Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Attraction or Repulsion? Theoretical Assessment of Bulky Alkyl Groups by Employing Dispersion-Corrected DFT

Mo Xie* and Wei Lu*

Department of Chemistry, South University of Science and Technology of China, Shenzhen, Guangdong 518055 (China)

1. Geometries of folded products

In the experimental research, the authors synthesized lots of compounds and arranged them into different series. Among them, the crystal structure data of the folded configurations of several compounds in 3 series were provided. In our computational studies, in order to better control the variables, the 1 series with only one arm were chosen for further study. Herein, we choose the crystal structure data of compound 3i to benchmark against the calculated 1i structure (named B2 in the text). The related chemical strucutres, parameter definitions, and the main bond length and bond angle which characterize the relative positions of the arm and body were shown in Figure S1, Figure S2 and Table S1, respectively. It is worth noting that in the same unit cell in the 3i crystal structure, there were two molecules with slightly different structures and we both listed the parameters of them in Table S2.

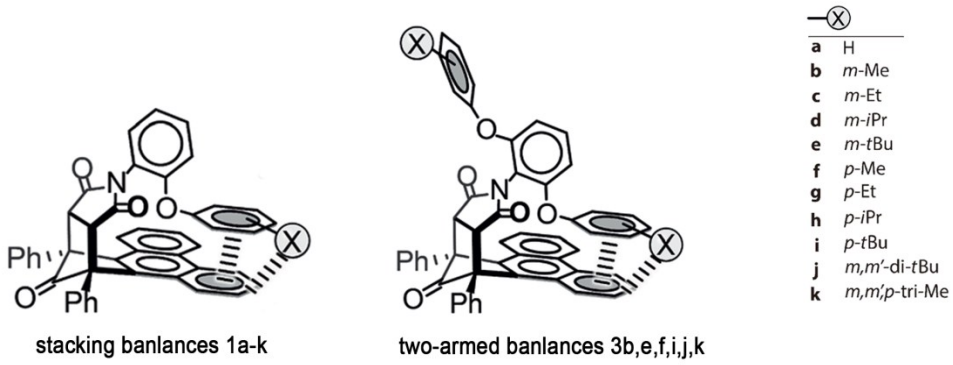


Figure S1. Chemical structures of folded configurations in the experimental study.

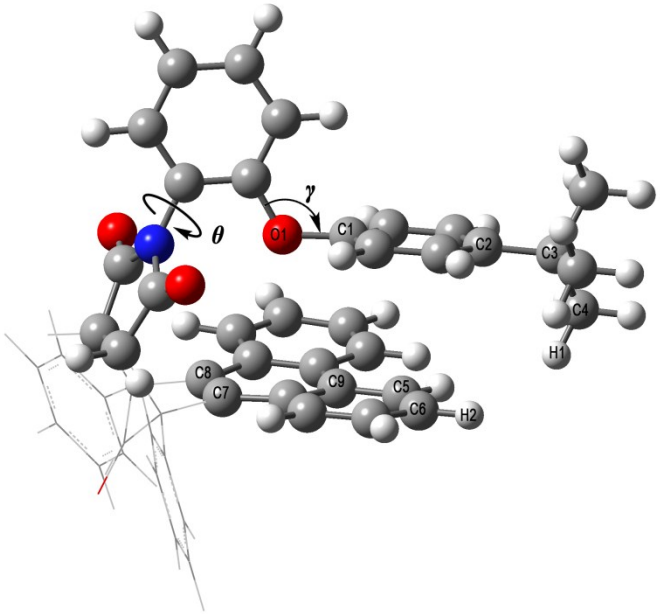


Figure S2. Geometries of B3LYP+D3 calculated B2 moelcule and the structural paremeter difination .

Table S1. Structural parameters of B2 (calculated by B3LYP and B3LYP+D3) and 3i (crystal structure). All distances are in Å and all angles are in deg.

parameter	B3LYP	B3LYP+D3	Exp1	Exp2
O1-C7	4.036	3.593	3.702	3.782
O1-C8	4.355	3.674	3.807	3.831
C1-C9	4.253	3.266	3.456	3.324
C2-C5	5.164	3.584	3.815	3.833
C2-C6	4.658	3.680	4.038	3.741
C3-C5	6.116	4.425	4.584	4.938
C3-C6	5.442	4.335	4.584	4.625
C4-C5	5.610	4.082	4.635	5.020
C4-C6	4.846	4.143	3.721	4.310
H1-H2	3.454	2.548	2.671	2.795
θ	118.64	118.21	115.02	115.87
γ	64.00	73.70	80.79	75.03

2. NCI analysis of O-B2

Figure S3. Scatter diagram of reduced density gradient (RGD) of folded conformation **O-B2.**

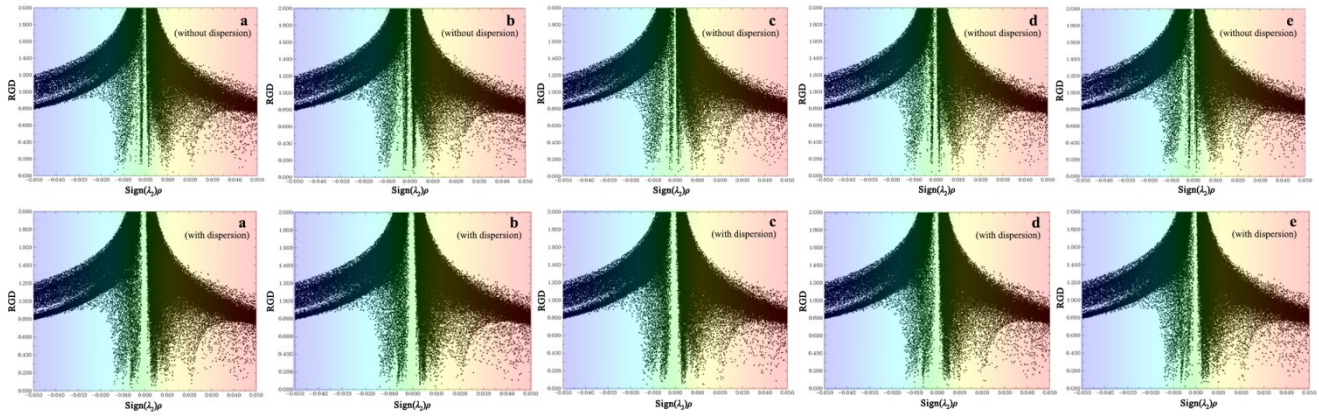
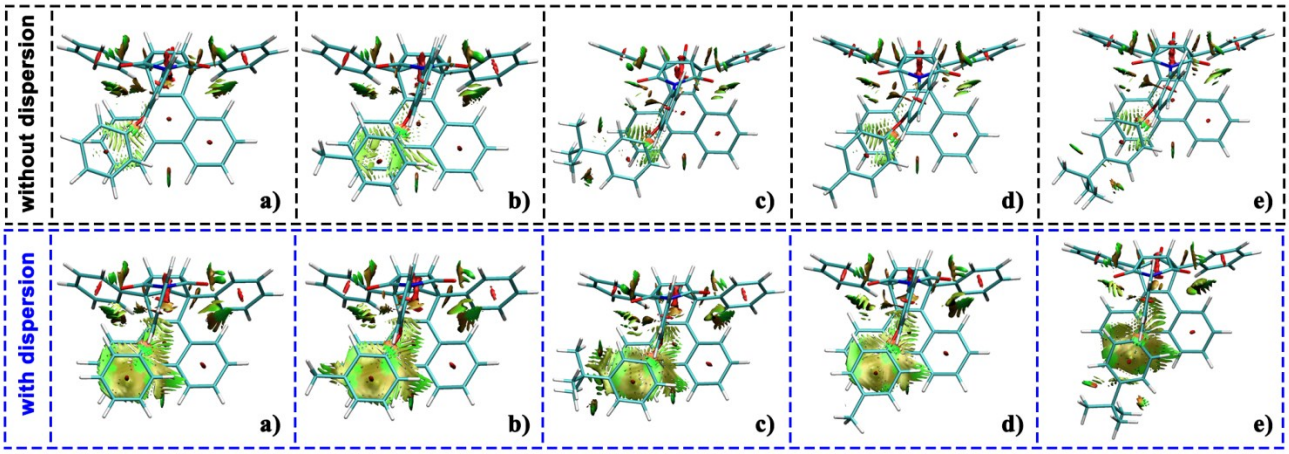


Figure S4. Colored contour surface of reduced density gradient (RDG) of folded conformation **O-B2.**



3. DFT optimized coordinates

O/RC

B3LYP/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	0.4299	0.62551	-1.69974
C	-0.25052	-0.7159	-1.32126
C	-1.29378	-0.35182	-0.27233
C	-0.27107	1.68257	-0.85541
N	-1.23083	1.03218	-0.06597
O	-2.05858	-1.0973	0.28751
O	-0.06999	2.87025	-0.85419
C	1.95975	0.41035	-1.40542
C	0.91656	-1.65174	-0.83437
C	2.00922	-1.10024	-1.80728
O	2.68098	-1.66269	-2.61286
C	3.8399	3.06539	1.78491
C	3.23637	2.30097	0.81036
C	2.71783	1.01656	1.10085
C	2.78414	0.52807	2.44176
C	3.42534	1.33533	3.40906
C	3.94843	2.57138	3.09293
C	2.10703	0.17602	0.10571
C	2.16011	-0.74328	2.78945
C	1.47002	-1.49967	1.79331
C	1.50718	-1.02174	0.43665
C	0.7778	-2.67229	2.17824
H	0.21768	-3.22482	1.43974
C	0.79777	-3.11919	3.48126
C	1.51463	-2.40695	4.45335
C	2.17181	-1.24418	4.11117
H	4.22657	4.04838	1.53723
H	3.1502	2.69425	-0.19106
H	3.50546	0.99236	4.43232
H	4.4314	3.16522	3.86238
H	0.257	-4.02029	3.75107
H	1.54286	-2.76034	5.47915
H	2.69928	-0.70697	4.88856
C	0.69511	-3.14192	-0.93236
C	1.80158	-4.00155	-0.88918
C	-0.57795	-3.70154	-1.08647
C	1.63915	-5.37827	-0.9978
H	2.79817	-3.59271	-0.77147
C	-0.73955	-5.08218	-1.19633
H	-1.4554	-3.06703	-1.07028
C	0.36667	-5.92523	-1.1548
H	2.50996	-6.02513	-0.96326
H	-1.73695	-5.49544	-1.3081
H	0.24006	-6.99976	-1.2407
C	2.94066	1.28002	-2.15402
C	4.28459	0.88754	-2.22373
C	2.55532	2.4564	-2.80602
C	5.21381	1.64803	-2.92495
H	4.60757	-0.02071	-1.72856
C	3.48784	3.21773	-3.50983
H	1.53575	2.81284	-2.7266
C	4.81857	2.81635	-3.57445
H	6.24885	1.32428	-2.96738
H	3.16843	4.13071	-4.00222
H	5.54347	3.40896	-4.12336
C	-2.10707	1.71857	0.82963
C	-1.61476	2.28966	1.99891
C	-3.46863	1.81065	0.51821
C	-2.47823	2.93932	2.87469
H	-0.5559	2.21169	2.21636
C	-4.33611	2.45026	1.40267
C	-3.83702	3.01047	2.57476
H	-2.09248	3.3823	3.78587
H	-5.39081	2.51501	1.16315
H	-4.51817	3.51244	3.25407
O	-3.86816	1.30851	-0.6953
C	-5.12843	0.73281	-0.81327
C	-5.98801	1.23902	-1.78215
C	-5.48388	-0.36756	-0.03566
C	-7.22987	0.63496	-1.97332
H	-5.6737	2.0906	-2.37521
C	-6.73032	-0.95601	-0.23094
H	-4.77809	-0.76079	0.68676
C	-7.60618	-0.45817	-1.196
H	-7.01268	-1.81608	0.3676
H	-8.57405	-0.92506	-1.34519
H	-0.75728	-1.17725	-2.17177
H	0.29434	0.87617	-2.75409
H	-7.90387	1.02477	-2.72918

O/RC

B3LYP+D3/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	-0.2382	0.70219	-1.46213
C	-0.17542	-0.84388	-1.38503
C	-1.14243	-1.22814	-0.27621
C	-1.2492	1.11599	-0.40919
N	-1.67811	-0.04392	0.24882
O	-1.4166	-2.3358	0.10679
O	-1.62613	2.23154	-0.1539
C	1.22176	1.18507	-1.13763
C	1.32385	-1.18058	-1.0483
C	1.97331	0.00516	-1.82493
O	2.79925	0.01067	-2.68195
C	1.33112	3.69452	2.64641
C	1.32228	2.95834	1.48263
C	1.53065	1.55883	1.49845
C	1.72557	0.89721	2.74951
C	1.73844	1.68996	3.92044
C	1.55035	3.0554	3.87575
C	1.49962	0.75367	0.30937
C	1.84553	-0.55499	2.79977
C	1.72383	-1.32673	1.60358
C	1.57257	-0.62149	0.36113
C	1.73448	-2.73855	1.691
H	1.60432	-3.32724	0.79734
C	1.9015	-3.37742	2.89941
C	2.06651	-2.6249	4.07133
C	2.03276	-1.24775	4.01738
H	1.16157	4.76537	2.60851
H	1.13687	3.45669	0.54453
H	1.88416	1.22543	4.88686
H	1.56126	3.6311	4.79573
H	1.9033	-4.46153	2.9402
H	2.20997	-3.12368	5.02446
H	2.15096	-0.69699	4.9413
C	1.83286	-2.54197	-1.43493
C	3.21597	-2.75431	-1.49484
C	0.97563	-3.60766	-1.72546
C	3.72877	-4.0012	-1.83458
H	3.89347	-1.93874	-1.27154
C	1.49089	-4.85771	-2.06512
H	-0.09554	-3.48455	-1.62717
C	2.86715	-5.05907	-2.12228
H	4.80339	-4.14719	-1.87493
H	0.81061	-5.67684	-2.27527
H	3.26701	-6.03316	-2.38527
C	1.6315	2.55124	-1.61396
C	2.99331	2.87776	-1.62356
C	0.70712	3.50872	-2.04173
C	3.42054	4.13077	-2.04787
H	3.72092	2.14506	-1.29389
C	1.13648	4.76511	-2.46712
H	-0.35416	3.30171	-1.98762
C	2.49224	5.0805	-2.47307
H	4.47999	4.36592	-2.04788
H	0.40435	5.50048	-2.78523
H	2.82456	6.05956	-2.80306
C	-2.60008	-0.01292	1.33524
C	-2.20403	0.56401	2.53984
C	-3.88751	-0.5501	1.2014
C	-3.07621	0.59507	3.62128
H	-1.20326	0.97433	2.61528
C	-4.75402	-0.52707	2.2921
C	-4.34883	0.03884	3.49613
H	-2.75919	1.04133	4.55702
H	-5.73956	-0.96095	2.16986
H	-5.0343	0.05088	4.33696
O	-4.33173	-1.17712	0.06166
C	-4.11022	-0.61952	-1.18472
C	-4.22397	0.7483	-1.4221
C	-3.7855	-1.501	-2.21393
C	-3.97835	1.23659	-2.7034
H	-4.45392	1.423	-0.60635
C	-3.55411	-1.00153	-3.49276
H	-3.69791	-2.55635	-1.98499
C	-3.64103	0.36908	-3.7416
H	-3.29625	-1.68557	-4.29479
H	-3.45272	0.75638	-4.73714
H	-0.47965	-1.32275	-2.31628
H	-0.55923	1.06464	-2.43921
H	-4.04734	2.30403	-2.88416

O/TS

B3LYP/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	1.25605	0.56995	-1.80234
C	0.16257	-0.50347	-1.71655
C	-1.02482	0.19195	-1.0773
C	0.59862	1.84882	-1.3162
N	-0.74368	1.58942	-0.9006
O	-1.9926	-0.37951	-0.65848
O	1.15479	2.91963	-1.32367
C	2.45856	0.00859	-0.95685
C	0.77993	-1.67578	-0.86559
C	2.25469	-1.49309	-1.348
O	3.00432	-2.26387	-1.85825
C	3.66262	2.35322	2.75359
C	3.27766	1.68989	1.60888
C	2.38115	0.59643	1.661
C	1.83478	0.20438	2.92074
C	2.26634	0.89962	4.0732
C	3.16319	1.94444	3.99853
C	1.97695	-0.13868	0.49251
C	0.82765	-0.84853	2.98569
C	0.37179	-1.48088	1.78855
C	1.01273	-1.12399	0.55088
C	-0.68404	-2.41913	1.86561
H	-1.06488	-2.86449	0.95978
C	-1.24422	-2.76669	3.07541
C	-0.76728	-2.18542	4.259
C	0.23897	-1.24398	4.20827
H	4.34912	3.19085	2.68755
H	3.66299	2.01589	0.65443
H	1.88137	0.62468	5.04649
H	3.46918	2.45772	4.90454
H	-2.05499	-3.48697	3.10721
H	-1.19756	-2.46333	5.21591
H	0.57025	-0.79829	5.13713
C	0.22838	-3.06424	-1.08121
C	0.98003	-4.16876	-0.65605
C	-0.99743	-3.29794	-1.71335
C	0.51953	-5.46516	-0.8575
H	1.93326	-4.01501	-0.16435
C	-1.45785	-4.5982	-1.91689
H	-1.62583	-2.46598	-2.00494
C	-0.70146	-5.68626	-1.4924
H	1.11866	-6.30506	-0.52054
H	-2.41592	-4.75521	-2.40207
H	-1.06043	-6.69821	-1.65076
C	3.84179	0.5305	-1.26262
C	4.95178	-0.18333	-0.78899
C	4.06705	1.67747	-2.03083
C	6.24566	0.23783	-1.07329
H	4.80357	-1.07702	-0.19379
C	5.36568	2.09841	-2.31702
H	3.23193	2.27685	-2.37058
C	6.45892	1.38102	-1.84213
H	7.08955	-0.3314	-0.69685
H	5.51703	2.99537	-2.90918
H	7.46895	1.70926	-2.06587
C	-1.72716	2.66445	-0.84901
C	-1.26313	3.95648	-0.52276
C	-3.12853	2.46867	-0.76502
C	-2.11884	5.00007	-0.20031
H	-0.20426	4.13919	-0.50415
C	-3.9776	3.52157	-0.41405
C	-3.48859	4.78248	-0.11877
H	-1.6971	5.97394	0.02328
H	-5.04371	3.32746	-0.41552
H	-4.17015	5.58288	0.14894
O	-3.70294	1.33679	-1.29657
C	-4.75361	0.70842	-0.65819
C	-5.73391	0.14922	-1.47519
C	-4.82142	0.57363	0.72734
C	-6.79338	-0.54646	-0.89913
H	-5.64973	0.26521	-2.54999
C	-5.89076	-0.11703	1.29144
H	-4.0389	0.98905	1.35054
C	-6.87993	-0.67866	0.48563
H	-5.94138	-0.22568	2.37017
H	-7.70827	-1.21786	0.93286
H	-0.13755	-0.87374	-2.70011
H	1.5936	0.75003	-2.82568
H	-7.55614	-0.9814	-1.53712

