	8	0	-5.327550	-2.406710	0.051901
51	1	0	-7.751432	-2.185753	0.163411

52	1	0	4.298363	5.126309	-0.308561
53	1	0	6.191064	3.189518	0.015168

1:G Counterpoise Corrected Energy: -1715.723273018754
BSSE Energy: 0.001156798156

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.023521	-1.191358	0.083270
2	8	0	-4.002964	-0.880314	-0.900378
3	1	0	-2.672632	-2.218167	-0.029922
4	6	0	-3.728044	-1.022351	1.437449
5	6	0	-5.332724	-1.054471	-0.357706
6	6	0	-5.146106	-1.503046	1.105702
7	1	0	-3.750926	0.025867	1.738965
8	1	0	-3.251094	-1.611530	2.225882
9	6	0	-6.111301	0.248993	-0.534462
10	1	0	-5.833965	-1.858846	-0.909980
11	1	0	-5.898056	-1.048515	1.762663
12	1	0	-6.077090	0.523099	-1.600774
13	1	0	-7.161606	0.074313	-0.272434
14	8	0	-5.636383	1.293499	0.294888
15	1	0	-4.669943	1.376034	0.139490
16	8	0	-5.244649	-2.926565	1.109057
17	1	0	-5.104028	-3.233988	2.014525
18	7	0	-1.857684	-0.337078	-0.130333
19	6	0	-0.534361	-0.734236	-0.386295
20	6	0	-1.830915	1.030217	-0.012278
21	7	0	0.294450	0.300583	-0.385700
22	6	0	-0.500092	1.405012	-0.156664
23	7	0	-2.901108	1.840005	0.178663
24	6	0	-0.170125	2.795887	-0.117775
25	6	0	-2.612641	3.121427	0.240397
26	8	0	0.913774	3.366407	-0.244597
27	7	0	-1.332379	3.590618	0.107524
28	7	0	-3.613225	4.019268	0.488808
29	1	0	-1.137791	4.581148	0.191542
30	1	0	-3.516612	4.963289	0.145770
31	1	0	-4.546145	3.627255	0.430522
32	6	0	-0.158902	-2.107399	-0.652350
33	6	0	-0.811923	-3.116360	-1.365680
34	6	0	0.053222	-4.232582	-1.398722
35	1	0	-1.772546	-3.027273	-1.853475
36	6	0	1.201954	-3.876479	-0.708732
37	7	0	1.069098	-2.596022	-0.270780
38	1	0	1.780083	-2.094098	0.284729
39	7	0	7.343400	0.320690	0.259392
40	6	0	7.463157	-0.845816	0.999498
41	1	0	8.429809	-1.224186	1.302963
42	7	0	6.311006	-1.399917	1.268697
43	6	0	5.379978	-0.560122	0.680932
44	6	0	3.953521	-0.650647	0.610203
45	8	0	3.215291	-1.526308	1.078537
46	7	0	3.403787	0.432663	-0.112067
47	1	0	2.383202	0.408373	-0.237941

48	6	0	4.124148	1.461803	-0.675985
49	7	0	3.415357	2.409596	-1.346444
50	1	0	2.472813	2.633266	-1.023274
51	1	0	3.978283	3.204000	-1.613827
52	7	0	5.443372	1.544592	-0.625706
53	6	0	6.003036	0.516720	0.045533
54	1	0	8.082750	0.922669	-0.069719
55	1	0	2.097720	-4.439332	-0.491760
56	1	0	-0.135447	-5.183280	-1.876385

2:C Counterpoise Corrected Energy: -1721.746488808867
BSSE Energy: 0.001078116843

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.665842	-1.937530	-0.248860
2	8	0	2.472129	-2.158118	0.909548
3	1	0	0.886489	-2.706745	-0.294728
4	6	0	2.624937	-2.085851	-1.448224
5	6	0	3.326342	-3.253231	0.569017
6	6	0	3.733865	-3.021827	-0.904033
7	1	0	3.024951	-1.115985	-1.748510
8	1	0	2.117324	-2.539175	-2.303295
9	6	0	4.466105	-3.313922	1.575264
10	1	0	2.763879	-4.201328	0.601476
11	1	0	4.711420	-2.525926	-0.942441
12	1	0	4.063111	-3.578122	2.563599
13	1	0	5.156401	-4.107141	1.271370
14	8	0	5.215054	-2.109838	1.630106
15	1	0	4.613549	-1.423168	1.951498
16	8	0	3.796614	-4.299894	-1.527511
17	1	0	4.259371	-4.199774	-2.368802
18	7	0	0.935918	-0.694197	-0.133979
19	6	0	1.339318	0.653122	-0.090017
20	6	0	-0.447978	-0.672170	-0.105518
21	7	0	0.306288	1.474121	-0.051721
22	6	0	-0.809323	0.673855	-0.062204
23	7	0	-1.245206	-1.756394	-0.136340
24	6	0	-2.202548	1.002460	-0.034911
25	6	0	-2.536046	-1.447792	-0.109659
26	8	0	-2.728032	2.125515	0.004135
27	7	0	-3.001347	-0.155340	-0.059235
28	7	0	-3.462331	-2.426805	-0.141695
29	1	0	-4.023431	0.006234	-0.031386
30	1	0	-4.466694	-2.244332	-0.075770
31	1	0	-3.118099	-3.372317	-0.134592
32	6	0	2.687819	1.191515	-0.080189
33	6	0	3.961464	0.669850	0.058672
34	6	0	4.877354	1.769366	0.016137
35	1	0	4.218783	-0.364199	0.208322
36	6	0	4.100731	2.952960	-0.148831
37	7	0	2.784482	2.568985	-0.208459
38	1	0	1.961202	3.149664	-0.274587
39	6	0	4.685720	4.222308	-0.225244

40	6	0	6.070241	4.295780	-0.131900
41	6	0	6.858458	3.136617	0.033855
42	6	0	6.277008	1.878681	0.108584
43	1	0	4.080736	5.115363	-0.351047
44	1	0	6.555853	5.265734	-0.186479
45	1	0	7.937647	3.235636	0.104529
46	1	0	6.887782	0.989931	0.239744
47	7	0	-8.083872	-0.456121	0.134909
48	6	0	-8.599390	0.802261	0.186898
49	1	0	-9.679537	0.883264	0.237478
50	6	0	-7.775161	1.878921	0.174641
51	1	0	-8.165262	2.887468	0.215652
52	6	0	-6.356570	1.618144	0.105302
53	7	0	-5.480541	2.626992	0.090663
54	1	0	-4.461174	2.441186	0.052939
55	1	0	-5.807076	3.578320	0.136258
56	7	0	-5.871502	0.370839	0.052664
57	6	0	-6.698338	-0.707750	0.066685
58	8	0	-6.319923	-1.882560	0.024254
59	1	0	-8.676298	-1.274575	0.144091

2:G Counterpoise Corrected Energy: -1869.413726348051
BSSE Energy: 0.001251061735

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.114668	0.924798	0.245950
2	8	0	4.089370	0.780296	-0.778426
3	1	0	2.673397	1.922378	0.226133
4	6	0	3.865865	0.706612	1.567368
5	6	0	5.413668	1.027645	-0.249342
6	6	0	5.227597	1.337893	1.249520
7	1	0	3.987865	-0.357187	1.776638
8	1	0	3.360520	1.182393	2.412639
9	6	0	6.298392	-0.181670	-0.549992
10	1	0	5.826593	1.915973	-0.742688
11	1	0	6.033622	0.901017	1.852079
12	1	0	6.257720	-0.371315	-1.634200
13	1	0	7.336182	0.065742	-0.297074
14	8	0	5.941554	-1.328227	0.200490
15	1	0	4.982381	-1.484516	0.057530
16	8	0	5.199884	2.759140	1.368669
17	1	0	5.056268	2.979378	2.298759
18	7	0	2.021147	-0.010111	-0.018587
19	6	0	0.662060	0.281786	-0.210480
20	6	0	2.122297	-1.378756	-0.037022
21	7	0	-0.069141	-0.818990	-0.299946
22	6	0	0.828081	-1.860710	-0.200057
23	7	0	3.264868	-2.100678	0.060966
24	6	0	0.626494	-3.274033	-0.296245
25	6	0	3.095919	-3.403560	-0.003437
26	8	0	-0.403583	-3.925787	-0.465276
27	7	0	1.861163	-3.975038	-0.167433
28	7	0	4.179313	-4.222390	0.139151
29	1	0	1.760354	-4.982906	-0.183287

30	1	0	4.159478	-5.140894	-0.277546
31	1	0	5.072383	-3.743946	0.109037
32	6	0	0.139199	1.632069	-0.329013
33	6	0	0.678302	2.755017	-0.943912
34	6	0	-0.300130	3.790014	-0.848529
35	1	0	1.627196	2.805155	-1.458872
36	6	0	-1.416288	3.230939	-0.160638
37	7	0	-1.125369	1.924933	0.135446
38	1	0	-1.759908	1.289303	0.640089
39	6	0	-2.573454	3.972199	0.119650
40	6	0	-2.599948	5.290218	-0.309192
41	6	0	-1.506627	5.865526	-0.999859
42	6	0	-0.362998	5.132992	-1.272829
43	1	0	-3.406043	3.518065	0.647279
44	1	0	-3.480024	5.895914	-0.113548
45	1	0	-1.570018	6.901695	-1.319325
46	1	0	0.471704	5.583360	-1.802770
47	7	0	-7.117684	-1.546396	0.220202
48	6	0	-7.353680	-0.478582	1.072730
49	1	0	-8.355311	-0.219048	1.387375
50	7	0	-6.260224	0.142107	1.427883
51	6	0	-5.248312	-0.547514	0.781758
52	6	0	-3.834709	-0.327603	0.760181
53	8	0	-3.183627	0.551990	1.337988
54	7	0	-3.178526	-1.276792	-0.056431
55	1	0	-2.164916	-1.146303	-0.160018
56	6	0	-3.794588	-2.298992	-0.743630
57	7	0	-2.992769	-3.103999	-1.491540
58	1	0	-2.037016	-3.273058	-1.175645
59	1	0	-3.476681	-3.911608	-1.856077
60	7	0	-5.101223	-2.501670	-0.735411
61	6	0	-5.761905	-1.601920	0.022841
62	1	0	-7.794833	-2.171940	-0.189098

Absolute Energies and Cartesian Coordinates of B3LYP/6-311+G(2df,p)/B3LYP/6-31G(d) Minima and Transition State Conformations of 1

TS (1 imaginary frequency) $\chi = 55.0°$ $\theta = 2.0°$
Energy= -1172.9356798

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.221276	-1.340952	0.009968
2	8	0	-0.630663	-1.649780	-1.080505
3	1	0	1.180031	-1.840283	-0.136060
4	6	0	-0.472612	-1.922060	1.251186
5	6	0	-1.443371	-2.805329	-0.768555
6	6	0	-1.092322	-3.203142	0.680257
7	1	0	-1.253517	-1.243330	1.600146
8	1	0	0.227885	-2.112915	2.070516
9	6	0	-2.910660	-2.440392	-0.992911
10	1	0	-1.156775	-3.624645	-1.439747
11	1	0	-1.982987	-3.518872	1.236331
12	1	0	-3.013747	-2.060575	-2.022186