O/TS

B3LYP+D3/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	0.43719	0.85095	-1.48829
C	-0.57543	-0.24159	-1.11001
C	-1.3021	0.31604	0.09057
C	0.10129	2.0335	-0.59657
N	-1.05652	1.73541	0.18282
O	-1.87241	-0.33448	0.91716
O	0.72496	3.06564	-0.58569
C	1.83999	0.17961	-1.30713
C	0.26538	-1.52281	-0.80165
C	1.42673	-1.24837	-1.80678
O	1.87992	-1.92152	-2.67683
C	4.50028	1.97716	1.9049
C	3.667	1.48127	0.92656
C	2.83878	0.36097	1.1711
C	2.83337	-0.23584	2.46847
C	3.71366	0.29286	3.43971
C	4.53404	1.36767	3.16792
C	1.97616	-0.2021	0.17161
C	1.90401	-1.31841	2.77168
C	0.9789	-1.77039	1.78108
C	1.08019	-1.2083	0.46398
C	0.00469	-2.73289	2.13371
H	-0.73174	-3.03273	1.40573
C	-0.03029	-3.28121	3.39659
C	0.90943	-2.8818	4.35829
C	1.84554	-1.91724	4.05064
H	5.12471	2.8396	1.69645
H	3.63959	1.96205	-0.03927
H	3.74577	-0.13639	4.43262
H	5.194	1.74995	3.94009
H	-0.78802	-4.01706	3.64477
H	0.89226	-3.31808	5.35196
H	2.54137	-1.61498	4.82244
C	-0.424	-2.84878	-0.96598
C	0.34887	-4.01237	-1.06453
C	-1.81699	-2.96067	-1.01463
C	-0.2564	-5.25655	-1.20386
H	1.42949	-3.94229	-1.02852
C	-2.42228	-4.20758	-1.15625
H	-2.44542	-2.08765	-0.89471
C	-1.64621	-5.3595	-1.25121
H	0.35864	-6.14769	-1.27701
H	-3.5054	-4.27257	-1.18451
H	-2.11861	-6.33068	-1.35926
C	3.0128	0.76658	-2.04371
C	4.18733	0.00837	-2.1358
C	2.9796	2.02814	-2.64356
C	5.30037	0.50029	-2.80672
H	4.22842	-0.97106	-1.67329
C	4.09649	2.5212	-3.31752
H	2.10426	2.65587	-2.53993
C	5.25887	1.76069	-3.40245
H	6.20171	-0.10119	-2.86579
H	4.05601	3.5075	-3.76872
H	6.12809	2.14653	-3.92541
C	-2.02553	2.75071	0.53261
C	-1.63702	4.10346	0.48582
C	-3.29252	2.48386	1.11117
C	-2.46078	5.12964	0.93095
H	-0.65499	4.3532	0.12443
C	-4.09846	3.52325	1.57053
C	-3.69496	4.8476	1.50179
H	-2.10561	6.15189	0.858
H	-5.06693	3.24444	1.9694
H	-4.33733	5.6381	1.87376
O	-3.88304	1.23803	1.17278
C	-4.3321	0.64054	0.0173
C	-4.29387	1.23979	-1.24135
C	-4.81458	-0.66184	0.1658
C	-4.73502	0.51756	-2.35377
H	-3.93592	2.25526	-1.35715
C	-5.25439	-1.36352	-0.94772
H	-4.80266	-1.10527	1.15383
C	-5.21108	-0.782	-2.21817
H	-5.62324	-2.37698	-0.82592
H	-5.54626	-1.33735	-3.08719
H	-1.304	-0.4269	-1.90315
H	0.32533	1.19055	-2.52139
H	-4.70498	0.98689	-3.33201

O/PD

B3LYP/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	1.80048	0.58758	-1.72114
C	0.89105	-0.62718	-2.04125
C	-0.51823	-0.05327	-2.14356
C	0.86096	1.78391	-1.64322
N	-0.43992	1.32747	-1.90928
O	-1.52936	-0.64517	-2.42893
O	1.15806	2.93382	-1.44062
C	2.56559	0.19817	-0.40751
C	1.17736	-1.6731	-0.90059
C	2.69473	-1.32868	-0.72477
O	3.65929	-2.02166	-0.80313
C	1.84572	2.75846	3.28874
C	2.03853	2.03578	2.13158
C	1.33712	0.83029	1.89438
C	0.38234	0.3802	2.85582
C	0.22339	1.14164	4.03582
C	0.93982	2.29942	4.25566
C	1.52839	0.03397	0.71211
C	-0.4282	-0.80112	2.58472
C	-0.30496	-1.48415	1.33655
C	0.73147	-1.05748	0.43477
C	-1.18864	-2.54994	1.04703
H	-1.13395	-3.03906	0.08658
C	-2.1221	-2.97512	1.96698
C	-2.20485	-2.34836	3.21802
C	-1.38105	-1.2821	3.51063
H	2.3917	3.6829	3.44532
H	2.72782	2.40447	1.38691
H	-0.48826	0.82897	4.78894
H	0.78815	2.86154	5.17169
H	-2.79011	-3.79342	1.71984
H	-2.92786	-2.68875	3.95226
H	-1.48243	-0.80714	4.47788
C	0.90516	-3.12434	-1.21713
C	1.51811	-4.12086	-0.44478
C	0.07299	-3.51599	-2.27156
C	1.30594	-5.46721	-0.72043
H	2.16659	-3.84367	0.3775
C	-0.13921	-4.86651	-2.54671
H	-0.45429	-2.76899	-2.85209
C	0.47759	-5.84669	-1.77535
H	1.79211	-6.22202	-0.11062
H	-0.7949	-5.14781	-3.3647
H	0.31335	-6.89771	-1.99093
C	3.88296	0.88476	-0.13989
C	4.76922	0.32053	0.78793
C	4.26826	2.05502	-0.80257
C	6.00301	0.90834	1.0438
H	4.49335	-0.58592	1.31394
C	5.50619	2.64343	-0.54594
H	3.58341	2.54362	-1.48457
C	6.37888	2.07221	0.37499
H	6.67421	0.4534	1.76523
H	5.78129	3.55587	-1.06543
H	7.34246	2.53043	0.57391
C	-1.55811	2.20642	-2.06018
C	-1.55939	3.14958	-3.08505
C	-2.6459	2.12317	-1.18201
C	-2.64475	4.0001	-3.25968
H	-0.70274	3.20674	-3.74662
C	-3.74165	2.96839	-1.36745
C	-3.73609	3.90017	-2.39988
H	-2.63859	4.73038	-4.0609
H	-4.58746	2.89714	-0.69479
H	-4.59154	4.55547	-2.52701
O	-2.55546	1.22976	-0.14942
C	-3.73045	0.68473	0.36176
C	-4.47847	-0.20133	-0.40938
C	-4.10014	1.00061	1.66351
C	-5.62617	-0.7683	0.13756
H	-4.14224	-0.4461	-1.41038
C	-5.24916	0.42234	2.20182
H	-3.48466	1.6833	2.23812
C	-6.01629	-0.45651	1.44035
H	-5.54405	0.66325	3.21805
H	-6.91112	-0.90289	1.86154
H	1.13699	-1.08124	-3.00433
H	2.52651	0.7779	-2.51576
H	-6.21325	-1.46271	-0.45482

O/PD

B3LYP+D3/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	-2.01538	-0.52416	-1.68742
C	-1.33513	0.84467	-1.94631
C	0.11725	0.51009	-2.26114
C	-0.94335	-1.56561	-1.95959
N	0.23468	-0.8856	-2.29088
O	1.01727	1.28308	-2.47148
O	-1.05857	-2.76428	-1.91864
C	-2.50399	-0.45025	-0.20113
C	-1.55157	1.68004	-0.63541
C	-2.92492	1.05624	-0.22321
O	-3.97068	1.56918	0.01984
C	-0.49857	-3.37903	2.63426
C	-1.08774	-2.5271	1.72583
C	-0.67716	-1.17864	1.61758
C	0.39215	-0.70331	2.43475
C	0.95703	-1.6017	3.3676
C	0.5225	-2.90713	3.47293
C	-1.27103	-0.25849	0.69109
C	0.91297	0.64451	2.24647
C	0.40202	1.46969	1.19936
C	-0.73668	0.99104	0.46761
C	1.0226	2.71273	0.93624
H	0.67653	3.31574	0.11179
C	2.06738	3.16465	1.71159
C	2.53185	2.38662	2.78147
C	1.97026	1.15382	3.03249
H	-0.82314	-4.41248	2.69507
H	-1.86306	-2.90007	1.07381
H	1.7686	-1.27779	4.00575
H	0.98409	-3.57179	4.19642
H	2.52949	4.12097	1.48937
H	3.35308	2.73867	3.3966
H	2.37656	0.56234	3.84142
C	-1.54773	3.17854	-0.76498
C	-2.11797	3.95075	0.25486
C	-0.97549	3.83073	-1.86172
C	-2.11661	5.33901	0.17908
H	-2.56104	3.46138	1.11351
C	-0.97504	5.22274	-1.93689
H	-0.47297	3.25858	-2.63177
C	-1.54639	5.98159	-0.91912
H	-2.56251	5.92055	0.97955
H	-0.5172	5.71175	-2.79085
H	-1.54445	7.06534	-0.97775
C	-3.59369	-1.39236	0.23209
C	-4.255	-1.13754	1.44019
C	-3.97148	-2.50966	-0.51771
C	-5.2673	-1.97798	1.88791
H	-3.97088	-0.2761	2.03374
C	-4.98726	-3.35257	-0.06793
H	-3.43798	-2.76315	-1.42497
C	-5.63911	-3.09027	1.13334
H	-5.7674	-1.76423	2.82703
H	-5.26005	-4.2217	-0.65801
H	-6.42824	-3.74844	1.48272
C	1.45813	-1.55506	-2.59062
C	1.60341	-2.24465	-3.78825
C	2.50808	-1.50853	-1.6667
C	2.8039	-2.88012	-4.08964
H	0.76849	-2.27288	-4.47919
C	3.71872	-2.12973	-1.97537
C	3.85771	-2.81103	-3.18174
H	2.91556	-3.41752	-5.02442
H	4.53952	-2.08274	-1.27138
H	4.8023	-3.29462	-3.40821
O	2.25586	-0.86074	-0.4893
C	3.33992	-0.48448	0.29699
C	3.99015	0.71127	0.02066
C	3.71745	-1.29202	1.36282
C	5.05194	1.10232	0.83216
H	3.64188	1.31828	-0.80665
C	4.77875	-0.88896	2.17052
H	3.16676	-2.20491	1.55466
C	5.45002	0.30378	1.90367
H	5.08014	-1.50893	3.00881
H	6.27603	0.61475	2.53487
H	-1.77028	1.36903	-2.79946
H	-2.86851	-0.70498	-2.34439
H	5.56106	2.03935	0.63247

A1/RC

B3LYP/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	0.4618	0.70329	-1.61895
C	-0.12785	-0.68672	-1.26382
C	-1.0908	-0.42851	-0.11127
C	-0.21117	1.68029	-0.66263
N	-1.06803	0.94405	0.16797
O	-1.77262	-1.23756	0.46693
O	-0.06536	2.87515	-0.61453
C	2.01882	0.54313	-1.46281
C	1.11435	-1.59391	-0.93346
C	2.09631	-0.93793	-1.95789
O	2.7191	-1.42168	-2.84948
C	4.03679	3.10488	1.71907
C	3.39274	2.36574	0.75101
C	2.95304	1.04507	1.00698
C	3.1428	0.48992	2.3096
C	3.82275	1.27368	3.26975
C	4.26704	2.54768	2.98524
C	2.30211	0.23167	0.0146
C	2.60149	-0.82539	2.63108
C	1.87291	-1.56084	1.64688
C	1.78301	-1.00952	0.32102
C	1.26517	-2.78476	2.014
H	0.67726	-3.324	1.28746
C	1.40087	-3.29742	3.28551
C	2.15344	-2.60181	4.24251
C	2.73141	-1.39245	3.91936
H	4.36139	4.11647	1.49895
H	3.21204	2.80629	-0.21753
H	3.998	0.88043	4.26261
H	4.78316	3.12149	3.74836
H	0.92298	-4.23697	3.54246
H	2.272	-3.00569	5.2429
H	3.28887	-0.87086	4.68641
C	0.94624	-3.08445	-1.10374
C	2.08585	-3.89323	-1.21419
C	-0.31208	-3.69181	-1.17907
C	1.96984	-5.26717	-1.3951
H	3.07154	-3.44625	-1.16175
C	-0.4271	-5.06937	-1.36134
H	-1.20954	-3.10022	-1.04622
C	0.71146	-5.86169	-1.47242
H	2.86557	-5.87405	-1.48029
H	-1.41303	-5.52063	-1.41008
H	0.62091	-6.93379	-1.61534
C	2.89621	1.49875	-2.23486
C	4.24468	1.17341	-2.43684
C	2.40947	2.69191	-2.77983
C	5.08016	2.01522	-3.1626
H	4.64453	0.25386	-2.02577
C	3.24814	3.53503	-3.50806
H	1.38649	2.99626	-2.59599
C	4.58422	3.19989	-3.70466
H	6.1205	1.74259	-3.30852
H	2.85169	4.45967	-3.91542
H	5.2358	3.85642	-4.27249
C	-1.90202	1.54288	1.16158
C	-1.34902	2.07272	2.32296
C	-3.28538	1.59078	0.9526
C	-2.1719	2.63674	3.29234
H	-0.27478	2.03116	2.4604
C	-4.11103	2.14536	1.92978
C	-3.5506	2.66421	3.09315
H	-1.73893	3.04755	4.19737
H	-5.182	2.17647	1.76884
H	-4.19992	3.09944	3.84575
O	-3.74963	1.13519	-0.25538
C	-4.99908	0.52705	-0.32255
C	-5.92233	1.04609	-1.22005
C	-5.27795	-0.61287	0.42942
C	-7.16856	0.42994	-1.38706
H	-5.65493	1.93048	-1.78996
C	-6.5182	-1.22043	0.27098
H	-4.52401	-1.01635	1.09503
C	-7.45481	-0.70579	-0.62634
H	-6.7527	-2.11258	0.84281
H	-8.41563	-1.19854	-0.74034
H	-0.68763	-1.12341	-2.09382
H	0.22911	1.00359	-2.64296
C	-8.17248	0.99847	-2.36061
H	-9.04976	0.35512	-2.45224
H	-8.51966	1.98721	-2.04373
H	-7.7396	1.11543	-3.35847

A1/RC

B3LYP+D3/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	-0.59213	0.82612	-1.13713
C	0.00279	-0.55016	-1.52358
C	-0.58195	-1.53351	-0.52505
C	-1.45984	0.56044	0.07748
N	-1.36046	-0.80167	0.38267
O	-0.41718	-2.72484	-0.48305
O	-2.11866	1.35902	0.69539
C	0.64647	1.73295	-0.8121
C	1.55815	-0.37285	-1.38742
C	1.62722	1.11486	-1.85549
O	2.24076	1.62305	-2.73893
C	0.57409	3.17723	3.4922
C	0.60777	2.77728	2.17556
C	1.2497	1.57705	1.79274
C	1.8452	0.75353	2.79586
C	1.79959	1.20476	4.13384
C	1.1841	2.38888	4.4787
C	1.29186	1.11557	0.43557
C	2.42322	-0.53469	2.43853
C	2.37772	-0.99158	1.08642
C	1.82156	-0.11091	0.10037
C	2.84519	-2.2901	0.78036
H	2.77367	-2.65542	-0.23126
C	3.37913	-3.1014	1.7558
C	3.46577	-2.64222	3.07787
C	2.99215	-1.39061	3.40677
H	0.06976	4.09835	3.76307
H	0.12387	3.38241	1.42613
H	2.24489	0.60972	4.9197
H	1.16333	2.70246	5.51713
H	3.72721	-4.0958	1.49861
H	3.89381	-3.27551	3.84775
H	3.058	-1.07165	4.43825
C	2.43678	-1.31561	-2.1549
C	3.79033	-0.99581	-2.30951
C	1.956	-2.50213	-2.71258
C	4.64389	-1.84418	-3.00371
H	4.17656	-0.08002	-1.87807
C	2.81262	-3.3524	-3.409
H	0.92728	-2.79771	-2.55291
C	4.15705	-3.02679	-3.55826
H	5.69083	-1.58176	-3.11321
H	2.4259	-4.27621	-3.82627
H	4.82332	-3.69057	-4.09913
C	0.4682	3.21836	-0.91442
C	1.60563	4.03339	-0.91912
C	-0.79034	3.81745	-0.99963
C	1.48674	5.41523	-1.00182
H	2.5881	3.58134	-0.85142
C	-0.9093	5.2031	-1.08252
H	-1.68375	3.20971	-0.94322
C	0.22693	6.00613	-1.08441
H	2.37882	6.03256	-1.00237
H	-1.89513	5.65303	-1.13659
H	0.13337	7.08523	-1.14642
C	-2.06334	-1.3953	1.46919
C	-1.68906	-1.06412	2.76862
C	-3.10552	-2.30522	1.24678
C	-2.3347	-1.6435	3.85327
H	-0.87898	-0.35841	2.91022
C	-3.74143	-2.89249	2.33785
C	-3.35537	-2.56674	3.6328
H	-2.03476	-1.38372	4.86175
H	-4.537	-3.60178	2.14334
H	-3.86072	-3.03152	4.47235
O	-3.51053	-2.70835	-0.00249
C	-3.64396	-1.78069	-1.02027
C	-4.18929	-0.52244	-0.80077
C	-3.2057	-2.16494	-2.28484
C	-4.25188	0.40825	-1.84177
H	-4.50595	-0.24154	0.19709
C	-3.29205	-1.25022	-3.32806
H	-2.77915	-3.1516	-2.4155
C	-3.79541	0.03214	-3.10747
H	-2.9474	-1.53263	-4.31731
H	-3.83628	0.74418	-3.92546
H	-0.26278	-0.85325	-2.53599
H	-1.19952	1.25835	-1.93198
C	-4.78171	1.79232	-1.5711
H	-4.61409	2.45838	-2.41972
H	-5.85752	1.77324	-1.37171
H	-4.29495	2.2243	-0.69286