13	1	0	-3.522549	-3.346910	-0.910514
14	8	0	-3.394201	-1.515482	-0.037625
15	1	0	-2.771484	-0.748068	-0.039721
16	8	0	-0.133885	-4.262361	0.596005
17	1	0	0.050493	-4.564220	1.499413
18	7	0	0.471702	0.092240	0.035421
19	6	0	1.685716	0.813406	-0.033258
20	6	0	-0.527081	1.047149	0.069492
21	7	0	1.473633	2.115987	-0.030581
22	6	0	0.114611	2.276748	0.027226
23	7	0	-1.864379	0.807433	0.117297
24	6	0	-0.673339	3.484413	0.046088
25	6	0	-2.608532	1.892393	0.132104
26	8	0	-0.344577	4.656419	0.030110
27	7	0	-2.075785	3.150238	0.098724
28	7	0	-3.972563	1.765657	0.235053
29	1	0	-2.679941	3.961579	0.169149
30	1	0	-4.544128	2.481793	-0.193329
31	1	0	-4.306959	0.818760	0.083376
32	6	0	3.049351	0.303778	-0.073310
33	6	0	4.187241	1.104787	-0.093876
34	6	0	5.320767	0.260888	-0.129728
35	1	0	4.163552	2.184176	-0.081123
36	6	0	4.863770	-1.041472	-0.130356
37	1	0	6.356907	0.569492	-0.150703
38	1	0	5.392480	-1.983465	-0.154834
39	7	0	3.492667	-1.009704	-0.090856
40	1	0	2.921538	-1.837133	-0.115976

TS (1 imaginary frequency) $\chi = 57.0°$ $\theta = 84.5°$
Energy= -1172.9392628

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.718675	1.086106	-0.087174
2	8	0	0.115149	1.703440	1.042899
3	1	0	1.809761	1.123240	-0.007874
4	6	0	0.236588	1.890851	-1.302943
5	6	0	-0.257683	3.066798	0.738383
6	6	0	0.151155	3.309859	-0.727703
7	1	0	-0.753669	1.553407	-1.617272
8	1	0	0.925244	1.812270	-2.150269
9	6	0	-1.748408	3.248213	1.026710
10	1	0	0.324972	3.737307	1.382480
11	1	0	-0.589210	3.924726	-1.254738
12	1	0	-1.935567	2.926367	2.064134
13	1	0	-1.997024	4.314469	0.960827
14	8	0	-2.580421	2.567582	0.106084
15	1	0	-2.300509	1.621758	0.100226
16	8	0	1.425880	3.954015	-0.693823
17	1	0	1.712103	4.092458	-1.610398
18	7	0	0.367019	-0.327124	-0.092115
19	6	0	1.254793	-1.417453	-0.035394
20	6	0	-0.892826	-0.869246	-0.095287
21	7	0	0.623882	-2.569917	-0.021291

22	6	0	-0.714514	-2.249703	-0.056491
23	7	0	-2.064409	-0.178601	-0.110056
24	6	0	-1.873023	-3.108022	-0.046761
25	6	0	-3.136876	-0.939592	-0.099057
26	8	0	-1.975000	-4.320144	-0.026533
27	7	0	-3.073445	-2.305130	-0.070748
28	7	0	-4.372427	-0.347219	-0.165720
29	1	0	-3.923527	-2.855741	-0.120591
30	1	0	-5.152022	-0.822835	0.268395
31	1	0	-4.353390	0.656522	-0.015639
32	6	0	2.710600	-1.234049	-0.004695
33	6	0	3.652838	-1.251602	-1.017838
34	6	0	4.926255	-1.025004	-0.429344
35	1	0	3.437524	-1.419822	-2.064216
36	6	0	4.731576	-0.873994	0.928307
37	1	0	5.877760	-0.980453	-0.941358
38	1	0	5.432783	-0.693356	1.730227
39	7	0	3.389238	-0.993425	1.176379
40	1	0	2.955993	-0.978517	2.087640

TS (1 imaginary frequency) $\chi = 51.9°$ $\theta = 281.5°$
Energy= -1172.9379326

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.698466	1.103689	0.021546
2	8	0	-0.021362	1.678370	1.102413
3	1	0	1.776064	1.161546	0.207155
4	6	0	0.303779	1.925433	-1.215357
5	6	0	-0.393395	3.041431	0.800716
6	6	0	0.123323	3.329049	-0.623107
7	1	0	-0.644128	1.565004	-1.622719
8	1	0	1.066320	1.890113	-2.000477
9	6	0	-1.905721	3.187431	0.972381
10	1	0	0.123433	3.706421	1.503946
11	1	0	-0.595058	3.928011	-1.196535
12	1	0	-2.168616	2.837387	1.983680
13	1	0	-2.171962	4.249582	0.909276
14	8	0	-2.644076	2.510148	-0.027980
15	1	0	-2.340735	1.570886	-0.027026
16	8	0	1.366989	4.016368	-0.477696
17	1	0	1.701504	4.214530	-1.366409
18	7	0	0.382041	-0.317829	-0.049579
19	6	0	1.285489	-1.390848	0.071252
20	6	0	-0.867388	-0.884243	-0.087284
21	7	0	0.674907	-2.554111	0.089220
22	6	0	-0.666747	-2.259298	-0.000734
23	7	0	-2.049561	-0.217727	-0.173253
24	6	0	-1.808999	-3.139079	-0.015501
25	6	0	-3.108210	-0.997794	-0.178528
26	8	0	-1.889465	-4.352148	0.031319
27	7	0	-3.021775	-2.360435	-0.108097
28	7	0	-4.350565	-0.429900	-0.307948
29	1	0	-3.859587	-2.928188	-0.171400
30	1	0	-5.136703	-0.908632	0.110865

31	1	0	-4.353535	0.577260	-0.179126
32	6	0	2.735490	-1.183834	0.145911
33	6	0	3.600571	-1.196311	1.224578
34	6	0	4.911180	-0.949802	0.732825
35	1	0	3.308001	-1.360165	2.252436
36	6	0	4.816607	-0.795292	-0.634468
37	1	0	5.820120	-0.889626	1.315617
38	1	0	5.574183	-0.607110	-1.381659
39	7	0	3.495625	-0.920857	-0.981961
40	1	0	3.142642	-0.966105	-1.926120

TS (1 imaginary frequency) $\chi = 57.7°$ $\theta = 187.5°$
Energy= -1172.9474414

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.072975	-1.400630	0.036211
2	8	0	-0.781580	-1.658619	-1.068428
3	1	0	0.994366	-1.974408	-0.058586
4	6	0	-0.707435	-1.864723	1.275634
5	6	0	-1.727550	-2.701296	-0.739119
6	6	0	-1.452596	-3.088262	0.728327
7	1	0	-1.419737	-1.098509	1.588430
8	1	0	-0.047950	-2.104947	2.115742
9	6	0	-3.139815	-2.182577	-1.010204
10	1	0	-1.524912	-3.570580	-1.377353
11	1	0	-2.384183	-3.284308	1.273524
12	1	0	-3.178007	-1.827856	-2.052863
13	1	0	-3.850733	-3.012363	-0.915381
14	8	0	-3.541875	-1.178176	-0.097229
15	1	0	-2.843481	-0.481308	-0.107067
16	8	0	-0.620413	-4.250047	0.695493
17	1	0	-0.437765	-4.508302	1.612650
18	7	0	0.449999	0.006688	0.023074
19	6	0	1.729902	0.573065	-0.037582
20	6	0	-0.427908	1.070900	0.057121
21	7	0	1.687092	1.894134	-0.019062
22	6	0	0.354235	2.218840	0.035533
23	7	0	-1.783581	0.989120	0.084460
24	6	0	-0.286487	3.508944	0.061467
25	6	0	-2.395371	2.153368	0.104459
26	8	0	0.179687	4.634353	0.065495
27	7	0	-1.718390	3.341115	0.094235
28	7	0	-3.765545	2.185439	0.188641
29	1	0	-2.224780	4.216506	0.168535
30	1	0	-4.245894	2.966440	-0.238294
31	1	0	-4.204512	1.284406	0.025346
32	6	0	3.006594	-0.118868	-0.089556
33	6	0	3.466890	-1.424382	-0.253730
34	6	0	4.883863	-1.384263	-0.241892
35	1	0	2.873091	-2.315014	-0.394631
36	6	0	5.259689	-0.064276	-0.074116
37	1	0	5.551254	-2.228423	-0.347032
38	1	0	6.237163	0.391773	-0.012225

39	7	0	4.124011	0.684076	0.018293
40	1	0	4.042520	1.687761	0.113738

TS (1 imaginary frequency) $\chi = 161.1°$ $\theta = 172.1°$
Energy= -1172.9300033

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.666448	-1.096460	-0.735756
2	8	0	-1.998473	-0.754127	-0.414131
3	1	0	-0.576107	-1.271898	-1.816095
4	6	0	-0.388591	-2.380792	0.064290
5	6	0	-2.743703	-1.909781	0.033019
6	6	0	-1.748451	-3.079836	0.029775
7	1	0	-0.137777	-2.115316	1.095132
8	1	0	0.422876	-2.975997	-0.354782
9	6	0	-3.349823	-1.560251	1.390898
10	1	0	-3.539686	-2.119832	-0.691584
11	1	0	-1.893959	-3.737069	0.897487
12	1	0	-4.079357	-0.748065	1.255322
13	1	0	-3.883370	-2.428320	1.792721
14	8	0	-2.359438	-1.206591	2.342465
15	1	0	-1.953283	-0.388807	2.009377
16	8	0	-1.962862	-3.791599	-1.190467
17	1	0	-1.300203	-4.498341	-1.240777
18	7	0	0.215458	0.028808	-0.376046
19	6	0	-0.047220	1.399094	-0.177276
20	6	0	1.581861	-0.118807	-0.205532
21	7	0	1.053542	2.056037	0.157514
22	6	0	2.064841	1.136665	0.144387
23	7	0	2.288136	-1.271827	-0.364917
24	6	0	3.473184	1.314403	0.387184
25	6	0	3.575164	-1.124321	-0.161975
26	8	0	4.112871	2.305095	0.697151
27	7	0	4.154228	0.064173	0.196833
28	7	0	4.425832	-2.193344	-0.367599
29	1	0	5.162879	0.136688	0.271125
30	1	0	5.231433	-2.259257	0.242561
31	1	0	3.927771	-3.069278	-0.464924
32	6	0	-1.285552	2.155271	-0.317712
33	6	0	-2.545259	1.993865	-0.891334
34	6	0	-3.228661	3.229930	-0.781946
35	1	0	-2.919979	1.089248	-1.338780
36	6	0	-2.378801	4.121366	-0.151575
37	1	0	-4.233256	3.441575	-1.122298
38	1	0	-2.514855	5.157207	0.124747
39	7	0	-1.217709	3.464594	0.124919
40	1	0	-0.361567	3.844098	0.507006

TS (1 imaginary frequency) $\chi = 163.0°$ $\theta = 345.2°$
Energy= -1172.926514