A1/TS

B3LYP/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	1.36193	0.53731	-1.81383
C	0.24091	-0.49946	-1.66083
C	-0.88934	0.23938	-0.96848
C	0.77786	1.83749	-1.29182
N	-0.55345	1.628	-0.81725
O	-1.8534	-0.29589	-0.49668
O	1.37531	2.88556	-1.31757
C	2.59328	-0.06108	-1.0392
C	0.86606	-1.68535	-0.83436
C	2.31535	-1.55724	-1.40452
O	3.00642	-2.35709	-1.9515
C	4.09385	2.26588	2.57297
C	3.61858	1.60943	1.45866
C	2.6919	0.54622	1.57337
C	2.20973	0.18023	2.86667
C	2.73327	0.86682	3.98565
C	3.65785	1.88075	3.84893
C	2.19395	-0.18192	0.43739
C	1.17233	-0.83617	3.00003
C	0.62217	-1.45742	1.83722
C	1.20065	-1.13168	0.5608
C	-0.46231	-2.35374	1.9848
H	-0.91478	-2.78831	1.10704
C	-0.96085	-2.67355	3.22873
C	-0.39104	-2.1056	4.37716
C	0.64511	-1.20357	4.25888
H	4.8016	3.0804	2.45922
H	3.95458	1.91783	0.48001
H	2.39827	0.61097	4.98233
H	4.0348	2.38882	4.73081
H	-1.79541	-3.36152	3.31467
H	-0.77255	-2.36238	5.3603
H	1.04911	-0.76649	5.16271
C	0.25548	-3.05563	-1.00272
C	0.9931	-4.18218	-0.61249
C	-1.01486	-3.25083	-1.55488
C	0.47567	-5.4631	-0.77017
H	1.97981	-4.05791	-0.18249
C	-1.53276	-4.53557	-1.71384
H	-1.63031	-2.39905	-1.81487
C	-0.78998	-5.64604	-1.3248
H	1.06472	-6.32086	-0.46163
H	-2.52456	-4.66272	-2.13593
H	-1.19365	-6.64594	-1.44845
C	3.97288	0.41117	-1.43022
C	5.08376	-0.33828	-1.01767
C	4.1916	1.54601	-2.218
C	6.37238	0.0369	-1.37957
H	4.94006	-1.2235	-0.40888
C	5.48486	1.92137	-2.58136
H	3.35882	2.17217	-2.51222
C	6.57903	1.16895	-2.16646
H	7.21703	-0.55929	-1.04938
H	5.63178	2.81018	-3.18678
H	7.58481	1.46157	-2.45063
C	-1.49706	2.73683	-0.74007
C	-0.97774	4.01542	-0.44684
C	-2.9	2.5888	-0.60132
C	-1.7855	5.09114	-0.10648
H	0.08682	4.16145	-0.46816
C	-3.69965	3.67385	-0.23258
C	-3.15779	4.92079	0.02805
H	-1.32347	6.05259	0.08955
H	-4.77084	3.51577	-0.1915
H	-3.80175	5.74681	0.31068
O	-3.52845	1.47006	-1.09659
C	-4.58405	0.89049	-0.41929
C	-5.6071	0.36433	-1.20192
C	-4.61543	0.77583	0.96922
C	-6.69106	-0.29041	-0.61026
H	-5.54142	0.47291	-2.27998
C	-5.69908	0.13496	1.56015
H	-3.80193	1.16675	1.56772
C	-6.72881	-0.39297	0.7831
H	-5.73468	0.03871	2.64076
H	-7.56576	-0.89079	1.26344
H	-0.12184	-0.86781	-2.62382
H	1.64256	0.70594	-2.85628
C	-7.78175	-0.88462	-1.46862
H	-8.68419	-1.08649	-0.88764
H	-8.0555	-0.21833	-2.2911
H	-7.46113	-1.83217	-1.915

A1/TS

B3LYP+D3/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	0.58308	0.93666	-1.44265
C	-0.44812	-0.15677	-1.11433
C	-1.14171	0.34548	0.12804
C	0.26613	2.0782	-0.49251
N	-0.91461	1.76555	0.23806
O	-1.67058	-0.34047	0.95102
O	0.91038	3.09354	-0.40542
C	1.96844	0.22727	-1.30532
C	0.3647	-1.46994	-0.89544
C	1.52357	-1.15979	-1.89577
O	1.95142	-1.78089	-2.81519
C	4.65619	1.79501	1.99381
C	3.81793	1.36743	0.98867
C	2.97253	0.2496	1.17199
C	2.95724	-0.41856	2.43306
C	3.84126	0.04203	3.43303
C	4.67736	1.1175	3.22145
C	2.09979	-0.24153	0.14653
C	2.01735	-1.50575	2.6735
C	1.08933	-1.89256	1.65958
C	1.19129	-1.25058	0.38166
C	0.11286	-2.87099	1.95327
H	-0.62253	-3.12594	1.20803
C	0.07583	-3.49119	3.18172
C	1.01446	-3.15053	4.16606
C	1.95495	-2.17464	3.91554
H	5.29415	2.65749	1.83418
H	3.79846	1.89998	0.05073
H	3.86362	-0.44305	4.39964
H	5.34077	1.44728	4.01407
H	-0.68341	-4.23845	3.38588
H	0.99382	-3.64273	5.13277
H	2.65166	-1.91876	4.70246
C	-0.36642	-2.75963	-1.12417
C	0.36625	-3.93862	-1.29855
C	-1.76233	-2.8228	-1.15359
C	-0.28196	-5.15289	-1.4912
H	1.44861	-3.90508	-1.27553
C	-2.41081	-4.03951	-1.34851
H	-2.36041	-1.9387	-0.97724
C	-1.67448	-5.20833	-1.51722
H	0.30137	-6.05822	-1.62179
H	-3.49531	-4.06637	-1.35808
H	-2.17997	-6.15681	-1.66601
C	3.15119	0.83624	-1.99915
C	4.31511	0.06923	-2.12635
C	3.13682	2.12915	-2.52507
C	5.43857	0.58488	-2.7594
H	4.34123	-0.93462	-1.71913
C	4.26423	2.64661	-3.16041
H	2.26757	2.75887	-2.39066
C	5.41711	1.87773	-3.28069
H	6.33292	-0.02287	-2.84674
H	4.23978	3.65772	-3.55312
H	6.29505	2.28216	-3.77338
C	-1.85702	2.7717	0.66407
C	-1.54382	4.12435	0.438
C	-3.04723	2.51332	1.38541
C	-2.35583	5.15819	0.88286
H	-0.62489	4.37465	-0.06137
C	-3.84333	3.56327	1.83706
C	-3.50739	4.88781	1.60988
H	-2.05917	6.18032	0.67575
H	-4.75009	3.29061	2.36393
H	-4.13976	5.68675	1.97992
O	-3.566	1.25986	1.62889
C	-4.1702	0.57841	0.59659
C	-4.25514	1.0651	-0.70477
C	-4.65514	-0.69011	0.91308
C	-4.81028	0.27362	-1.71881
H	-3.89289	2.05869	-0.94061
C	-5.20799	-1.47029	-0.09034
H	-4.54612	-1.05119	1.92785
C	-5.27867	-1.00103	-1.40355
H	-5.57242	-2.46409	0.14814
H	-5.70154	-1.62797	-2.18181
H	-1.19085	-0.27821	-1.90623
H	0.47411	1.32656	-2.45821
C	-4.91742	0.81751	-3.12114
H	-4.96334	0.01446	-3.85949
H	-5.8221	1.42312	-3.23917
H	-4.06759	1.45776	-3.37129

A1/PD

B3LYP/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	2.06331	0.50373	-1.67975
C	1.24735	-0.78234	-1.97269
C	-0.18039	-0.30061	-2.21662
C	1.07041	1.65056	-1.81839
N	-0.17631	1.10048	-2.15031
O	-1.14586	-0.97376	-2.47591
O	1.29475	2.82968	-1.71266
C	2.69496	0.273	-0.26143
C	1.48927	-1.72477	-0.73743
C	2.95327	-1.26075	-0.43666
O	3.96344	-1.88567	-0.35893
C	1.37746	3.07837	3.07317
C	1.75827	2.27072	2.0238
C	1.16685	1.00134	1.8228
C	0.1288	0.57005	2.70296
C	-0.22434	1.42088	3.77499
C	0.38611	2.64319	3.96447
C	1.55015	0.12245	0.751
C	-0.56361	-0.68904	2.45763
C	-0.23851	-1.47371	1.30958
C	0.86442	-1.04615	0.49134
C	-0.99978	-2.63365	1.03323
H	-0.79038	-3.20799	0.14414
C	-2.0082	-3.0452	1.87706
C	-2.29709	-2.30637	3.03291
C	-1.59391	-1.15254	3.30602
H	1.84261	4.04993	3.20336
H	2.51384	2.61928	1.33585
H	-1.00297	1.12504	4.46601
H	0.08704	3.27194	4.79722
H	-2.57452	-3.94114	1.64427
H	-3.08362	-2.63046	3.70666
H	-1.85471	-0.59374	4.19515
C	1.34263	-3.20931	-0.97191
C	1.94753	-4.10942	-0.08366
C	0.634	-3.72529	-2.06286
C	1.84792	-5.48224	-0.28233
H	2.50246	-3.73638	0.76847
C	0.53475	-5.10194	-2.26085
H	0.11198	-3.05618	-2.73601
C	1.14279	-5.98552	-1.37419
H	2.32632	-6.16062	0.4169
H	-0.02626	-5.47988	-3.10974
H	1.06668	-7.05702	-1.52962
C	3.93057	1.06682	0.08824
C	4.73218	0.64342	1.15737
C	4.32518	2.19913	-0.63245
C	5.89266	1.33109	1.49435
H	4.44819	-0.23147	1.73065
C	5.48965	2.88778	-0.29409
H	3.69977	2.58177	-1.4295
C	6.27864	2.45619	0.76744
H	6.49925	0.98425	2.32484
H	5.77249	3.76872	-0.8616
H	7.1853	2.99212	1.02973
C	-1.32302	1.90132	-2.45077
C	-1.35247	2.6477	-3.62473
C	-2.4105	1.93518	-1.56773
C	-2.46318	3.42186	-3.94209
H	-0.49633	2.61239	-4.28915
C	-3.53048	2.70307	-1.89267
C	-3.5504	3.44025	-3.07261
H	-2.47876	4.00063	-4.85862
H	-4.37606	2.72682	-1.21707
H	-4.42557	4.03712	-3.30793
O	-2.28587	1.2264	-0.40561
C	-3.43594	0.90444	0.31208
C	-4.25507	-0.1235	-0.13693
C	-3.70563	1.58852	1.49195
C	-5.38868	-0.48787	0.59662
H	-3.98847	-0.64131	-1.05288
C	-4.83334	1.22795	2.22456
H	-3.03615	2.37526	1.81975
C	-5.6681	0.2046	1.77892
H	-5.06412	1.75033	3.14756
H	-6.54519	-0.06311	2.36061
H	1.59101	-1.28559	-2.87982
H	2.86617	0.65786	-2.40521
C	-6.26912	-1.61803	0.12099
H	-7.16364	-1.71723	0.73923
H	-6.59254	-1.46678	-0.91292
H	-5.73564	-2.57327	0.15314

A1/PD

B3LYP+D3/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	2.23389	0.27757	-1.6697
C	1.34421	-0.95956	-1.95564
C	-0.03417	-0.38851	-2.25951
C	1.35432	1.48143	-1.95243
N	0.08276	1.0058	-2.29094
O	-1.0522	-0.99988	-2.46522
O	1.66528	2.64464	-1.91511
C	2.6694	0.10961	-0.17612
C	1.41726	-1.84283	-0.66237
C	2.86548	-1.4442	-0.22252
O	3.82093	-2.11057	0.01712
C	1.07846	3.2622	2.6745
C	1.54843	2.34723	1.7586
C	0.94199	1.07875	1.6219
C	-0.19705	0.75536	2.41718
C	-0.63661	1.71147	3.35751
C	-0.014	2.9349	3.49099
C	1.40421	0.09531	0.68812
C	-0.90605	-0.49799	2.20494
C	-0.50399	-1.37956	1.1569
C	0.69585	-1.05886	0.44069
C	-1.283	-2.52626	0.88397
H	-1.01263	-3.17081	0.06359
C	-2.3842	-2.83524	1.65046
C	-2.75395	-2.00027	2.71342
C	-2.03355	-0.85574	2.97379
H	-0.26938	-5.59685	-2.89053
H	0.52488	-7.1385	-1.11242
C	3.86984	0.87435	0.29904
C	4.43307	0.52846	1.53247
C	4.4447	1.91138	-0.43758
C	5.54377	1.20524	2.01919
H	3.99217	-0.27138	2.11595
C	5.55976	2.59012	0.05105
H	3.99046	2.23364	-1.36517
C	6.11331	2.23977	1.27816
H	5.96682	0.92509	2.97809
H	5.9877	3.40122	-0.5287
H	6.97984	2.77045	1.65846
C	-1.01439	1.86767	-2.58078
C	-1.06445	2.56088	-3.78317
C	-2.04549	1.99347	-1.64566
C	-2.15502	3.37233	-4.07664
H	-0.24627	2.45053	-4.48531
C	-3.15023	2.78874	-1.94729
C	-3.19658	3.47325	-3.15796
H	-2.19366	3.91308	-5.01497
H	-3.95996	2.87271	-1.23435
H	-4.05757	4.09462	-3.37995
O	-1.8809	1.3326	-0.46168
C	-3.02059	1.04946	0.28427
C	-3.76483	-0.07252	-0.04016
C	-3.35751	1.87236	1.35133
C	-4.89232	-0.40137	0.7164
H	-3.43806	-0.69021	-0.86942
C	-4.47932	1.54667	2.10637
H	-2.73805	2.73029	1.58014
C	-5.23978	0.42251	1.78926
H	-4.76222	2.17216	2.94673
H	-6.11112	0.17801	2.38875
H	1.69185	-1.52919	-2.81944
H	3.12099	0.31983	-2.30438
C	-5.68927	-1.63438	0.38163
H	-6.53644	-1.76198	1.05832
H	-6.07931	-1.59171	-0.63933
H	-5.06477	-2.52955	0.44952

A2/RC

B3LYP/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	0.35882	0.48343	-1.39733
C	1.27387	-0.73668	-1.68005
C	0.71804	-1.86273	-0.81719
C	-0.65711	-0.00934	-0.37384
N	-0.37162	-1.35213	-0.09689
O	1.11195	-2.99931	-0.75345
O	-1.56292	0.61755	0.1169
C	1.32596	1.62651	-0.91478
C	2.72888	-0.25101	-1.331
C	2.54354	1.22558	-1.81032
O	3.15052	1.85764	-2.61583
C	0.74354	3.24934	3.30524
C	0.86824	2.7485	2.02793
C	1.76167	1.69012	1.73802
C	2.51098	1.10355	2.80337
C	2.36719	1.65613	4.0964
C	1.51125	2.70775	4.34614
C	1.94932	1.16495	0.41169
C	3.35597	-0.05783	2.55097
C	3.44685	-0.60671	1.23506
C	2.75755	0.07291	0.17066
C	4.18987	-1.79455	1.03518
H	4.22764	-2.23777	0.05185
C	4.85773	-2.40369	2.07499
C	4.80767	-1.8447	3.36011
C	4.06779	-0.70361	3.58771
H	0.05023	4.0605	3.50156
H	0.26811	3.16875	1.23567
H	2.93147	1.24806	4.92477
H	1.42471	3.10519	5.35236
H	5.41822	-3.31527	1.89613
H	5.33929	-2.31507	4.18115
H	4.03143	-0.30986	4.59505
C	3.87765	-0.97543	-1.99055
C	5.13735	-0.36195	-2.03372
C	3.72842	-2.23351	-2.58455
C	6.214	-0.98773	-2.65262
H	5.27825	0.61347	-1.58312
C	4.80868	-2.85972	-3.20523
H	2.78145	-2.75528	-2.52195
C	6.0537	-2.23972	-3.24418
H	7.17992	-0.4934	-2.67615
H	4.67217	-3.83902	-3.65287
H	6.89377	-2.72734	-3.72847
C	0.8623	3.05052	-1.1041
C	1.80509	4.08721	-1.06443
C	-0.47698	3.37692	-1.34325
C	1.41944	5.40907	-1.25838
H	2.84891	3.86014	-0.88265
C	-0.86252	4.70266	-1.53856
H	-1.23508	2.60369	-1.33029
C	0.08286	5.72295	-1.49948
H	2.1665	6.19566	-1.22541
H	-1.90804	4.93384	-1.71614
H	-0.21767	6.75451	-1.65295
C	-1.17495	-2.14854	0.77636
C	-0.67124	-2.58721	1.99703
C	-2.47707	-2.48517	0.3881
C	-1.46757	-3.3477	2.84675
H	0.34176	-2.3204	2.27492
C	-3.27828	-3.23922	1.24489
C	-2.77046	-3.66551	2.46823
H	-1.07366	-3.68633	3.79834
H	-4.28713	-3.49455	0.94318
H	-3.39853	-4.25727	3.12613
O	-2.87706	-2.09832	-0.86573
C	-4.20205	-1.72616	-1.0769
C	-4.77638	-0.70702	-0.31776
C	-4.89296	-2.34243	-2.10903
C	-6.08253	-0.28323	-0.5731
H	-4.16947	-0.24522	0.44927
C	-6.19421	-1.91866	-2.37635
H	-4.41435	-3.12621	-2.68493
C	-6.78016	-0.91148	-1.61878
H	-6.75509	-2.38443	-3.1804
H	-7.79472	-0.60775	-1.85216
H	1.23756	-1.04968	-2.72578
H	-0.17855	0.81231	-2.28959
C	-6.74906	0.84649	0.23214
C	-8.06091	0.32755	0.86295
H	-8.5415	1.11828	1.44718
H	-8.77754	-0.00459	0.10829
H	-7.86898	-0.51557	1.53219
C	-7.06805	2.02677	-0.71322
H	-7.74342	1.7332	-1.52027
H	-7.54629	2.84102	-0.15981
H	-6.15583	2.42	-1.16991
C	-5.84689	1.36743	1.36452
H	-5.59922	0.58253	2.08433
H	-4.91068	1.78665	0.98766
H	-6.36311	2.161	1.91157