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.629127	-1.059706	-0.748096
2	8	0	-1.989353	-0.783952	-0.442953
3	1	0	-0.529491	-1.190884	-1.832754
4	6	0	-0.311257	-2.362727	0.008028
5	6	0	-2.665393	-1.933061	0.127530
6	6	0	-1.659769	-3.082580	0.020835
7	1	0	-0.012344	-2.125396	1.031696
8	1	0	0.486299	-2.934738	-0.465933
9	6	0	-3.118550	-1.571843	1.541454
10	1	0	-3.537671	-2.157065	-0.496959
11	1	0	-1.746429	-3.776329	0.868093
12	1	0	-3.846379	-0.749193	1.480549
13	1	0	-3.626328	-2.432869	1.989769
14	8	0	-2.039278	-1.241619	2.399466
15	1	0	-1.685033	-0.390628	2.092871
16	8	0	-1.935218	-3.744907	-1.214039
17	1	0	-1.255461	-4.424777	-1.343883
18	7	0	0.212448	0.080642	-0.339105
19	6	0	-0.064134	1.461203	-0.133674
20	6	0	1.585386	-0.046362	-0.194802
21	7	0	1.035026	2.122907	0.181807
22	6	0	2.054182	1.214855	0.150423
23	7	0	2.306083	-1.187943	-0.376704
24	6	0	3.465521	1.412424	0.367065
25	6	0	3.594452	-1.022491	-0.196509
26	8	0	4.098832	2.409012	0.667823
27	7	0	4.161426	0.171835	0.158859
28	7	0	4.457397	-2.078122	-0.424078
29	1	0	5.170011	0.259691	0.215398
30	1	0	5.274243	-2.133603	0.172181
31	1	0	3.970415	-2.961260	-0.511811
32	6	0	-1.317293	2.198875	-0.239117
33	6	0	-1.482397	3.532703	0.132544
34	6	0	-2.790824	3.924427	-0.228897
35	1	0	-0.712664	4.135758	0.590577
36	6	0	-3.397890	2.829455	-0.818113
37	1	0	-3.240395	4.896844	-0.080405
38	1	0	-4.392482	2.700319	-1.221135
39	7	0	-2.499014	1.799652	-0.830834
40	1	0	-2.687157	0.842020	-1.092267

TS (1 imaginary frequency) $\chi = 228.8°$ $\theta = 266.0°$
Energy= -1172.9314645

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.409362	1.167656	-0.053569

2	8	0	1.421982	0.869768	-1.006489
3	1	0	-0.204170	2.012381	-0.387409
4	6	0	1.187269	1.557746	1.205892
5	6	0	2.519828	1.784139	-0.789046
6	6	0	2.289714	2.435369	0.596664
7	1	0	1.624042	0.666302	1.664844
8	1	0	0.573871	2.086413	1.942292
9	6	0	3.843906	1.032061	-0.904471
10	1	0	2.478511	2.573211	-1.552333
11	1	0	3.205759	2.423860	1.197428
12	1	0	3.830097	0.426711	-1.823223
13	1	0	4.646549	1.772172	-1.006815
14	8	0	4.161715	0.255313	0.235213
15	1	0	3.638088	-0.564492	0.217388
16	8	0	1.846322	3.773623	0.358457
17	1	0	1.742100	4.205379	1.220841
18	7	0	-0.507779	0.045312	0.051639
19	6	0	-0.259287	-1.333208	0.159560
20	6	0	-1.874656	0.179123	-0.001453
21	7	0	-1.371427	-2.035316	0.172833
22	6	0	-2.387310	-1.113523	0.082282
23	7	0	-2.548061	1.356310	-0.096758
24	6	0	-3.814885	-1.305820	0.040489
25	6	0	-3.849025	1.196088	-0.144803
26	8	0	-4.492218	-2.317210	0.077117
27	7	0	-4.465465	-0.026750	-0.076122
28	7	0	-4.662048	2.294425	-0.324677
29	1	0	-5.471197	-0.095194	-0.185526
30	1	0	-5.570298	2.277271	0.121808
31	1	0	-4.167123	3.169517	-0.205790
32	6	0	1.084604	-1.924419	0.193198
33	6	0	1.946250	-2.199125	1.241041
34	6	0	3.104021	-2.824540	0.695683
35	1	0	1.749737	-1.992161	2.284078
36	6	0	2.914271	-2.918954	-0.670654
37	1	0	3.968404	-3.176784	1.241724
38	1	0	3.540972	-3.334094	-1.446606
39	7	0	1.689039	-2.379369	-0.958719
40	1	0	1.288055	-2.280290	-1.879339

TS (1 imaginary frequency) $\chi = 332.7°$ $\theta = 54.2°$
Energy= -1172.9198292

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.866072	0.715222	-0.677195
2	8	0	-0.320500	1.980770	-0.344175
3	1	0	-1.069823	0.676509	-1.757808
4	6	0	-2.173860	0.659097	0.130319
5	6	0	-1.389671	2.926441	-0.140558
6	6	0	-2.683315	2.099081	-0.007223
7	1	0	-1.938409	0.443742	1.176578
8	1	0	-2.898090	-0.072321	-0.230062
9	6	0	-1.018017	3.746257	1.090737
10	1	0	-1.480572	3.576678	-1.020696

11	1	0	-3.268293	2.403608	0.869508
12	1	0	-0.098270	4.313370	0.880411
13	1	0	-1.814009	4.464725	1.312696
14	8	0	-0.868567	2.925145	2.236810
15	1	0	-0.166909	2.291620	2.010270
16	8	0	-3.428416	2.300333	-1.210301
17	1	0	-4.269188	1.825220	-1.117917
18	7	0	0.128056	-0.315107	-0.341880
19	6	0	-0.108264	-1.638185	0.090507
20	6	0	1.503048	-0.152708	-0.305510
21	7	0	1.000106	-2.258368	0.427772
22	6	0	2.004690	-1.352328	0.202098
23	7	0	2.210784	0.928679	-0.727812
24	6	0	3.426118	-1.507743	0.391916
25	6	0	3.503124	0.799467	-0.563159
26	8	0	4.074025	-2.438155	0.839243
27	7	0	4.100632	-0.316797	-0.035371
28	7	0	4.335836	1.853839	-0.884169
29	1	0	5.099370	-0.327187	0.139491
30	1	0	5.239709	1.618792	-1.276063
31	1	0	3.850229	2.575875	-1.402540
32	6	0	-1.419318	-2.280452	0.085156
33	6	0	-2.100989	-2.940845	1.091040
34	6	0	-3.322261	-3.420460	0.545775
35	1	0	-1.750275	-3.046338	2.108014
36	6	0	-3.355603	-3.051714	-0.783305
37	1	0	-4.091414	-3.972685	1.068334
38	1	0	-4.090124	-3.235635	-1.554230
39	7	0	-2.204416	-2.351824	-1.053947
40	1	0	-1.900923	-2.070446	-1.974343