A2/RC

B3LYP+D3/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z

C	0.50268300	0.68873500	-1.02785800
C	0.24789600	-0.59540600	-1.46103900
C	0.01614700	-1.59090500	-0.33499300
C	-1.18400800	0.33126800	0.27968100
N	-0.78190000	-0.96059300	0.63299600
O	0.43725400	-2.71455200	-0.25239700
O	-1.93055100	1.02501600	0.92582700
C	0.62579300	1.77284700	-0.86571900
C	1.75880200	-0.17376900	-1.60095700
C	1.51704800	1.29708400	-2.05400900
O	1.90035600	1.88743100	-3.01373500
C	0.88070200	3.15196800	3.44673800
C	0.81046700	2.77145600	2.12486500
C	1.62425800	1.73103700	1.61738400
C	2.51605300	1.04887200	2.50011400
C	2.56605700	1.47600600	3.84701900
C	1.77324900	2.50374500	4.31349700
C	1.54563000	1.27655600	0.25741800
C	3.28915100	-0.09127700	2.02290900
C	3.10852000	-0.57348400	0.69002300
C	2.22746000	0.16032500	-0.17602000
C	3.78225800	-1.75011500	0.28708600
H	3.61976600	-2.14355000	-0.70331300
C	4.63999800	-2.40868700	1.13983800
C	4.85895600	-1.91230400	2.43307300
C	4.19232900	-0.78383700	2.86060200
H	0.23938200	3.94588000	3.81451000
H	0.10769900	3.26307000	1.47088800
H	3.22412200	0.97933800	4.54784300
H	1.83336200	2.79984600	5.35589100
H	5.14337000	-3.31037700	0.80735400
H	5.54439500	-2.42021000	3.10387000
H	4.37546000	-0.43184400	3.86744000
C	2.61950100	-0.99052200	-2.52504700
C	3.83109000	-0.45285400	-2.97729600
C	2.25896500	-2.27685700	-2.93792600
C	4.66093300	-1.18352800	-3.82057500
H	4.12548800	0.54213200	-2.66572600
C	3.09151100	-3.00838200	-3.78334400
H	1.35812900	-2.73775500	-2.55267700
C	4.29338400	-2.46514000	-4.22877700
H	5.59636900	-0.75074900	-4.16030200
H	2.80072100	-4.00977200	-4.08428800
H	4.94168800	-3.03613500	-4.88570100
C	0.23469600	3.22352000	-0.92745000
C	1.24370300	4.18201700	-1.08502900
C	-1.09070900	3.65408800	-0.83175200
C	0.93422100	5.53594500	-1.14484800
H	2.27717600	3.86298400	-1.15889600
C	-1.40160500	5.01165200	-0.89286600
H	-1.88101100	2.93925900	-0.64856700
C	-0.39211800	5.95668200	-1.05089000
H	1.72960800	6.26413900	-1.26648200
H	-2.43676800	5.32644100	-0.80767600
H	-0.63429100	7.01361000	-1.09682700
C	-1.14923800	-1.57727100	1.86539400
C	-0.70069200	-1.01462200	3.05884200
C	-1.93815000	-2.73620400	1.88692100
C	-1.01456800	-1.60861300	4.27516600
H	-0.09556200	-0.11636000	3.01796000
C	-2.23848000	-3.33453400	3.10895000
C	-1.77538600	-2.77697600	4.29578300
H	-0.65623800	-1.16668700	5.19798500
H	-2.83862600	-4.23687200	3.09946600
H	-2.01813600	-3.25348900	5.23973000
O	-2.38834100	-3.36569200	0.75267300
C	-2.97042500	-2.63125400	-0.26734800
C	-3.81427000	-1.55425700	-0.00288200
C	-2.69039600	-3.02946800	-1.56793800
C	-4.37566200	-0.81651500	-1.04695800
H	-3.98834500	-1.28356700	1.02898800
C	-3.26086500	-2.30973200	-2.61546700
H	-2.02457500	-3.86764500	-1.73333100
C	-4.08118800	-1.21440300	-2.36121200
H	-3.05366300	-2.60145000	-3.64025200
H	-4.49989800	-0.66863600	-3.19919500
H	-0.13091000	-1.00584900	-2.39745100
H	-1.24794700	1.01482700	-1.75410900
C	-5.28207000	0.39836200	-0.79148100
C	-6.67389800	0.13363400	-1.40475300
H	-7.33535600	0.98799700	-1.23129200
H	-6.62096400	-0.03087400	-2.48356700
H	-7.13665000	-0.74956400	-0.95612900
C	-4.65498900	1.64624400	-1.45045400
H	-4.52617800	1.52473600	-2.52834300
H	-5.29015800	2.52261000	-1.29002200
H	-3.67824400	1.85396000	-1.01029900
C	-5.45377100	0.69353600	0.70861500
H	-5.93200900	-0.13740100	1.23490700
H	-4.49590200	0.90591700	1.18816600
H	-6.09338600	1.57059600	0.83935100

A2/TS

B3LYP/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	1.8064	0.42791	-1.85654
C	0.64791	-0.53864	-1.57752
C	-0.38779	0.28751	-0.83788
C	1.32633	1.7796	-1.35996
N	0.03196	1.65917	-0.76607
O	-1.34205	-0.17588	-0.27808
O	1.96382	2.79542	-1.49284
C	3.05763	-0.20294	-1.14041
C	1.2694	-1.72259	-0.74576
C	2.67866	-1.69531	-1.4195
O	3.28717	-2.55189	-1.97855
C	4.92379	2.18785	2.25318
C	4.34039	1.51063	1.20461
C	3.36905	0.50658	1.4295
C	2.95731	0.22433	2.76747
C	3.5903	0.92966	3.81607
C	4.55518	1.88399	3.5716
C	2.75751	-0.24166	0.3641
C	1.88103	-0.72787	3.01635
C	1.22345	-1.37029	1.92291
C	1.72899	-1.13145	0.59738
C	0.10767	-2.20018	2.18303
H	-0.42475	-2.64783	1.35821
C	-0.32146	-2.43727	3.47057
C	0.3518	-1.84951	4.55107
C	1.42162	-1.01006	4.32288
H	5.66472	2.95532	2.05495
H	4.62616	1.75578	0.19273
H	3.31104	0.73626	4.84355
H	5.01695	2.40839	4.40209
H	-1.18149	-3.07576	3.64336
H	0.02474	-2.04151	5.56804
H	1.90671	-0.55516	5.17665
C	0.58052	-3.06409	-0.81319
C	1.2866	-4.21225	-0.42777
C	-0.73306	-3.21376	-1.27067
C	0.69737	-5.46967	-0.49888
H	2.30571	-4.1239	-0.07059
C	-1.32299	-4.47501	-1.34284
H	-1.32257	-2.34195	-1.52463
C	-0.61074	-5.60738	-0.96012
H	1.26366	-6.34473	-0.19638
H	-2.34639	-4.56616	-1.69262
H	-1.07041	-6.58895	-1.01673
C	4.42813	0.17892	-1.64543
C	5.52677	-0.61087	-1.27789
C	4.64715	1.26975	-2.49303
C	6.80399	-0.31687	-1.74103
H	5.38277	-1.46315	-0.62392
C	5.92882	1.56319	-2.95849
H	3.82791	1.92666	-2.75645
C	7.01097	0.7719	-2.58676
H	7.63931	-0.94283	-1.44378
H	6.07658	2.41932	-3.6091
H	8.00783	1.00099	-2.9497
C	-0.84325	2.82059	-0.6589
C	-0.23408	4.07558	-0.44745
C	-2.23675	2.7557	-0.40717
C	-0.9531	5.20466	-0.08215
H	0.83193	4.16055	-0.55441
C	-2.94514	3.89447	-0.01409
C	-2.31795	5.11584	0.16232
H	-0.42576	6.14358	0.04672
H	-4.01675	3.79867	0.11449
H	-2.8923	5.98472	0.46584
O	-2.96078	1.66039	-0.81617
C	-3.9977	1.16643	-0.04686
C	-5.10165	0.68187	-0.74803
C	-3.93889	1.09361	1.33939
C	-6.18785	0.11419	-0.07817
H	-5.0769	0.76438	-1.8267
C	-5.02182	0.53686	2.01527
H	-3.06482	1.44688	1.8724
C	-6.12812	0.05617	1.32322
H	-4.99371	0.46831	3.09832
H	-6.9504	-0.37187	1.88598
H	0.19599	-0.92438	-2.49477
H	2.02164	0.5344	-2.92235
C	-7.42401	-0.4238	-0.82091
C	-8.67368	0.3697	-0.37712
H	-9.56676	-0.00416	-0.88769
H	-8.84836	0.28838	0.69798
H	-8.56892	1.43166	-0.61612
C	-7.62005	-1.91859	-0.48117
H	-7.77509	-2.07879	0.58806
H	-8.49377	-2.31844	-1.00526
H	-6.74835	-2.50673	-0.78058
C	-7.29306	-0.2949	-2.34842
H	-7.18667	0.7463	-2.66461
H	-6.43809	-0.8565	-2.73464
H	-8.18992	-0.69164	-2.83183

A2/TS

B3LYP+D3/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	0.5861	1.05289	-1.18756
C	-0.33058	-0.11163	-0.77511
C	-0.78937	0.24792	0.61573
C	0.42952	2.0883	-0.08772
N	-0.59055	1.66497	0.81191
O	-1.13076	-0.52538	1.46007
O	1.05616	3.1156	-0.01901
C	1.98808	0.39769	-1.39265
C	0.54212	-1.40105	-0.84916
C	1.47162	-0.94793	-2.0201
O	1.72437	-1.46158	-3.06245
C	5.21612	1.79002	1.46938
C	4.21285	1.413	0.60511
C	3.45609	0.24158	0.83497
C	3.70871	-0.53862	2.00285
C	4.75406	-0.12537	2.85744
C	5.49733	1.00634	2.59779
C	2.41482	-0.19576	-0.04717
C	2.86908	-1.68957	2.30867
C	1.76911	-2.02404	1.46152
C	1.59872	-1.26334	0.25834
C	0.8987	-3.07105	1.83984
H	0.03704	-3.28936	1.23047
C	1.12587	-3.80528	2.98202
C	2.23333	-3.51533	3.79186
C	3.07641	-2.47583	3.46288
H	5.78211	2.69512	1.27752
H	3.9939	2.02753	-0.25409
H	4.97773	-0.69221	3.75123
H	6.28993	1.29737	3.27913
H	0.44399	-4.60368	3.25423
H	2.42088	-4.09795	4.68772
H	3.91051	-2.26328	4.11808
C	-0.19006	-2.69281	-1.0612
C	0.51873	-3.82009	-1.49032
C	-1.56442	-2.80698	-0.83449
C	-0.13066	-5.03427	-1.68049
H	1.58446	-3.74685	-1.66979
C	-2.21437	-4.02314	-1.02676
H	-2.13691	-1.96819	-0.46319
C	-1.50116	-5.14094	-1.44908
H	0.43452	-5.89937	-2.01089
H	-3.27989	-4.0894	-0.83434
H	-2.00688	-6.08959	-1.59596
C	2.99487	1.12026	-2.2383
C	4.13394	0.42282	-2.65685
C	2.84089	2.45173	-2.62789
C	5.09797	1.04354	-3.44047
H	4.26825	-0.61009	-2.35781
C	3.8077	3.0744	-3.41538
H	1.9965	3.02697	-2.27207
C	4.93787	2.37418	-3.82424
H	5.9761	0.48835	-3.75277
H	3.67771	4.11339	-3.69956
H	5.69151	2.86081	-4.43438
C	-1.50347	2.59323	1.43279
C	-1.28431	3.9715	1.25704
C	-2.55806	2.22815	2.30294
C	-2.06476	4.93197	1.8847
H	-0.45956	4.29924	0.64935
C	-3.32342	3.20545	2.93536
C	-3.0828	4.55713	2.75157
H	-1.84659	5.9791	1.70709
H	-4.12954	2.85397	3.56839
H	-3.68755	5.29769	3.26241
O	-2.98335	0.93701	2.53436
C	-3.69242	0.27743	1.55479
C	-3.85342	0.77274	0.26116
C	-4.18873	-0.97338	1.90369
C	-4.47794	0.00352	-0.72578
H	-3.47624	1.75652	0.02644
C	-4.83816	-1.72753	0.93557
H	-4.0271	-1.34227	2.90877
C	-4.97491	-1.25455	-0.36735
H	-5.2267	-2.70673	1.19563
H	-5.4687	-1.87608	-1.10492
H	-1.20849	-0.19341	-1.41912
H	0.26519	1.5279	-2.11881
C	-4.61078	0.50098	-2.17137
C	-6.10479	0.66488	-2.51565
H	-6.22677	1.01118	-3.54627
H	-6.64601	-0.27791	-2.41391
H	-6.57899	1.39342	-1.85324
C	-3.97432	-0.52742	-3.12913
H	-4.46172	-1.50168	-3.06878
H	-4.05028	-0.18205	-4.16399
H	-2.91599	-0.68175	-2.90297
C	-3.91273	1.85179	-2.39126
H	-4.34546	2.64394	-1.7757
H	-2.84245	1.79874	-2.17065
H	-4.01597	2.15573	-3.43545

A2/PD

B3LYP/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	2.41807	0.29196	-1.7766
C	1.31717	-0.77624	-2.00447
C	0.01004	0.00774	-2.07553
C	1.68259	1.62448	-1.73495
N	0.31646	1.36938	-1.93263
O	-1.09421	-0.43106	-2.27933
O	2.16498	2.72105	-1.60565
C	3.16023	-0.15297	-0.46765
C	1.48986	-1.81114	-0.83114
C	3.04691	-1.69312	-0.71893
O	3.89339	-2.5263	-0.79733
C	2.94568	2.66274	3.10335
C	2.99865	1.85624	1.98761
C	2.11461	0.76302	1.8295
C	1.12688	0.51717	2.83065
C	1.11247	1.35922	3.96584
C	2.00151	2.40408	4.10723
C	2.14965	-0.11076	0.68794
C	0.1455	-0.54473	2.64494
C	0.13503	-1.30883	1.43848
C	1.19153	-1.0833	0.48842
C	-0.89629	-2.25551	1.23509
H	-0.93726	-2.80533	0.30748
C	-1.85342	-2.48854	2.19846
C	-1.81376	-1.78168	3.40829
C	-0.84036	-0.82792	3.61659
H	3.63054	3.49888	3.19844
H	3.72014	2.07197	1.21421
H	0.38021	1.20153	4.74711
H	1.95786	3.03321	4.99065
H	-2.63343	-3.22091	2.01829
H	-2.55704	-1.97106	4.17593
H	-0.84658	-0.28625	4.55349
C	0.99195	-3.21514	-1.07826
C	1.48048	-4.26581	-0.28916
C	0.06857	-3.51304	-2.0866
C	1.05968	-5.57361	-0.50421
H	2.19617	-4.06198	0.49804
C	-0.35207	-4.82505	-2.3017
H	-0.36595	-2.71571	-2.67696
C	0.14291	-5.86016	-1.51441
H	1.45264	-6.37182	0.11739
H	-1.07421	-5.03238	-3.08512
H	-0.1838	-6.88138	-1.68304
C	4.57531	0.33605	-0.27017
C	5.39775	-0.31691	0.65839
C	5.10945	1.40511	-0.99748
C	6.71378	0.08719	0.85301
H	5.00708	-1.14836	1.23324
C	6.42969	1.80936	-0.80191
H	4.48313	1.96209	-1.68312
C	7.2371	1.15183	0.12098
H	7.33318	-0.43338	1.57639
H	6.82122	2.64672	-1.37078
H	8.26467	1.46682	0.27241
C	-0.65433	2.41033	-2.07363
C	-0.54937	3.30795	-3.13338
C	-1.70657	2.52732	-1.15569
C	-1.49205	4.31539	-3.30196
H	0.27792	3.20666	-3.82627
C	-2.66073	3.53132	-1.33515
C	-2.54921	4.41762	-2.40109
H	-1.40267	5.00959	-4.12985
H	-3.47877	3.61928	-0.63113
H	-3.29451	5.19704	-2.52184
O	-1.71289	1.66494	-0.09545
C	-2.92609	1.38952	0.53396
C	-3.87803	0.61574	-0.12733
C	-3.12769	1.84882	1.8254
C	-5.08223	0.28572	0.49877
H	-3.63922	0.27084	-1.12458
C	-4.32541	1.52037	2.46006
H	-2.36077	2.43847	2.31387
C	-5.28592	0.75738	1.80671
H	-4.50888	1.86619	3.47245
H	-6.20623	0.52088	2.32958
H	1.44432	-1.29761	-2.95645
H	3.13582	0.32496	-2.60027
C	-6.15658	-0.57724	-0.18678
C	-7.48794	0.2049	-0.24564
H	-8.2614	-0.39399	-0.73623
H	-7.85609	0.46595	0.74917
H	-7.37298	1.13354	-0.81127
C	-6.36157	-1.87627	0.62516
H	-6.68703	-1.67173	1.64788
H	-7.12289	-2.50619	0.1546
H	-5.43436	-2.45291	0.6813
C	-5.76584	-0.96488	-1.62371
H	-5.62781	-0.08731	-2.26108
H	-4.84563	-1.55357	-1.65686
H	-6.5583	-1.57151	-2.0704