TS (1 imaginary frequency) $\chi = 326.2°$ $\theta = 203.9°$
Energy= -1172.9251975

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.839190	-0.870799	-0.745239
2	8	0	0.276511	-2.034352	-0.147525
3	1	0	0.906028	-1.010857	-1.832756
4	6	0	2.233933	-0.795145	-0.106737
5	6	0	1.307561	-3.022041	0.033741
6	6	0	2.649646	-2.272429	-0.085701
7	1	0	2.141455	-0.417892	0.916117
8	1	0	2.950539	-0.175510	-0.642906
9	6	0	1.054615	-3.673494	1.389077
10	1	0	1.254079	-3.770620	-0.768189
11	1	0	3.308768	-2.488697	0.764167
12	1	0	0.084598	-4.193344	1.363964
13	1	0	1.831574	-4.417455	1.593611
14	8	0	1.104573	-2.722204	2.439795
15	1	0	0.425008	-2.062267	2.221641
16	8	0	3.248632	-2.689239	-1.313673
17	1	0	4.118426	-2.264479	-1.377214
18	7	0	-0.074564	0.245485	-0.465210
19	6	0	0.193364	1.553729	-0.026300

20	6	0	-1.454259	0.105677	-0.384071
21	7	0	-0.895896	2.178546	0.378558
22	6	0	-1.922527	1.293016	0.173351
23	7	0	-2.185149	-0.952547	-0.819936
24	6	0	-3.333302	1.456043	0.420545
25	6	0	-3.470293	-0.815573	-0.610811
26	8	0	-3.952007	2.377190	0.927059
27	7	0	-4.035457	0.288357	-0.023299
28	7	0	-4.327672	-1.846737	-0.943474
29	1	0	-5.027369	0.302319	0.186512
30	1	0	-5.234379	-1.583673	-1.310685
31	1	0	-3.865355	-2.558709	-1.496121
32	6	0	1.460227	2.264829	-0.095507
33	6	0	2.520291	2.293968	-0.995041
34	6	0	3.376432	3.360349	-0.616066
35	1	0	2.636396	1.655117	-1.859537
36	6	0	2.814690	3.966301	0.491865
37	1	0	4.296412	3.654386	-1.102560
38	1	0	3.145616	4.807431	1.083544
39	7	0	1.664989	3.293660	0.798822
40	1	0	0.965374	3.559161	1.478292

Minimum (0 imaginary frequencies) $\chi = 47.3°$ $\theta = 165.6°$
Energy= -1172.9477857

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.189628	-1.376830	0.035977
2	8	0	0.726681	-1.579060	1.101306
3	1	0	-1.145341	-1.846720	0.278666
4	6	0	0.461450	-2.031141	-1.191325
5	6	0	1.571663	-2.720107	0.831826
6	6	0	1.175678	-3.235790	-0.567235
7	1	0	1.190300	-1.348368	-1.635140
8	1	0	-0.269889	-2.314383	-1.955250
9	6	0	3.031278	-2.287127	0.966840
10	1	0	1.348774	-3.500959	1.569877
11	1	0	2.056720	-3.539092	-1.146094
12	1	0	3.161564	-1.837314	1.964464
13	1	0	3.674649	-3.173989	0.916362
14	8	0	3.442604	-1.408885	-0.064414
15	1	0	2.798887	-0.659958	-0.076264
16	8	0	0.288890	-4.337696	-0.363041
17	1	0	0.047777	-4.688034	-1.234969
18	7	0	-0.454510	0.052870	-0.092432
19	6	0	-1.688195	0.710999	-0.015870
20	6	0	0.497716	1.051377	-0.111997
21	7	0	-1.553790	2.024565	0.016716
22	6	0	-0.199514	2.251666	-0.034460
23	7	0	1.842466	0.875073	-0.183880
24	6	0	0.532660	3.492520	-0.030541
25	6	0	2.536148	1.992435	-0.179479
26	8	0	0.149889	4.647681	0.023156
27	7	0	1.947546	3.224345	-0.108258
28	7	0	3.902285	1.927941	-0.300860

29	1	0	2.513688	4.063763	-0.163731
30	1	0	4.449777	2.659640	0.132353
31	1	0	4.277057	0.992546	-0.173876
32	6	0	-2.995981	0.085178	0.013087
33	6	0	-3.524037	-1.161818	-0.313733
34	6	0	-4.926883	-1.097150	-0.115715
35	1	0	-2.978758	-2.014798	-0.690808
36	6	0	-5.224866	0.181264	0.317883
37	1	0	-5.637353	-1.896407	-0.275325
38	1	0	-6.168285	0.638508	0.578758
39	7	0	-4.055347	0.880888	0.393863
40	1	0	-3.929555	1.856623	0.627326

Minimum (0 imaginary frequencies) $\chi = 47.8°$ $\theta = 322.9°$
Energy= -1172.9385676