A2/PD

B3LYP+D3/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z

C	2.63142400	0.00917300	1.68790300
C	1.51977600	1.05635400	1.95222300
C	0.25675900	0.23420100	2.18496400
C	1.98097900	-1.34112900	1.92903500
N	0.62639300	-1.11598400	2.20192500
O	-0.86463400	0.64525300	2.35047800
O	2.50816000	-2.42429400	1.90865500
C	3.07643100	0.27971600	0.21093500
C	1.48635500	1.97744700	0.67921700
C	2.99232200	1.84006400	0.28615600
O	3.82557900	2.66591100	0.08641700
C	2.09971800	-3.10945500	-2.64555300
C	2.39831400	-2.11167500	-1.74380700
C	1.58422700	-0.96105600	-1.63288800
C	0.41723500	-0.84668700	-2.44574900
C	0.15391500	-1.88291400	-3.36942900
C	0.97458700	-2.98709600	-3.47455800
C	1.85470900	0.09227700	-0.69771900
C	-0.48882900	0.28037700	-2.26990000
C	-0.26097100	1.22840200	-1.22635500
C	0.95277400	1.10850700	-0.46879500
C	-1.21639000	2.24658400	-1.00169000
H	-1.07402300	2.94139100	-0.19015000
C	-2.32785900	2.37053800	-1.80498900
C	-2.53508000	1.46854200	-2.85804000
C	-1.63831600	0.44543600	-3.07377100
H	2.73219700	-3.98876400	-2.70751400
H	3.25751200	-2.21984200	-1.09904200
H	-0.72267300	-1.83372200	-4.00177700
H	0.73787300	-3.76794500	-4.19044500
H	-3.03961400	3.16728000	-1.61687500
H	-3.41115300	1.55836200	-3.49112800
H	-1.84088500	-0.25065600	-3.87614500
C	0.99416300	3.38592100	0.87336900
C	1.34278400	4.37061000	-0.05966800
C	0.16876500	3.73893300	1.94626200
C	0.87686200	5.67392900	0.07736000
H	1.97760900	4.11442500	-0.89848400
C	-0.29757400	5.04524700	2.08207600
H	-0.16605800	2.98177000	2.64436100
C	0.05505300	6.01745900	1.14989000
H	1.15639600	6.42308100	-0.65639300
H	-0.94649200	5.29735100	2.91475400
H	-0.30976500	7.03421400	1.25504500
C	4.41365100	-0.24466100	-0.23600500
C	4.94323700	0.23016800	-1.44264000
C	5.14693000	-1.18011100	0.49849700
C	6.17359400	-0.22071600	-1.90501300
H	4.38292500	0.95395600	-2.02372500
C	6.38222400	-1.63154100	0.03436400
H	4.73432300	-1.60557300	1.40431400
C	6.89991100	-1.15423300	-1.16597900
H	6.56707200	0.15717800	-2.84318300
H	6.93349100	-2.36646900	0.61220400
H	7.86026800	-1.50841100	-1.52691700
C	0.29890100	-2.17196200	2.45418200
C	0.22365700	-2.89967200	3.63676100
C	1.28352200	-2.46105800	1.50438200
C	1.14681400	-3.90650000	3.89814400
H	0.55973200	-2.66293900	4.34767600
C	2.22421200	-3.45566000	1.77651300
C	2.14969900	-4.17127000	2.96758200
H	-1.08737800	-4.47264400	4.82072900
H	-3.00109700	-3.66598000	1.05248000
H	-2.88231000	-4.94705200	3.16480000
O	-1.24199000	-1.75557400	0.33293800
C	-2.44331700	-1.59224800	-0.35521200
C	-3.32755100	-0.61536600	0.08639800
C	-2.70711300	-2.38200300	-1.46223700
C	-4.54015700	-0.41174600	-0.57508600
H	-3.02360000	-0.02793800	0.94264700
C	-3.91393200	-2.18326200	-2.13109000
H	-1.97717900	-3.11483800	-1.78372900
C	-4.81694700	-1.22228300	-1.68795700
H	-4.15246800	-2.78685500	-3.00127900
H	-5.75232400	-1.10332700	-2.22330100
H	1.71947000	1.65504400	2.84329600
H	3.49010400	0.12024700	2.35307800
C	-5.56688800	0.62447800	-0.09210200
C	-6.78531000	-0.12701100	0.48876100
H	-7.54021500	0.58108300	0.84497800
H	-7.25449200	-0.76942900	-0.26081400
H	-6.48879900	-0.75911000	1.33012200
C	-6.03231500	1.51120400	-1.26676600
H	-6.51295400	0.93288300	-2.05848900
H	-6.75898900	2.25068900	-0.91762700
H	-5.18961300	2.04604700	-1.70767200
C	-4.98918500	1.54329700	0.99887400
H	-4.72967500	0.99214000	1.90591200
H	-4.09213000	2.06306400	0.65365700
H	-5.72974200	2.29750300	1.27816000

B1/RC

B3LYP/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	-0.61697	-0.60871	-1.69307
C	0.11698	0.68833	-1.26323
C	1.1016	0.2518	-0.18648
C	0.00131	-1.71651	-0.84898
N	0.96722	-1.13211	-0.01624
O	1.87709	0.94856	0.41929
O	-0.25841	-2.89238	-0.88015
C	-2.14396	-0.31913	-1.45101
C	-1.01722	1.67383	-0.79969
C	-2.09922	1.19881	-1.82363
O	-2.70899	1.81071	-2.64246
C	-4.30778	-2.91429	1.6077
C	-3.61897	-2.1712	0.674
C	-3.0356	-0.92649	1.01096
C	-3.12732	-0.45914	2.35794
C	-3.85636	-1.24236	3.28185
C	-4.44039	-2.43786	2.91993
C	-2.33768	-0.1049	0.05793
C	-2.44262	0.7652	2.75649
C	-1.67421	1.50047	1.80275
C	-1.68704	1.05178	0.4357
C	-0.93043	2.6228	2.23811
H	-0.31235	3.1568	1.53271
C	-0.97163	3.0426	3.54965
C	-1.76208	2.3526	4.47982
C	-2.47247	1.23769	4.08833
H	-4.74381	-3.86649	1.3243
H	-3.51732	-2.55081	-0.3312
H	-3.95931	-0.91257	4.3074
H	-4.9909	-3.01383	3.65691
H	-0.39003	3.90482	3.85877
H	-1.8061	2.6849	5.51209
H	-3.05632	0.71503	4.83472
C	-0.71708	3.15222	-0.85758
C	-1.77973	4.06612	-0.835
C	0.58704	3.64928	-0.95643
C	-1.5447	5.43462	-0.90907
H	-2.79917	3.70623	-0.76124
C	0.82159	5.02178	-1.03156
H	1.43069	2.97095	-0.92461
C	-0.24163	5.91921	-1.01058
H	-2.38271	6.12409	-0.89147
H	1.84187	5.38563	-1.10035
H	-0.05843	6.98736	-1.06978
C	-3.13852	-1.1226	-2.25368
C	-4.45608	-0.65803	-2.36897
C	-2.79013	-2.30828	-2.9097
C	-5.39551	-1.35768	-3.11823
H	-4.75007	0.25864	-1.87135
C	-3.73302	-3.00883	-3.66122
H	-1.79456	-2.71945	-2.79687
C	-5.03715	-2.53618	-3.77071
H	-6.40951	-0.97854	-3.19565
H	-3.44303	-3.93059	-4.15545
H	-5.77007	-3.0814	-4.35684
C	1.79302	-1.88047	0.87756
C	1.24787	-2.48594	2.00528
C	3.16244	-1.99362	0.60742
C	2.06575	-3.19129	2.88188
H	0.18444	-2.39052	2.19091
C	3.98397	-2.68836	1.4941
C	3.43207	-3.2828	2.62502
H	1.639	-3.66093	3.76088
H	5.04446	-2.76847	1.28741
H	4.07788	-3.82748	3.30598
O	3.6129	-1.4527	-0.5702
C	4.90001	-0.92641	-0.62973
C	5.77943	-1.43833	-1.57367
C	5.27095	0.14359	0.18271
C	7.04887	-0.87443	-1.70212
H	5.46339	-2.26347	-2.20234
C	6.54281	0.68669	0.04576
H	4.55617	0.55095	0.88836
C	7.45558	0.18951	-0.8945
H	6.82757	1.52434	0.67656
H	0.67747	1.13794	-2.08591
H	-0.4561	-0.84595	-2.74705
H	7.73223	-1.27684	-2.44415
C	8.83358	0.79287	-1.02241
H	9.38437	0.36123	-1.86066
H	8.78464	1.87447	-1.18018
H	9.42814	0.62755	-0.11801

B1/RC

B3LYP+D3/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z

C	0.69754900	1.07095400	-0.77181100
C	-0.37717500	-0.27730300	-1.46330100
C	-0.86744900	-1.34637500	-0.49920300
C	-1.34728500	0.70163800	0.54864900
N	-1.36672900	-0.69599600	0.63763000
O	-0.84393700	-2.54009100	-0.65298500
O	-1.76888100	1.45181400	1.39176500
C	0.69288400	1.78002100	-0.59486400
C	1.18371300	-0.27682600	-1.66298800
C	1.35025700	1.25436600	-1.90583200
O	1.83785000	1.84583400	-2.81654000
C	1.64906700	2.44457200	3.79539700
C	1.37620200	2.27997100	2.45569500
C	1.78512500	1.11680600	1.76160800
C	2.47092900	0.08515900	2.47331100
C	2.74047400	0.29669200	3.84531500
C	2.34497500	1.44721400	4.49455300
C	1.49407300	0.89625200	0.37239800
C	2.81966200	-1.16118800	1.80183300
C	2.43876500	-1.37427000	0.44140200
C	1.78866400	-0.29671700	-0.25153800
C	2.69178100	-2.63152500	-0.15579000
H	2.37083800	-2.81312000	-1.16894500
C	3.33431500	-3.63386400	0.53623800
C	3.75070600	-3.41531000	1.85745900
C	3.49148800	-2.20870300	2.47202100
H	1.31793200	3.34216400	4.30686000
H	0.82685900	3.04582000	1.93168600
H	3.25758500	-0.46171600	4.41836200
H	2.56441200	1.57271400	5.55001600
H	3.51453000	-4.59014300	0.05663200
H	4.26725000	-4.19821200	2.40342200
H	3.81443600	-2.07694800	3.49647700
C	1.74367700	-1.15131900	-2.75094100
C	3.04844700	-0.91604700	-3.20239500
C	1.01323000	-2.19847200	-3.32071900
C	3.60909100	-1.70909400	-4.19720700
H	3.62758700	-0.10876400	-2.76984000
C	1.57629300	-2.99295100	-4.31839800
H	0.02631600	-2.43778600	-2.94530600
C	2.87381300	-2.75111700	-4.76117700
H	4.62189100	-1.51240000	-4.53383900
H	0.99891800	-3.80902800	-4.74097800
H	3.31171300	-3.37115200	-5.53686100
C	0.70164900	3.27597700	-0.44431900
C	1.91306100	3.96032400	-0.60301300
C	0.45099200	4.00868900	-0.14589600
C	1.97132000	5.34239900	-0.46495600
H	2.81511500	3.40481900	-0.83237700
C	0.39188200	5.39482300	-0.00847200
H	-1.38561600	3.49604500	0.04324200
C	0.81698500	6.06633400	-0.16834900
H	2.91920000	5.85573500	-0.59043600
H	-1.29421700	5.94683800	0.23464300
H	0.86194200	7.14521700	-0.05932900
C	1.89597100	-1.38534200	1.76734100
C	1.22376000	-1.29727300	2.98434600
C	3.07518700	-2.13702600	1.66606100
C	1.70562700	-1.96888900	4.10134200
H	-0.31726100	-0.70419800	3.03453300
C	3.54642900	-2.81916700	2.78621600
C	2.86363400	-2.73854200	3.99496500
H	-1.17471500	-1.89872200	5.04393600
H	-4.45186300	-3.40550200	2.68172500
H	-3.24405000	-3.27356100	4.85873400
O	-3.77494500	-2.30326500	0.49468100
C	-4.00892800	-1.22352700	-0.34104100
C	-4.39004200	0.02429100	0.14316300
C	-3.85531500	-1.43338700	-1.70822400
C	-4.57457300	1.07398300	-0.75204400
H	-4.48454800	0.18629100	1.21028200
C	-4.05631300	-0.37505600	-2.58980000
H	-3.54603900	-2.41272100	-2.05345200
C	-4.40685600	0.89970900	-2.12981900
H	-3.92285800	-0.54233000	-3.65481500
H	-0.88848500	-0.38961700	-2.41968100
H	-1.38231100	1.68982300	-1.35279300
H	-4.84234400	2.05184700	-0.36313700
C	-4.62661300	2.04363100	-3.08973800
H	-4.34170000	3.00110300	-2.64616000
H	-4.04811200	1.91643800	-4.00800200
H	-5.68037900	2.12161500	-3.37825900

B1/TS

B3LYP/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	-1.54741	-0.66652	-1.72461
C	-0.42253	0.37622	-1.77356
C	0.78247	-0.31532	-1.16433
C	-0.90414	-1.92378	-1.16651
N	0.4861	-1.70419	-0.93136
O	1.7768	0.25417	-0.81328
O	-1.51593	-2.94819	-0.98394
C	-2.69396	-0.0077	-0.8736
C	-0.95846	1.61783	-0.96967
C	-2.46009	1.45723	-1.37134
O	-3.20708	2.22095	-1.8961
C	-3.81943	-2.03776	3.0429
C	-3.4597	-1.4736	1.83848
C	-2.51895	-0.41876	1.77457
C	-1.90072	0.03595	2.97885
C	-2.30756	-0.5578	4.19528
C	-3.24841	-1.56527	4.23332
C	-2.14131	0.21734	0.54107
C	-0.85047	1.04657	2.9258
C	-0.42713	1.57692	1.66869
C	-1.13988	1.16528	0.48861
C	0.66897	2.47042	1.63285
H	1.02561	2.83476	0.68199
C	1.3001	2.87337	2.78935
C	0.85691	2.39434	4.03053
C	-0.18796	1.49661	4.09039
H	-4.54102	-2.84773	3.06585
H	-3.89846	-1.84912	0.92646
H	-1.86848	-0.23247	5.12935
H	-3.53363	-2.0005	5.18578
H	2.14102	3.55677	2.7348
H	1.3438	2.71636	4.9456
H	-0.49142	1.12827	5.06169
C	-0.37654	2.97147	-1.29767
C	-1.06948	4.1236	-0.90021
C	0.81827	3.1261	-2.00839
C	-0.58255	5.38975	-1.20509
H	-1.99742	4.03036	-0.34845
C	1.3051	4.39598	-2.31586
H	1.40396	2.25761	-2.28177
C	0.60674	5.53184	-1.91803
H	-1.13616	6.26768	-0.8878
H	2.23849	4.49221	-2.86131
H	0.98633	6.52007	-2.15742
C	-4.10543	-0.50009	-1.08501
C	-5.17123	0.28638	-0.62489
C	-4.40041	-1.69284	-1.75332
C	-6.48887	-0.10876	-0.82542
H	-4.97009	1.21646	-0.10614
C	-5.72254	-2.08786	-1.95581
H	-3.60035	-2.34627	-2.07705
C	-6.77124	-1.29821	-1.49535
H	-7.29734	0.51678	-0.46077
H	-5.92739	-3.02109	-2.47083
H	-7.79985	-1.60627	-1.6535
C	1.44341	-2.8048	-0.90899
C	0.95973	-4.10031	-0.63147
C	2.8526	-2.64694	-0.87548
C	1.80003	-5.17456	-0.37463
H	-0.10162	-4.26153	-0.58698
C	3.68461	-3.7322	-0.58708
C	3.17594	-4.99201	-0.32296
H	1.36102	-6.14724	-0.18093
H	4.75439	-3.56115	-0.61468
H	3.84569	-5.81704	-0.10489
O	3.44543	-1.51379	-1.37966
C	4.51308	-0.9277	-0.72708
C	5.51086	-0.37337	-1.52287
C	4.58287	-0.81948	0.65986
C	6.58262	0.28417	-0.92562
H	5.43124	-0.45639	-2.60119
C	5.66605	-0.16643	1.23929
H	3.78938	-1.2249	1.27628
C	6.68648	0.39474	0.46399
H	5.70793	-0.08098	2.32164
H	-0.17297	0.67374	-2.79541
H	-1.93318	-0.91675	-2.71632
H	7.35417	0.71583	-1.55707
C	7.86878	1.07692	1.10945
H	8.33224	1.80092	0.43505
H	7.57878	1.60909	2.0192
H	8.64336	0.35495	1.39173

B1/TS

B3LYP+D3/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	0.67353	0.83455	-1.51407
C	-0.45671	-0.12028	-1.09152
C	-1.07252	0.54388	0.11496
C	0.48847	2.07266	-0.65443
N	-0.70635	1.93951	0.10839
O	-1.64949	-0.01756	0.99807
O	1.23415	3.02008	-0.65153
C	1.98169	0.00203	-1.33101
C	0.22336	-1.49059	-0.78333
C	1.39269	-1.37318	-1.81243
O	1.74411	-2.10104	-2.68479
C	4.84823	1.5446	1.82302
C	3.95484	1.13055	0.86056
C	3.01856	0.1068	1.12972
C	2.96749	-0.47342	2.43244
C	3.90996	-0.03207	3.38657
C	4.83491	0.94691	3.09167
C	2.08625	-0.36908	0.15084
C	1.93405	-1.44784	2.75851
C	0.94919	-1.8044	1.78798
C	1.08821	-1.26447	0.46709
C	-0.11354	-2.65702	2.16245
H	-0.88789	-2.88281	1.44784
C	-0.18318	-3.19048	3.42967
C	0.80911	-2.88602	4.37237
C	1.83617	-2.02815	4.04195
H	5.55615	2.33498	1.59834
H	3.95945	1.60315	-0.10935
H	3.90731	-0.45222	4.38341
H	5.5415	1.26534	3.85091
H	-1.00869	-3.84167	3.69611
H	0.76311	-3.31174	5.36928
H	2.57423	-1.79518	4.79773
C	-0.63861	-2.71172	-0.9096
C	-0.03376	-3.96891	-1.01096
C	-2.03415	-2.63345	-0.91093
C	-0.80593	-5.12085	-1.10667
H	1.04657	-4.04538	-1.00789
C	-2.80699	-3.78811	-1.00536
H	-2.53468	-1.6826	-0.78666
C	-2.19699	-5.03535	-1.10374
H	-0.32016	-6.0879	-1.18262
H	-3.88852	-3.70594	-0.98762
H	-2.79928	-5.93501	-1.17477
C	3.21149	0.43308	-2.07421
C	4.29523	-0.45078	-2.13343
C	3.3176	1.67039	-2.71131
C	5.45858	-0.10294	-2.8072
H	4.22769	-1.41304	-1.63953
C	4.48467	2.01893	-3.38898
H	2.5142	2.39096	-2.63452
C	5.55774	1.1354	-3.4398
H	6.28964	-0.79948	-2.83965
H	4.5542	2.98922	-3.8695
H	6.46686	1.40895	-3.9649
C	-1.5491	3.06421	0.43469
C	-1.09955	4.35733	0.11188
C	-2.76331	2.98166	1.15751
C	-1.80933	5.49766	0.4615
H	-0.15457	4.47548	-0.38786
C	-3.45587	4.13681	1.51262
C	-2.98876	5.39989	1.18764
H	-1.41062	6.46627	0.18134
H	-4.38937	3.99667	2.04465
H	-3.54228	6.28383	1.48322
O	-3.40328	1.80741	1.49041
C	-4.05214	1.10194	0.50119
C	-4.09332	1.48861	-0.83511
C	-4.64465	-0.09577	0.89855
C	-4.70267	0.64957	-1.77067
H	-3.66088	2.42947	-1.15149
C	-5.24992	-0.9109	-0.04498
H	-4.58361	-0.38301	1.94092
C	-5.27869	-0.56501	-1.40286
H	-5.69724	-1.84643	0.27769
H	-1.22332	-0.22278	-1.8631
H	0.58749	1.15263	-2.55649
H	-4.72505	0.95823	-2.81176
C	-5.87884	-1.49245	-2.42877
H	-6.21884	-0.94811	-3.31257
H	-5.14901	-2.2364	-2.76683
H	-6.73488	-2.03829	-2.02453

B1/PD

B3LYP/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	-2.11096	-0.56019	-1.63075
C	-1.17985	0.61386	-2.02976
C	0.19827	-0.01473	-2.21155
C	-1.21388	-1.79047	-1.59493
N	0.08154	-1.38961	-1.95698
O	1.21003	0.53467	-2.56939
O	-1.53956	-2.92461	-1.35078
C	-2.77218	-0.12334	-0.2768
C	-1.35411	1.68823	-0.89321
C	-2.86758	1.40238	-0.61195
O	-3.8099	2.12909	-0.639
C	-1.89206	-2.65729	3.40286
C	-2.1396	-1.94207	2.25148
C	-1.41271	-0.76712	1.94748
C	-0.37745	-0.34083	2.83333
C	-0.16306	-1.09346	4.01025
C	-0.90368	-2.22101	4.29679
C	-1.65695	0.01979	0.76878
C	0.45234	0.80781	2.4903
C	0.2658	1.48024	1.24426
C	-0.84301	1.07796	0.42095
C	1.16165	2.51277	0.88092
H	1.05747	2.99278	-0.07998
C	2.16945	2.91673	1.72918
C	2.31824	2.30117	2.97968
C	1.48246	1.26609	3.34188
H	-2.45918	-3.55853	3.61115
H	-2.89345	-2.29324	1.56299
H	0.61074	-0.79836	4.70706
H	-0.70835	-2.77729	5.20812
H	2.84469	3.70991	1.42597
H	3.10084	2.62517	3.65813
H	1.63476	0.79851	4.30603
C	-1.05218	3.12312	-1.25451
C	-1.57712	4.15426	-0.46301
C	-0.27764	3.46632	-2.36815
C	-1.33596	5.48714	-0.77767
H	-2.17937	3.91465	0.40504
C	-0.03669	4.80336	-2.68262
H	0.18493	2.69125	-2.96677
C	-0.56632	5.8183	-1.89173
H	-1.75395	6.26938	-0.1521
H	0.57337	5.04667	-3.54681
H	-0.37975	6.85884	-2.13786
C	-4.09325	-0.75683	0.08823
C	-4.89567	-0.1451	1.06124
C	-4.56426	-1.92133	-0.5277
C	-6.13131	-0.68116	1.40618
H	-4.55294	0.75816	1.55222
C	-5.80378	-2.45815	-0.1813
H	-3.94425	-2.44503	-1.24468
C	-6.59282	-1.84	0.78376
H	-6.73702	-0.18984	2.16093
H	-6.1459	-3.36697	-0.66614
H	-7.55786	-2.25785	1.05229
C	1.15466	-2.31445	-2.1537
C	1.04978	-3.28853	-3.14364
C	2.3078	-2.24006	-1.3614
C	2.09055	-4.18206	-3.3681
H	0.14523	-3.33659	-3.7388
C	3.35898	-3.12805	-1.59925
C	3.24595	-4.09174	-2.59571
H	2.00063	-4.93705	-4.14092
H	4.25488	-3.06496	-0.99435
H	4.06844	-4.77942	-2.76328
O	2.32005	-1.31234	-0.35686
C	3.54941	-0.83644	0.09397
C	4.29532	0.02796	-0.7032
C	3.98602	-1.19007	1.36241
C	5.49827	0.52716	-0.21769
H	3.91471	0.31064	-1.67817
C	5.19349	-0.67598	1.83504
H	3.37814	-1.85156	1.96932
C	5.97198	0.18205	1.05522
H	5.53199	-0.9518	2.82956
H	-1.47039	1.06085	-2.98366
H	-2.89502	-0.73304	-2.37249
H	6.077	1.20599	-0.83804
C	7.29003	0.72079	1.55756
H	7.36674	1.80121	1.40526
H	7.4236	0.52577	2.62377
H	8.135	0.26249	1.03263

B1/PD

B3LYP+D3/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z

C	2.34631600	-0.49192700	1.53152700
C	1.64242500	0.84176500	1.88944400
C	0.24199500	0.44134400	2.33595300
C	1.35122000	-1.58241100	1.89086400
N	0.18605400	-0.95855500	2.35208200
O	-0.66431200	1.17238000	2.64549900
O	1.51111600	-2.77440100	1.81595300
C	2.67735200	-0.36759500	0.00504400
C	1.69728600	1.71406900	0.58592700
C	3.04436000	1.15304100	0.02410000
O	4.04183900	1.71042100	-0.30782800
C	0.51260800	-3.30073600	-2.70830900
C	1.15382500	-2.45127700	-1.83326100
C	0.70958800	-1.12176700	-1.64946100
C	-0.44651100	-0.66548700	-2.35099000
C	-1.06385100	-1.55968700	-3.25412000
C	-0.59655700	-2.84506100	-3.43666500
C	1.35630600	-0.20334800	-0.75693100
C	-0.99473400	0.65644300	-2.07645900
C	-0.41525800	1.47479000	-1.05991500
C	0.80286700	1.02018300	-0.45065500
C	-1.04986900	2.68817900	-0.70707200
H	-0.64744300	3.28372100	0.09683400
C	-2.17844400	3.11979300	-1.36813600
C	-2.71620500	2.34988500	-2.40923000
C	-2.13966500	1.14431000	-2.74435800
H	0.86524700	-4.31973000	-2.82820600
H	1.99802900	-2.81244600	-1.26545800
H	-1.94168900	-1.24984400	-3.80545200
H	-1.09998100	-3.50733000	-4.13397900
H	-2.64945800	4.05329600	-1.07805300
H	-3.60238500	2.68768900	-2.93644100
H	-2.60024500	0.55720100	-3.52688200
C	1.65194800	3.20794500	0.75519300
C	2.09729700	4.02537500	-0.29135800
C	1.15989900	3.81213700	1.91640000
C	2.05266100	5.41049100	-0.17858400
H	2.47817500	3.57438800	-1.19943500
C	1.11552000	5.20095000	2.02843400
H	0.75110900	3.20349000	2.71332000
C	1.56292300	6.00492800	0.98363900
H	2.40175000	6.02723800	-1.00049800
H	0.72035500	5.65173100	2.93322500
H	1.52709000	7.08614000	1.07121000
C	3.75077600	-1.25708100	-0.56034900
C	4.27363400	-0.95137300	-1.82329400
C	4.24449900	-2.37387900	0.11941500
C	5.26329700	-1.74320700	-2.39331800
H	3.89804800	-0.08926500	-2.36256600
C	5.23788900	-3.16774800	-0.45301800
H	3.81628100	-2.66488600	1.06999500
C	5.75120500	-2.85580700	-1.70845600
H	5.65542600	-1.49120000	-3.37336800
H	5.60183500	-4.03767200	0.08430800
H	6.52316600	-3.47559900	-2.15333800
C	-0.97504000	-1.68399800	2.75292100
C	-0.97926500	-2.40116900	3.94281700
C	-2.10819200	-1.66410900	1.93190400
C	-2.12071900	-3.09058800	4.34048400
H	-0.08221700	-2.40891400	4.55161300
C	-3.25979200	-2.33862800	2.33849900
C	-3.25774800	-3.04700200	3.53729700
H	-2.12253100	-3.64989900	5.26909600
H	-4.14386900	-2.31162600	1.71459000
H	-4.15722200	-3.57269800	3.84068800
O	-1.98996300	-0.98687600	0.75130800
C	-3.15136300	-0.64790300	0.06469400
C	-3.82974900	0.51307000	0.41074600
C	-3.58380100	-1.44934700	-0.98213100
C	-4.96091100	0.87336000	-0.31313100
H	-3.44890300	1.12182000	1.22241800
C	-4.71568000	-1.07083400	-1.70032500
H	-3.02124300	-2.33979300	-1.23553900
C	-5.42079000	0.09299200	-1.37973900
H	-5.05131800	-1.69229600	-2.52574000
H	2.13823500	1.36466400	2.70989200
H	3.26942700	-0.64895500	2.09321800
H	-5.48613700	1.78787000	-0.05331800
C	-6.61591300	0.52974200	-2.19098000
H	-7.39152900	0.97242900	1.56067200
H	-6.33199200	1.28645400	2.93113800
H	-7.06368400	-0.30523200	-2.73469100

B2/RC

B3LYP/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	1.18279	0.5579	-1.70013
C	0.41335	-0.68929	-1.19119
C	-0.49785	-0.1716	-0.08595
C	0.65498	1.72085	-0.86888
N	-0.29158	1.20901	0.0307
O	-1.27579	-0.8103	0.57775
O	0.96195	2.88235	-0.95671
C	2.70533	0.20698	-1.51579
C	1.52371	-1.71033	-0.74596
C	2.57619	-1.31833	-1.83382
O	3.1184	-1.98319	-2.65888
C	5.10541	2.80974	1.35396
C	4.3497	2.06328	0.47638
C	3.72917	0.85781	0.88275
C	3.85672	0.4355	2.2416
C	4.65251	1.22088	3.10676
C	5.26985	2.37671	2.67755
C	2.95818	0.03425	-0.01044
C	3.14197	-0.74546	2.71177
C	2.30542	-1.48088	1.81737
C	2.2763	-1.07921	0.436
C	1.53841	-2.55738	2.32265
H	0.87013	-3.08921	1.66303
C	1.61989	-2.93445	3.6452
C	2.47553	-2.24573	4.51674
C	3.21056	-1.17364	4.0571
H	5.56896	3.73136	1.01795
H	4.22404	2.41017	-0.53787
H	4.7821	0.92498	4.13958
H	5.87195	2.95561	3.37062
H	1.01958	-3.76204	4.00841
H	2.55147	-2.54495	5.55724
H	3.84622	-0.65053	4.75956
C	1.15609	-3.17446	-0.74007
C	2.17671	-4.1353	-0.73799
C	-0.17226	-3.61357	-0.75931
C	1.87753	-5.49325	-0.75372
H	3.21346	-3.82032	-0.7261
C	-0.47109	-4.97546	-0.77608
H	-0.98263	-2.89663	-0.71137
C	0.55075	-5.91997	-0.77543
H	2.68382	-6.21976	-0.75331
H	-1.50872	-5.29387	-0.78349
H	0.31727	-6.97984	-0.78935
C	3.69692	0.93785	-2.38849
C	4.98667	0.41093	-2.54274
C	3.37157	2.11455	-3.07173
C	5.92175	1.04142	-3.35604
H	5.26203	-0.50027	-2.02474
C	4.30997	2.74577	-3.88756
H	2.4007	2.57369	-2.93192
C	5.58638	2.21176	-4.03502
H	6.91399	0.61473	-3.46264
H	4.03872	3.66214	-4.40208
H	6.31572	2.70323	-4.67103
C	-1.03852	2.02374	0.93587
C	-0.41352	2.63771	2.0164
C	-2.41253	2.19302	0.72513
C	-1.15579	3.40807	2.90562
H	0.65208	2.49798	2.15578
C	-3.15856	2.95336	1.62455
C	-2.52712	3.55589	2.70871
H	-0.66675	3.88419	3.74791
H	-4.22285	3.0772	1.46395
H	-3.1145	4.15133	3.40002
O	-2.9411	1.63722	-0.41212
C	-4.25661	1.18468	-0.40254
C	-5.14479	1.71081	-1.32755
C	-4.6578	0.16743	0.46058
C	-6.4495	1.21797	-1.38811
H	-4.81163	2.49519	-1.99836
C	-5.96253	-0.30409	0.39029
H	-3.94298	-0.25721	1.15607
C	-6.89268	0.20593	-0.53115
H	-6.253	-1.09939	1.06857
H	-0.20568	-1.13998	-1.97011
H	0.98433	0.76659	-2.75372
H	-7.11981	1.64745	-2.12211
C	-8.32427	-0.35689	-0.57114
C	-9.19411	0.33427	-1.63577
H	-9.2946	1.40722	-1.45016
H	-8.79316	0.19921	-2.64401
H	-10.20022	-0.09333	-1.62618
C	-8.27536	-1.86669	-0.89786
H	-7.7092	-2.42864	-0.1515
H	-9.28619	-2.28523	-0.92945
H	-7.80721	-2.04295	-1.87014
C	-8.99832	-0.15386	0.80472
H	-10.0185	-0.54973	0.79354
H	-8.45656	-0.6628	1.60527
H	-9.0517	0.90723	1.06341

B2/RC

B3LYP+D3/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	-0.90655	0.55456	0.10413
C	-0.39117	0.0562	-1.26725
C	0.03357	-1.38349	-1.03555
C	-0.69546	-0.60406	1.05814
N	-0.15913	-1.66677	0.32163
O	0.45476	-2.16747	-1.84639
O	-0.93352	-0.63646	2.23826
C	-0.03059	1.80662	0.44802
C	0.78935	1.02517	-1.62885
C	0.16695	2.31775	-1.01212
O	-0.08862	3.36886	-1.50756
C	2.33501	1.24907	4.28587
C	1.60725	1.45283	3.13546
C	2.11887	1.0787	1.87179
C	3.39816	0.44852	1.79469
C	4.11788	0.267	2.99667
C	3.60573	0.66004	4.21446
C	1.3902	1.26538	0.65094
C	3.90353	-0.03025	0.51531
C	3.11675	0.1149	-0.66739
C	1.86408	0.80462	-0.55771
C	3.58115	-0.44538	-1.87939
H	2.97204	-0.37268	-2.76596
C	4.79447	-1.09246	-1.94435
C	5.59027	-1.20371	-0.79526
C	5.14784	-0.6888	0.40412
H	1.92014	1.53965	5.24483
H	0.62556	1.89359	3.20087
H	5.09399	-0.19891	2.97698
H	4.18493	0.50217	5.11817
H	5.12864	-1.51789	-2.88429
H	6.55056	-1.7062	-0.84393
H	5.77763	-0.80565	1.27583
C	1.17611	1.14221	-3.07351
C	1.9885	2.21159	-3.46656
C	0.75922	0.22166	-4.03721
C	2.37863	2.35465	-4.79219
H	2.32129	2.93089	-2.72764
C	1.151	0.36567	-5.36673
H	0.18004	-0.64373	-3.74305
C	1.95984	1.43131	-5.74889
H	3.01026	3.18844	-5.07994
H	0.82911	-0.36526	-6.10106
H	2.26614	1.54122	-6.78388
C	-0.61203	2.81226	1.39644
C	-0.02021	4.07664	1.48773
C	-1.72668	2.53107	2.19034
C	-0.52828	5.03575	2.35552
H	0.84599	4.30704	0.87891
C	-2.23716	3.49376	3.05857
H	-2.16481	1.54154	2.17789
C	-1.64123	4.74829	3.14387
H	-0.05592	6.01054	2.41531
H	-3.09683	3.2551	3.67599
H	-2.03776	5.4968	3.82174
C	0.12551	-2.9334	0.90594
C	1.19099	-3.04107	1.79484
C	-0.66512	-4.05268	0.61293
C	1.49213	-4.2631	2.3826
H	1.77856	-2.15535	2.00781
C	-0.35237	-5.27798	1.19682
C	0.72144	-5.38248	2.07315
H	2.32622	-4.3414	3.07007
H	-0.96639	-6.13472	0.94598
H	0.95151	-6.34299	2.52123
O	-1.70223	-4.04008	-0.28871
C	-2.5895	-2.97784	-0.31579
C	-3.1437	-2.44267	0.83788
C	-2.92944	-2.45889	-1.56193
C	-3.99328	-1.34104	0.74269
H	-2.87031	-2.84006	1.80775
C	-3.78734	-1.36966	-1.63752
H	-2.48862	-2.89639	-2.44958
C	-4.32199	-0.76691	-0.48805
H	-4.02761	-0.9722	-2.61742
H	-1.16071	0.08804	-2.03826
H	-1.96402	0.8101	0.07918
H	-4.38162	-0.92389	1.66234
C	-5.22834	0.46446	-0.61945
C	-5.65978	1.01608	0.74724
H	-6.24139	0.28745	1.31739
H	-4.80158	1.31973	1.35238
H	-6.28841	1.89863	0.60654
C	-4.48301	1.58718	-1.37134
H	-4.14227	1.26632	-2.3577
H	-5.13908	2.44999	-1.51477
H	-3.61046	1.93229	-0.81053
C	-6.49441	0.07641	-1.41029
H	-7.16241	0.93679	-1.51084
H	-6.25151	-0.2754	-2.41534
H	-7.04089	-0.72193	-0.90201