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.536004	1.211635	0.030394
2	8	0	-0.286226	1.616875	1.114099
3	1	0	1.583464	1.432019	0.257357
4	6	0	0.045629	2.027721	-1.176862
5	6	0	-0.830559	2.933682	0.875609
6	6	0	-0.347433	3.359931	-0.526294
7	1	0	-0.829716	1.549145	-1.622716
8	1	0	0.812805	2.147721	-1.950208
9	6	0	-2.349863	2.868076	1.031225
10	1	0	-0.411058	3.624829	1.617464
11	1	0	-1.140963	3.871822	-1.083898
12	1	0	-2.572916	2.438367	2.021079
13	1	0	-2.756651	3.886431	1.012012
14	8	0	-2.976566	2.144346	-0.011653
15	1	0	-2.536258	1.260951	-0.053191
16	8	0	0.781023	4.215679	-0.334276
17	1	0	1.046543	4.553745	-1.203826
18	7	0	0.442010	-0.237000	-0.121577
19	6	0	1.473641	-1.191333	0.002932
20	6	0	-0.729758	-0.963331	-0.143704
21	7	0	1.009753	-2.422365	0.044052
22	6	0	-0.357326	-2.297989	-0.032870
23	7	0	-1.986300	-0.453478	-0.236073
24	6	0	-1.379197	-3.315081	-0.027236
25	6	0	-2.939449	-1.360134	-0.219166
26	8	0	-1.304588	-4.527662	0.046153
27	7	0	-2.680638	-2.698842	-0.129599
28	7	0	-4.245585	-0.954884	-0.343450
29	1	0	-3.439900	-3.369450	-0.175195
30	1	0	-4.957995	-1.525398	0.092367
31	1	0	-4.374386	0.044311	-0.214495
32	6	0	2.889492	-0.870842	0.074622
33	6	0	3.882538	-1.519905	0.790159
34	6	0	5.116309	-0.885357	0.495434
35	1	0	3.710752	-2.351309	1.458485
36	6	0	4.856212	0.131727	-0.399612
37	1	0	6.086423	-1.138065	0.900895

38	1	0	5.512412	0.846527	-0.874795
39	7	0	3.503772	0.148196	-0.638990
40	1	0	3.059783	0.690263	-1.364237

Minimum (0 imaginary frequencies) $\chi = 62.4°$ $\theta = 196.5°$
Energy= -1172.9474823

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.131213	-1.383399	0.074520
2	8	0	-0.667144	-1.737981	-1.046219
3	1	0	1.083708	-1.913913	0.051043
4	6	0	-0.673290	-1.821834	1.308500
5	6	0	-1.589053	-2.794712	-0.694559
6	6	0	-1.347089	-3.100825	0.797216
7	1	0	-1.428094	-1.075617	1.563411
8	1	0	-0.032803	-1.994578	2.179461
9	6	0	-3.009266	-2.338777	-1.031359
10	1	0	-1.338483	-3.685947	-1.283559
11	1	0	-2.287306	-3.311472	1.321952
12	1	0	-3.026689	-2.032089	-2.089697
13	1	0	-3.693620	-3.188711	-0.920608
14	8	0	-3.476133	-1.311130	-0.177399
15	1	0	-2.808996	-0.585406	-0.199045
16	8	0	-0.466717	-4.225720	0.845323
17	1	0	-0.292678	-4.425024	1.778734
18	7	0	0.445439	0.037420	0.001237
19	6	0	1.704283	0.649201	-0.053230
20	6	0	-0.468234	1.069729	0.037129
21	7	0	1.619120	1.967046	-0.015230
22	6	0	0.274320	2.244328	0.038742
23	7	0	-1.820480	0.939327	0.041799
24	6	0	-0.412072	3.510605	0.074356
25	6	0	-2.472868	2.081081	0.069240
26	8	0	0.013052	4.651665	0.102427
27	7	0	-1.837896	3.291732	0.084980
28	7	0	-3.844330	2.064594	0.134527
29	1	0	-2.375783	4.147595	0.165324
30	1	0	-4.346146	2.831788	-0.292827
31	1	0	-4.249126	1.150325	-0.041675
32	6	0	2.992889	-0.015973	-0.120739
33	6	0	3.465706	-1.272757	-0.491590
34	6	0	4.880335	-1.241460	-0.398049
35	1	0	2.876151	-2.107750	-0.841152
36	6	0	5.240439	0.026786	0.018422
37	1	0	5.557577	-2.055585	-0.616365
38	1	0	6.211202	0.460553	0.210005
39	7	0	4.096806	0.752416	0.185123
40	1	0	4.012135	1.731443	0.423292

Minimum (0 imaginary frequencies) $\chi = 74.3°$ $\theta = 37.1°$
Energy= -1172.9412346

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.705614	1.079388	0.314476
2	8	0	-0.435412	1.762259	-0.910333
3	1	0	-1.778008	1.100977	0.521811
4	6	0	0.038278	1.859758	1.408266
5	6	0	0.040350	3.104964	-0.649720
6	6	0	-0.047655	3.295641	0.874825
7	1	0	1.080148	1.546771	1.481397
8	1	0	-0.439751	1.741566	2.386060
9	6	0	1.446794	3.268657	-1.230745
10	1	0	-0.641839	3.809463	-1.140641
11	1	0	0.768952	3.925241	1.249600
12	1	0	1.419108	2.943783	-2.283328
13	1	0	1.710882	4.333135	-1.219567
14	8	0	2.448672	2.591300	-0.495687
15	1	0	2.205189	1.639278	-0.439587
16	8	0	-1.320487	3.889490	1.137856
17	1	0	-1.404899	3.995545	2.098508
18	7	0	-0.351745	-0.321604	0.158382
19	6	0	-1.233380	-1.418111	0.079976
20	6	0	0.914255	-0.861281	0.122608
21	7	0	-0.594727	-2.568940	0.066332
22	6	0	0.741112	-2.240624	0.102009
23	7	0	2.078448	-0.160179	0.061425
24	6	0	1.904736	-3.091176	0.068802
25	6	0	3.155477	-0.914604	0.019192
26	8	0	2.015327	-4.302951	0.071589
27	7	0	3.099734	-2.279656	0.035358
28	7	0	4.391713	-0.315686	0.004409
29	1	0	3.954920	-2.823939	0.063059
30	1	0	5.140084	-0.796468	-0.477446
31	1	0	4.356604	0.681986	-0.176061
32	6	0	-2.674235	-1.276796	-0.040327
33	6	0	-3.686274	-2.088903	0.445550
34	6	0	-4.919425	-1.568876	-0.023533
35	1	0	-3.531603	-2.954843	1.073324
36	6	0	-4.635498	-0.457077	-0.792156
37	1	0	-5.906367	-1.960265	0.181857
38	1	0	-5.284253	0.219183	-1.329877
39	7	0	-3.276402	-0.277524	-0.791277
40	1	0	-2.776618	0.397172	-1.354269