B2/TS

B3LYP/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	2.17672	0.60503	-1.71877
C	0.97696	-0.35078	-1.76687
C	-0.17224	0.42865	-1.15502
C	1.62473	1.91377	-1.18153
N	0.23142	1.7835	-0.89812
O	-1.21235	-0.0607	-0.81301
O	2.29476	2.90926	-1.05333
C	3.26284	-0.13316	-0.85298
C	1.41735	-1.63172	-0.96541
C	2.92952	-1.5774	-1.35505
O	3.62542	-2.39074	-1.87559
C	4.4712	1.84179	3.06497
C	4.09148	1.29276	1.85966
C	3.0872	0.29825	1.79063
C	2.42756	-0.10868	2.99
C	2.85589	0.46734	4.20758
C	3.85707	1.41463	4.25104
C	2.68178	-0.31781	0.55585
C	1.31829	-1.05353	2.93052
C	0.87452	-1.56208	1.67132
C	1.62007	-1.19728	0.4959
C	-0.272	-2.38958	1.6296
H	-0.6398	-2.73896	0.67753
C	-0.9363	-2.74916	2.78181
C	-0.4768	-2.2915	4.02502
C	0.61961	-1.45805	4.0907
H	5.2422	2.60475	3.09192
H	4.56482	1.63369	0.95113
H	2.38556	0.17733	5.13805
H	4.15712	1.83819	5.2042
H	-1.81448	-3.38356	2.72227
H	-0.98979	-2.5801	4.93696
H	0.93709	-1.10578	5.06348
C	0.73795	-2.93625	-1.30555
C	1.3486	-4.14174	-0.93245
C	-0.47477	-2.99251	-2.00082
C	0.76428	-5.36413	-1.24552
H	2.28876	-4.12595	-0.39426
C	-1.05941	-4.21841	-2.31574
H	-0.99804	-2.07933	-2.25439
C	-0.44245	-5.40822	-1.94176
H	1.25549	-6.28484	-0.94733
H	-2.0048	-4.23756	-2.84855
H	-0.89804	-6.3623	-2.18705
C	4.70804	0.25758	-1.04873
C	5.71004	-0.60096	-0.5746
C	5.09322	1.42531	-1.71542
C	7.05445	-0.29949	-0.75975
H	5.43724	-1.51347	-0.05735
C	6.44221	1.72651	-1.90171
H	4.34429	2.13167	-2.05015
C	7.42723	0.8663	-1.4273
H	7.81292	-0.97929	-0.38494
H	6.71825	2.64204	-2.41523
H	8.47675	1.10137	-1.57299
C	-0.64104	2.95103	-0.87576
C	-0.08012	4.1829	-0.4792
C	-2.05721	2.89242	-0.90707
C	-0.85422	5.29769	-0.18894
H	0.98704	4.25916	-0.37656
C	-2.82536	4.01407	-0.5844
C	-2.24069	5.2131	-0.21396
H	-0.35936	6.22037	0.09402
H	-3.902	3.92624	-0.67049
H	-2.86049	6.06973	0.02886
O	-2.69024	1.83481	-1.51644
C	-3.85797	1.31387	-0.99296
C	-4.83354	0.91066	-1.89509
C	-4.05674	1.12801	0.37355
C	-6.0108	0.32548	-1.43048
H	-4.66249	1.05497	-2.95632
C	-5.2405	0.55257	0.81799
H	-3.28532	1.41605	1.07771
C	-6.24861	0.13536	-0.06539
H	-5.36823	0.41646	1.88673
H	0.70452	-0.62695	-2.78886
H	2.58996	0.81404	-2.70867
H	-6.74925	0.02293	-2.1625
C	-7.53727	-0.50324	0.48097
C	-8.51672	-0.89238	-0.64014
H	-8.83433	-0.02583	-1.22672
H	-8.08419	-1.62645	-1.32558
H	-9.41607	-1.34006	-0.20874
C	-7.185	-1.78214	1.27428
H	-6.52856	-1.57067	2.12174
H	-8.09183	-2.25126	1.66887
H	-6.67698	-2.51136	0.63741
C	-8.25434	0.49547	1.41741
H	-9.17366	0.05568	1.81698
H	-7.62955	0.78071	2.26711
H	-8.52346	1.41068	0.88284

B2/TS

B3LYP+D3/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	0.79131	-0.59828	1.52726
C	-0.26966	0.20911	0.76154
C	-0.6053	-0.6464	-0.43563
C	0.88879	-1.92516	0.79815
N	-0.09999	-1.98181	-0.22727
O	-1.08261	-0.24608	-1.45653
O	1.6831	-2.78916	1.07481
C	2.06739	0.30342	1.52314
C	0.41071	1.56843	0.39619
C	1.32609	1.67888	1.65772
O	1.43877	2.54219	2.46791
C	5.64538	-1.41134	-0.67663
C	4.54418	-0.93997	0.00222
C	3.63122	-0.05599	-0.61655
C	3.82907	0.31508	-1.98026
C	4.97748	-0.17846	-2.63693
C	5.87102	-1.01509	-2.00283
C	2.48498	0.47613	0.05964
C	2.839	1.13476	-2.66643
C	1.65482	1.55316	-1.98673
C	1.53553	1.23047	-0.59456
C	0.65604	2.24987	-2.7038
H	-0.26095	2.52162	-2.20735
C	0.82919	2.57298	-4.03072
C	2.01026	2.20681	-4.69181
C	2.98479	1.49788	-4.02309
H	6.33221	-2.09168	-0.18492
H	4.36764	-1.25965	1.0172
H	5.16595	0.08678	-3.66855
H	6.74091	-1.37907	-2.53942
H	0.04837	3.10641	-4.562
H	2.15393	2.46675	-5.73535
H	3.87495	1.21062	-4.56638
C	-0.48604	2.74483	0.14983
C	0.06996	4.02886	0.15736
C	-1.85202	2.60308	-0.10655
C	-0.71875	5.145	-0.09303
H	1.12839	4.15228	0.35173
C	-2.64113	3.72286	-0.35992
H	-2.30423	1.62161	-0.16331
C	-2.0795	4.99588	-0.35486
H	-0.27015	6.13272	-0.08548
H	-3.69641	3.59241	-0.57042
H	-2.69592	5.86604	-0.55479
C	3.11209	0.06412	2.57289
C	4.11204	1.02799	2.74729
C	3.12499	-1.07168	3.38405
C	5.10379	0.85636	3.70419
H	4.11689	1.91303	2.1219
C	4.1193	-1.24328	4.3455
H	2.39466	-1.85527	3.23228
C	5.11093	-0.28173	4.50916
H	5.87273	1.61238	3.82282
H	4.12043	-2.13774	4.95959
H	5.88663	-0.41764	5.25541
C	-0.76301	-3.21694	-0.57952
C	-0.20717	-4.43027	-0.13516
C	-1.83538	-3.31962	-1.49949
C	-0.6932	-5.66467	-0.54532
H	0.65081	-4.40674	0.51232
C	-2.29732	-4.56456	-1.91714
C	-1.72851	-5.74498	-1.46627
H	-0.22376	-6.5631	-0.16046
H	-3.14149	-4.56425	-2.59648
H	-2.10027	-6.70231	-1.8134
O	-2.58753	-2.25447	-1.94837
C	-3.41973	-1.6174	-1.05534
C	-3.58342	-1.99576	0.27146
C	-4.09613	-0.4983	-1.54239
C	-4.40953	-1.23828	1.10791
H	-3.08442	-2.87307	0.6624
C	-4.91462	0.23287	-0.6988
H	-3.93865	-0.20524	-2.57306
C	-5.0877	-0.10904	0.6538
H	-5.42373	1.09969	-1.10552
H	-1.17919	0.36642	1.34585
H	0.49418	-0.81401	2.5566
H	-4.51372	-1.56022	2.13615
C	-6.00377	0.73324	1.54895
C	-5.99041	0.25322	3.00763
H	-6.35532	-0.77241	3.10419
H	-4.98827	0.30186	3.4421
H	-6.64196	0.88897	3.6121
C	-5.54572	2.20522	1.52597
H	-5.61455	2.63564	0.52504
H	-6.17349	2.81133	2.18544
H	-4.50938	2.30429	1.85738
C	-7.45035	0.64164	1.02189
H	-8.12485	1.24062	1.64117
H	-7.52924	1.00604	-0.0048
H	-7.80467	-0.39222	1.03451

B2/PD

B3LYP/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	2.80843	0.52503	-1.48119
C	1.87116	-0.59596	-1.9995
C	0.54603	0.09885	-2.2991
C	1.96543	1.79275	-1.49618
N	0.69874	1.46241	-2.00298
O	-0.44778	-0.39629	-2.76814
O	2.3122	2.90311	-1.18167
C	3.31661	0.02854	-0.08255
C	1.88771	-1.70183	-0.88086
C	3.37786	-1.49207	-0.44693
O	4.2856	-2.26063	-0.40072
C	2.19837	2.51241	3.56593
C	2.52395	1.81324	2.42424
C	1.77637	0.68311	2.01761
C	0.63927	0.28837	2.7856
C	0.34612	1.02246	3.95735
C	1.10723	2.10474	4.34654
C	2.09986	-0.08725	0.84725
C	-0.20507	-0.80975	2.33075
C	0.07557	-1.46514	1.09328
C	1.27796	-1.09832	0.39366
C	-0.8248	-2.44619	0.61624
H	-0.64448	-2.91259	-0.34012
C	-1.93141	-2.81743	1.34833
C	-2.17944	-2.21869	2.59124
C	-1.33783	-1.23298	3.06155
H	2.78414	3.37905	3.85407
H	3.35848	2.14264	1.82389
H	-0.50411	0.74892	4.56881
H	0.84974	2.64763	5.25049
H	-2.60738	-3.57185	0.95976
H	-3.041	-2.51811	3.17926
H	-1.56713	-0.77649	4.01571
C	1.56065	-3.11281	-1.30811
C	1.95967	-4.18416	-0.4969
C	0.8875	-3.39562	-2.5018
C	1.6945	-5.49737	-0.86928
H	2.48247	-3.99166	0.43222
C	0.6223	-4.7131	-2.87416
H	0.52168	-2.58702	-3.12281
C	1.02636	-5.76848	-2.06222
H	2.01464	-6.31142	-0.22677
H	0.09216	-4.90921	-3.80081
H	0.82116	-6.79372	-2.35353
C	4.62167	0.5927	0.4251
C	5.29542	-0.07399	1.45779
C	5.20122	1.74763	-0.11109
C	6.51099	0.39964	1.93875
H	4.86712	-0.97093	1.88967
C	6.42107	2.22124	0.37101
H	4.67991	2.31513	-0.87217
C	7.08148	1.54937	1.39486
H	7.01538	-0.13328	2.73845
H	6.84841	3.124	-0.05389
H	8.03086	1.91876	1.76938
C	-0.3099	2.44083	-2.26863
C	-0.05955	3.45155	-3.19351
C	-1.54637	2.38087	-1.6114
C	-1.03415	4.39824	-3.48665
H	0.9067	3.4865	-3.68309
C	-2.53026	3.32257	-1.91994
C	-2.27068	4.32332	-2.85043
H	-0.83034	5.18196	-4.20745
H	-3.48971	3.27286	-1.42069
H	-3.0431	5.05215	-3.07332
O	-1.70087	1.41264	-0.65896
C	-2.99007	1.01147	-0.31782
C	-3.72503	0.21102	-1.18109
C	-3.50799	1.37776	0.91821
C	-4.99899	-0.2113	-0.80367
H	-3.29144	-0.08532	-2.12961
C	-4.77969	0.94448	1.27914
H	-2.91115	1.98937	1.58557
C	-5.55978	0.14686	0.42827
H	-5.16604	1.24183	2.24826
H	2.23398	-1.03467	-2.93238
H	3.66668	0.67944	-2.14013
H	-5.55084	-0.83696	-1.49384
C	-6.96812	-0.29424	0.86524
C	-7.65886	-1.17725	-0.18923
H	-7.78883	-0.65481	-1.14084
H	-7.10292	-2.09917	-0.38049
H	-8.6535	-1.46378	0.16276
C	-6.87671	-1.10273	2.17892
H	-6.43887	-0.51785	2.991
H	-7.87236	-1.42229	2.50217
H	-6.2619	-1.99709	2.04605
C	-7.849	0.955	1.09469
H	-8.85589	0.66299	1.40912
H	-7.43842	1.60863	1.86792
H	-7.94075	1.54454	0.17833

B2/PD

B3LYP+D3/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	3.04282400	-0.50146300	1.20217700
C	2.44109200	0.84115000	1.69122000
C	1.16047900	0.45760700	2.42087200
C	2.11552000	-1.57911000	1.74069000
N	1.09326300	-0.94122900	2.45269500
O	0.34551400	1.19807000	2.90993600
O	2.22212200	-2.77180600	1.60750500
C	3.08708700	-0.37607200	-0.35766800
C	2.23974000	1.70865800	0.40002600
C	3.45465500	1.14478700	-0.40896500
O	4.37029300	1.70101000	-0.92657100
C	0.47685200	-3.25486500	-2.71625700
C	1.25324300	-2.43056700	-1.93096100
C	0.85445500	-1.10369200	-1.64997300
C	-0.39571900	-0.62767700	-2.14649400
C	-1.15200500	-1.49454300	-2.96647500
C	-0.72737400	-2.77539900	-3.25380200
C	1.64844000	-0.20397600	-0.86286500
C	-0.88750200	0.68541800	-1.75039800
C	-0.14038700	1.48151000	-0.82970000
C	1.16430200	1.01727200	-0.44937800
C	-0.70201100	2.68561700	-0.3463660
H	-0.16812800	3.26227700	0.3923650
C	-1.92389600	3.13330400	-0.7989640
C	-2.63258300	2.38613900	-1.7500900
C	-2.12829700	1.18612700	-2.2018400
H	0.79856500	-4.27184400	-2.9146240
H	2.17308000	-2.80834700	-1.5104970
H	-2.10398600	-1.16776900	-3.3635870
H	-1.33680900	-3.41682800	-3.8826990
H	-2.33472600	4.06122100	-0.4146630
H	-3.59421100	2.73552600	-2.11158200
H	-2.72137800	0.61321400	-2.9013920
C	2.22730500	3.20359500	0.56881200
C	2.45640500	4.01566100	-0.5491340
C	1.97256000	3.81298500	1.80124100
C	2.43200900	5.40127400	-0.43674100
H	2.65108400	3.55932900	-1.51198000
C	1.94813900	5.20234800	1.91278400
H	1.73005800	3.20742300	2.66548100
C	2.17895900	6.00111500	0.79619100
H	2.61068500	6.01408400	-1.31441600
H	1.73787600	5.65769000	2.87531000
H	2.15823100	7.08275500	0.88352600
C	4.03558200	-1.26983600	-1.1091750
C	4.33076100	-0.96132100	-2.4430710
C	4.63205500	-2.39415700	-0.5317210
C	5.19927700	-1.75657400	-3.1811380
H	3.87332900	-0.09409300	-2.9049900
C	5.50385200	-3.19139300	-1.2725850
H	4.37521300	-2.68798900	0.47799500
C	5.79165000	-2.87599600	-2.5972310
H	5.41514000	-1.50178400	-4.2137340
H	5.94974300	-4.06661900	-0.8109040
H	6.46892600	-3.49856300	-3.1731670
C	0.02081400	-1.64805200	3.07401800
C	0.21330800	-2.30382100	4.28286300
C	-1.23015300	-1.66535700	2.44729700
C	-0.84484500	-2.97281400	4.89139900
H	1.19583400	-2.27897300	4.74076000
C	-2.29612000	-2.32183400	3.06230400
C	-2.09526700	-2.97099400	4.27807700
H	-0.69460200	-3.48461500	5.83510800
H	-3.26862600	-2.32588600	2.58692000
H	-2.92970700	-3.48296600	4.74616800
O	-1.30507400	-1.03614500	1.23771500
C	-2.56082000	-0.76909800	0.70361000
C	-3.24131000	0.37263200	1.09178900
C	-3.08753500	-1.62175900	-0.2571640
C	-4.46669000	0.66930900	0.49861100
H	-2.79244800	1.03030800	1.82697800
C	-4.30739900	-1.30715100	-0.8428810
H	-2.52454300	-2.49737200	-0.5566670
C	-5.02400300	-0.15481800	-0.4844280
H	-4.69766500	-1.97491700	-1.6033520
H	3.10094300	1.36233500	2.38796900
H	4.05151900	-0.67564300	1.58279100
H	-4.96951300	1.57755600	0.80389300
C	-6.34948800	0.16975000	-1.1911840
C	-6.97680100	1.47963900	-0.6855490
H	-7.20806600	1.43562100	0.38202700
H	-6.32175400	2.33824800	-0.8571770
H	-7.91352900	1.67204600	-1.2153030
C	-6.09605500	0.31627200	-2.7085920
H	-5.70162500	-0.60288100	-3.1478230
H	-7.02578600	0.55908200	-3.2319680
H	-5.37782000	1.11598900	-2.9091530
C	-7.35885500	-0.97347300	-0.9489540
H	-8.30837100	-0.76100500	-1.4501390
H	-6.99096600	-1.92910400	-1.3292930
H	-7.55914900	-1.09606300	0.11886100