Minimum (0 imaginary frequencies) $\chi = 217.4°$ $\theta = 157.2°$
Energy= -1172.9367174

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.452103	-1.221800	-0.189316
2	8	0	-1.576843	-1.112201	-1.048943

3	1	0	0.179399	-2.063558	-0.491843
4	6	0	-1.059213	-1.493885	1.190943
5	6	0	-2.593320	-2.030322	-0.578292
6	6	0	-2.152213	-2.503727	0.826307
7	1	0	-1.508304	-0.577613	1.586512
8	1	0	-0.330045	-1.882928	1.908564
9	6	0	-3.955550	-1.340311	-0.582635
10	1	0	-2.618310	-2.899537	-1.248681
11	1	0	-2.989533	-2.481958	1.533067
12	1	0	-4.123950	-0.881421	-1.568807
13	1	0	-4.726508	-2.106927	-0.442187
14	8	0	-4.123097	-0.409227	0.471346
15	1	0	-3.599562	0.385660	0.259826
16	8	0	-1.638052	-3.828896	0.677205
17	1	0	-1.388425	-4.147546	1.558784
18	7	0	0.416839	-0.054003	-0.278399
19	6	0	0.176799	1.311958	-0.061422
20	6	0	1.790778	-0.200562	-0.210073
21	7	0	1.293463	1.988809	0.138595
22	6	0	2.304560	1.063627	0.056808
23	7	0	2.460942	-1.374088	-0.344267
24	6	0	3.729445	1.232127	0.182501
25	6	0	3.762123	-1.236348	-0.249278
26	8	0	4.403394	2.222990	0.405573
27	7	0	4.379490	-0.036669	-0.006654
28	7	0	4.577961	-2.328874	-0.451984
29	1	0	5.391647	0.023696	-0.008504
30	1	0	5.433746	-2.375480	0.086653
31	1	0	4.063605	-3.200572	-0.474319
32	6	0	-1.103322	1.998038	-0.089293
33	6	0	-2.294693	1.841609	-0.793862
34	6	0	-3.111601	2.968679	-0.504838
35	1	0	-2.486875	1.050935	-1.502469
36	6	0	-2.402277	3.783888	0.356919
37	1	0	-4.103971	3.162118	-0.888646
38	1	0	-2.663859	4.724631	0.819155
39	7	0	-1.196628	3.187348	0.599307
40	1	0	-0.413235	3.573666	1.108445

Minimum (0 imaginary frequencies) $\chi = 224.4°$ $\theta = 329.6°$
Energy= -1172.9337137

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-0.440984	-1.129478	-0.083569
2	8	0	-1.523977	-1.032257	-1.020230
3	1	0	0.180925	-1.993340	-0.336052
4	6	0	-1.141610	-1.367044	1.255997
5	6	0	-2.553789	-1.965562	-0.599935
6	6	0	-2.202300	-2.395629	0.844375
7	1	0	-1.613486	-0.442907	1.604872
8	1	0	-0.460990	-1.736925	2.028879
9	6	0	-3.929982	-1.314605	-0.722017
10	1	0	-2.505348	-2.848064	-1.250209
11	1	0	-3.085562	-2.363361	1.491478

12	1	0	-4.021465	-0.847453	-1.715859
13	1	0	-4.686757	-2.104596	-0.664896
14	8	0	-4.234514	-0.407242	0.323138
15	1	0	-3.675606	0.382336	0.224936
16	8	0	-1.669367	-3.718222	0.762994
17	1	0	-1.490628	-4.020052	1.667412
18	7	0	0.451833	0.011172	-0.162699
19	6	0	0.255944	1.392739	0.067102
20	6	0	1.823992	-0.171196	-0.154060
21	7	0	1.397053	2.034306	0.207805
22	6	0	2.377644	1.079969	0.088194
23	7	0	2.454657	-1.362724	-0.316136
24	6	0	3.811623	1.211596	0.147554
25	6	0	3.762296	-1.259743	-0.276046
26	8	0	4.522981	2.182872	0.332890
27	7	0	4.419356	-0.076446	-0.064349
28	7	0	4.539626	-2.374646	-0.508137
29	1	0	5.431754	-0.041997	-0.109121
30	1	0	5.415761	-2.440598	-0.005361
31	1	0	4.002259	-3.232605	-0.501019
32	6	0	-1.022564	2.081647	0.065779
33	6	0	-1.356585	3.283847	0.673704
34	6	0	-2.667044	3.626167	0.257514
35	1	0	-0.707195	3.839677	1.334547
36	6	0	-3.101997	2.636958	-0.604085
37	1	0	-3.233449	4.497769	0.555812
38	1	0	-4.029485	2.524950	-1.147650
39	7	0	-2.104113	1.695412	-0.703293
40	1	0	-2.078462	0.878444	-1.303488