C/RC

B3LYP/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	1.54651	1.27455	-1.25285
C	0.87596	-0.11977	-1.36224
C	-0.02797	-0.22505	-0.14022
C	0.98018	1.89162	0.01994
N	0.10475	0.95973	0.59621
O	-0.74537	-1.14627	0.15986
O	1.20903	2.98699	0.46632
C	3.09402	0.99225	-1.25968
C	2.06574	-1.14718	-1.43402
C	3.04717	-0.22955	-2.23359
O	3.59496	-0.40828	-3.27518
C	5.44443	2.18498	2.45874
C	4.70355	1.8618	1.34299
C	4.16951	0.563	1.16641
C	4.3704	-0.41465	2.18872
C	5.14827	-0.04834	3.3108
C	5.68058	1.21659	3.44496
C	3.41661	0.17764	0.00234
C	3.74605	-1.72793	2.07901
C	2.92833	-2.04162	0.95062
C	2.8229	-1.06376	-0.09969
C	2.25315	-3.2847	0.91548
H	1.60287	-3.51229	0.08494
C	2.40353	-4.20896	1.92602
C	3.23904	-3.92338	3.01519
C	3.88655	-2.70824	3.08756
H	5.84071	3.18874	2.57097
H	4.52269	2.61721	0.59378
H	5.33337	-0.76694	4.09858
H	6.27163	1.4625	4.3214
H	1.87299	-5.15409	1.87632
H	3.36861	-4.65135	3.8097
H	4.50885	-2.51123	3.95073
C	1.7918	-2.47836	-2.09158
C	2.87039	-3.25861	-2.53114
C	0.49407	-2.9567	-2.30259
C	2.6567	-4.4793	-3.16179
H	3.88522	-2.90952	-2.38118
C	0.28092	-4.18026	-2.93644
H	-0.35679	-2.40051	-1.92917
C	1.35947	-4.94498	-3.37018
H	3.50652	-5.06612	-3.49553
H	-0.73417	-4.53525	-3.08374
H	1.19281	-5.89684	-3.86437
C	3.99923	2.11215	-1.71383
C	5.307	1.8117	-2.1192
C	3.5747	3.44454	-1.76504
C	6.1633	2.81357	-2.56273
H	5.65885	0.78725	-2.09048
C	4.43416	4.44811	-2.2107
H	2.58861	3.71404	-1.40751
C	5.72936	4.1373	-2.61324
H	7.17141	2.55843	-2.87345
H	4.08685	5.47615	-2.23454
H	6.39751	4.91892	-2.96064
C	-0.66821	1.23435	1.76626
C	-0.05123	1.35952	3.00679
C	-2.05812	1.36591	1.6514
C	-0.81417	1.60008	4.1448
H	1.02591	1.259	3.0707
C	-2.82359	1.59235	2.79504
C	-2.1986	1.70769	4.03324
H	-0.33073	1.69646	5.11036
H	-3.89894	1.68831	2.7065
H	-2.80248	1.8905	4.91614
O	-2.58132	1.3274	0.38578
C	-3.88777	0.87872	0.1963
C	-4.79139	1.75585	-0.38611
C	-4.2288	-0.42979	0.51789
C	-6.09478	1.32757	-0.66065
H	-4.45111	2.75657	-0.6174
C	-5.52549	-0.88355	0.26345
H	-3.46589	-1.07002	0.93987
C	-6.43181	0.01208	-0.32098
H	-7.4387	-0.33358	-0.52474
H	0.25983	-0.21286	-2.25924
H	1.29348	1.92366	-2.09402
C	-7.14618	2.25078	-1.30435
C	-8.33363	2.43368	-0.33239
H	-9.09258	3.08777	-0.77289
H	-8.8155	1.48343	-0.09156
H	-8.00499	2.88567	0.60759
C	-7.65373	1.61991	-2.62059
H	-8.12428	0.64821	-2.4552
H	-8.39657	2.26946	-3.09382
H	-6.8335	1.47455	-3.3287
C	-6.57801	3.64283	-1.63194
H	-6.23424	4.16773	-0.73661
H	-5.74359	3.58862	-2.33636
H	-7.35405	4.26006	-2.09239
C	-5.9701	-2.32115	0.59167
C	-4.8403	-3.14913	1.22886

H	-3.97595	-3.24527	0.56688
H	-4.49632	-2.71557	2.17164
H	-5.1997	-4.15862	1.44627
C	-7.15363	-2.28082	1.58479
H	-8.01296	-1.74154	1.17946
H	-7.48468	-3.29582	1.82551
H	-6.86576	-1.79107	2.51915
C	-6.41428	-3.03348	-0.70573
H	-6.72923	-4.05905	-0.48947
H	-7.25327	-2.52598	-1.18768
H	-5.59501	-3.07803	-1.42836

C/RC

B3LYP+D3/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	-0.36922	0.01363	-1.00419
C	0.0848	-1.26241	-0.25335
C	0.08814	-0.88061	1.21563
C	-0.64136	1.0407	0.07917
N	-0.30791	0.4605	1.30755
O	0.38106	-1.57563	2.15332
O	-1.05611	2.16353	-0.06385
C	0.85116	0.38816	-1.91897
C	1.51727	-1.59161	-0.80985
C	1.28846	-1.0698	-2.26111
O	1.40039	-1.61547	-3.31237
C	2.47901	4.43097	-0.69032
C	1.99436	3.21218	-1.10847
C	2.5096	2.00379	-0.58559
C	3.53157	2.05194	0.41014
C	4.0092	3.32144	0.80484
C	3.50142	4.48543	0.26837
C	2.00325	0.71658	-0.96379
C	4.00645	0.82366	1.03192
C	3.41202	-0.42947	0.6922
C	2.41139	-0.43873	-0.33562
C	3.8132	-1.59375	1.38596
H	3.34107	-2.53592	1.15997
C	4.79403	-1.54393	2.35066
C	5.41286	-0.3238	2.6575
C	5.02041	0.83021	2.01446
H	2.06205	5.34545	-1.09773
H	1.19419	3.17911	-1.83079
H	4.78015	3.39733	1.55976
H	3.88707	5.44387	0.59965
H	5.08413	-2.45011	2.87112
H	6.19439	-0.28266	3.40883
H	5.5092	1.75796	2.27999
C	1.98041	-3.01484	-0.70989
C	3.0532	-3.43623	-1.50335
C	1.38231	-3.93284	0.15666
C	3.51719	-4.74431	-1.43003
H	3.52912	-2.73578	-2.17872
C	1.84746	-5.24399	0.22923
H	0.59461	-3.61124	0.82512
C	2.9145	-5.65481	-0.56388
H	4.35078	-5.05391	-2.0515
H	1.37811	-5.93992	0.91653
H	3.27766	-6.6755	-0.50584
C	0.60834	1.25639	-3.11683
C	1.64522	1.42175	-4.04202
C	-0.60923	1.89523	-3.34995
C	1.46988	2.2155	-5.16829
H	2.5971	0.93175	-3.87076
C	-0.7869	2.69081	-4.47994
H	-1.41152	1.81131	-2.63133
C	0.25097	2.85488	-5.39158
H	2.28505	2.33549	-5.87397
H	-1.73832	3.18745	-4.63903
H	0.11406	3.47684	-6.26987
C	-0.40597	1.15174	2.54818
C	0.44356	2.22534	2.79655
C	-1.33607	0.74723	3.51476
C	0.38687	2.8916	4.01486
H	1.15243	2.51742	2.03091
C	-1.37817	1.4079	4.73914
C	-0.51781	2.47188	4.9884
H	1.05348	3.72467	4.2051
H	-2.09524	1.07118	5.47833
H	-0.56254	2.98037	5.94538
O	-2.18159	-0.31982	3.33363
C	-2.87788	-0.42013	2.13692
C	-3.49775	0.68819	1.57708
C	-2.92908	-1.67148	1.53587
C	-4.16453	0.56349	0.35797
H	-3.42208	1.63971	2.08325
C	-3.59077	-1.82412	0.31573
H	-2.41812	-2.48771	2.02625
C	-4.19006	-0.69434	-0.25357
H	-4.70292	-0.79882	-1.20151
H	-0.58982	-2.10147	-0.41089
H	-1.27115	-0.14392	-1.59564
C	-4.84997	1.75735	-0.31941
C	-6.34423	1.43943	-0.52485
H	-6.85292	2.28786	-0.99168
H	-6.4921	0.56985	-1.16887
H	-6.83441	1.23312	0.43002
C	-4.18087	2.0204	-1.68343
H	-4.22281	1.14613	-2.33746
H	-4.6803	2.84561	-2.19975
H	-3.13507	2.29359	-1.53831
C	-4.73322	3.04124	0.51518
H	-5.20981	2.93618	1.49358
H	-3.69036	3.32838	0.6659
H	-5.23077	3.86383	-0.00461
C	-3.68454	-3.1777	-0.40259
C	-2.8865	-4.27595	0.31578

H	-1.82199	-4.03742	0.38054
H	-3.25588	-4.45189	1.32873
H	-2.97476	-5.21614	-0.23374
C	-5.16518	-3.60886	-0.45173
H	-5.7774	-2.88584	-0.99485
H	-5.26665	-4.57699	-0.9509
H	-5.57597	-3.70082	0.55675
C	-3.14477	-3.05382	-1.84193
H	-3.23203	-4.01064	-2.36364
H	-3.69186	-2.31018	-2.42396
H	-2.08903	-2.77098	-1.85092

C/TS

B3LYP/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	-2.4917	-0.23937	-1.92297
C	-1.32085	0.7315	-1.71817
C	-0.17969	-0.13165	-1.21127
C	-1.91858	-1.61935	-1.65451
N	-0.5506	-1.51951	-1.26096
O	0.82208	0.3022	-0.71539
O	-2.55665	-2.63444	-1.79349
C	-3.62799	0.27326	-0.96361
C	-1.83429	1.81452	-0.69735
C	-3.3297	1.79834	-1.1503
O	-4.03639	2.67983	-1.5245
C	-4.86227	-2.52188	2.40834
C	-4.47572	-1.71544	1.36014
C	-3.51345	-0.6932	1.53736
C	-2.90498	-0.52536	2.81822
C	-3.33907	-1.36253	3.87099
C	-4.29831	-2.33426	3.67841
C	-3.0984	0.18152	0.47365
C	-1.83677	0.45099	2.99861
C	-1.37755	1.22602	1.88991
C	-2.07108	1.0881	0.63706
C	-0.26694	2.08481	2.06473
H	0.11569	2.63655	1.22031
C	0.34401	2.22231	3.29213
C	-0.13343	1.50003	4.39548
C	-1.19317	0.63095	4.24413
H	-5.59935	-3.30154	2.24668
H	-4.90914	-1.87353	0.384
H	-2.90621	-1.25955	4.85744
H	-4.60394	-2.96198	4.50937
H	1.19328	2.88884	3.4004
H	0.33701	1.61281	5.36704
H	-1.52579	0.07393	5.11027
C	-1.19095	3.17917	-0.74107
C	-1.85569	4.26508	-0.15421
C	0.03813	3.41207	-1.36733
C	-1.30807	5.54258	-0.19319
H	-2.80963	4.11195	0.33619
C	0.58598	4.69354	-1.40778
H	0.60161	2.5865	-1.78363
C	-0.08456	5.76359	-0.8233
H	-1.8412	6.36842	0.26688
H	1.54464	4.849	-1.89235
H	0.34233	6.76093	-0.85514
C	-5.05313	-0.10728	-1.28577
C	-6.09449	0.5947	-0.6624
C	-5.38226	-1.10716	-2.20677
C	-7.42316	0.30391	-0.94917
H	-5.86414	1.375	0.05394
C	-6.71578	-1.39733	-2.49503
H	-4.60211	-1.69942	-2.66782
C	-7.74027	-0.69358	-1.87008
H	-8.21285	0.86084	-0.45512
H	-6.94874	-2.18255	-3.20726
H	-8.77751	-0.92024	-2.09538
C	0.35867	-2.64984	-1.41092
C	-0.18653	-3.94743	-1.31338
C	1.77139	-2.55969	-1.32901
C	0.6019	-5.08391	-1.20253
H	-1.2548	-4.06361	-1.30423
C	2.55191	-3.71099	-1.19005
C	1.9838	-4.97099	-1.11459
H	0.11922	-6.05363	-1.14803
H	3.62835	-3.58737	-1.17952
H	2.6139	-5.84793	-1.00994
O	2.41072	-1.38859	-1.65634
C	3.5268	-0.96945	-0.9517
C	4.53887	-0.37825	-1.69889
C	3.6102	-1.07527	0.43222
C	5.67644	0.12386	-1.06154
H	4.40748	-0.32493	-2.77137
C	4.73832	-0.58794	1.09693
H	2.78491	-1.51895	0.97092
C	5.75197	0.00279	0.33137
H	6.62982	0.38484	0.83956
H	-1.00968	1.21072	-2.64994
H	-2.86704	-0.24096	-2.94909
C	6.82793	0.78743	-1.83987
C	8.13921	0.00886	-1.58959
H	8.9661	0.46202	-2.14554
H	8.41671	0.00314	-0.53314
H	8.04612	-1.03147	-1.9131
C	7.00006	2.24654	-1.36094
H	7.23508	2.3021	-0.29571
H	7.81388	2.73561	-1.90565
H	6.08682	2.82401	-1.52842
C	6.57095	0.81088	-3.35697
H	6.4653	-0.196	-3.77007
H	5.67177	1.37811	-3.61207
H	7.41238	1.28659	-3.86787
C	4.88446	-0.67056	2.62854
C	3.67671	-1.35073	3.29727

H	2.74668	-0.80512	3.11896
H	3.54123	-2.37864	2.95007
H	3.82893	-1.39042	4.37946
C	6.14923	-1.48451	2.98374
H	7.05703	-1.03072	2.57973
H	6.26844	-1.55117	4.06977
H	6.08442	-2.50244	2.58941
C	5.01233	0.75485	3.21157
H	5.11642	0.71451	4.30055
H	5.88312	1.28241	2.816
H	4.12715	1.3526	2.97858

C/TS

B3LYP+D3/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	-0.90045	-1.07757	-0.94599
C	0.04375	0.09694	-0.65438
C	0.43032	-0.06719	0.79596
C	-0.98297	-1.85835	0.35341
N	-0.06826	-1.32096	1.31712
O	0.92744	0.78977	1.46942
O	-1.72098	-2.79769	0.51412
C	-2.24288	-0.43195	-1.43124
C	-0.79864	1.38593	-0.94614
C	-1.61526	0.80962	-2.14529
O	-1.73556	1.20319	-3.26178
C	-5.91724	-1.28634	1.11359
C	-4.78769	-1.07401	0.3546
C	-3.9706	0.0618	0.56165
C	-4.29622	0.97594	1.60997
C	-5.47298	0.73204	2.35399
C	-6.2713	-0.36597	2.11122
C	-2.8054	0.33863	-0.22964
C	-3.39937	2.08387	1.91999
C	-2.19448	2.26267	1.17389
C	-1.96122	1.38939	0.05837
C	-1.27727	3.26345	1.57026
H	-0.33961	3.35979	1.04655
C	-1.55104	4.10062	2.6289
C	-2.75681	3.96572	3.33292
C	-3.65131	2.97443	2.98828
H	-6.52783	-2.16602	0.93887
H	-4.51705	-1.79142	-0.40413
H	-5.76254	1.40955	3.14659
H	-7.16579	-0.52308	2.70549
H	-0.82996	4.85776	2.91855
H	-2.98081	4.62849	4.1627
H	-4.55861	2.87884	3.57026
C	-0.0718	2.66714	-1.24619
C	-0.80201	3.72435	-1.8042
C	1.28673	2.85608	-0.97599
C	-0.19501	4.94383	-2.0791
H	-1.85657	3.59059	-2.01553
C	1.89247	4.08344	-1.24624
H	1.86655	2.07191	-0.50405
C	1.15745	5.12899	-1.79756
H	-0.77907	5.75065	-2.50984
H	2.94146	4.22612	-1.01338
H	1.63393	6.08209	-2.00355
C	-3.14916	-1.25503	-2.30463
C	-4.16652	-0.60508	-3.01528
C	-3.01806	-2.64011	-2.43767
C	-5.03053	-1.32162	-3.83504
H	-4.28254	0.46828	-2.92184
C	-3.88414	-3.35851	-3.2608
H	-2.2777	-3.17351	-1.85563
C	-4.89171	-2.70328	-3.96272
H	-5.81318	-0.80014	-4.37654
H	-3.77311	-4.435	-3.34348
H	-5.56673	-3.26352	-4.60174
C	0.66438	-2.22131	2.18866
C	0.07447	-3.4529	2.53116
C	1.78363	-1.83224	2.97038
C	0.58334	-4.27156	3.53288
H	-0.82644	-3.75948	2.02993
C	2.26533	-2.64862	3.98944
C	1.66536	-3.86014	4.2991
H	0.08868	-5.21534	3.73557
H	3.15404	-2.30463	4.50575
H	2.05234	-4.47558	5.10381
O	2.59767	-0.7564	2.67342
C	3.26824	-0.74213	1.46493
C	3.19379	-1.7708	0.52965
C	4.00368	0.41159	1.20552
C	3.83762	-1.63915	-0.70575
H	2.63793	-2.66412	0.76539
C	4.67865	0.55468	-0.00541
H	3.99705	1.18258	1.96293
C	4.57393	-0.47876	-0.94863
H	5.08101	-0.37237	-1.89895
H	0.9518	0.07722	-1.26189
H	-0.50555	-1.75462	-1.70799
C	3.71698	-2.71519	-1.79796
C	5.12194	-3.19721	-2.2182
H	5.04717	-3.96959	-2.98976
H	5.72946	-2.38538	-2.62356
H	5.65912	-3.62035	-1.36529
C	2.99438	-2.10546	-3.02005
H	3.53332	-1.24662	-3.4254
H	2.89351	-2.84601	-3.81925
H	1.98937	-1.76638	-2.74952
C	2.91187	-3.94125	-1.33166
H	3.37233	-4.42956	-0.4688
H	1.88303	-3.68242	-1.06427
H	2.86025	-4.67852	-2.13697
C	5.54824	1.78364	-0.31411
C	5.30081	2.93163	0.68072

H	4.24984	3.23093	0.70437
H	5.59513	2.66204	1.69793
H	5.8927	3.80549	0.39589
C	7.03264	1.36557	-0.22102
H	7.26405	0.56434	-0.92738
H	7.68696	2.21409	-0.44546
H	7.27496	1.00516	0.78229
C	5.26128	2.30586	-1.73923
H	5.81022	3.23463	-1.92025
H	5.57268	1.59711	-2.50916
H	4.19827	2.505	-1.88663

C/PD

B3LYP/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	-3.12738	0.1041	-1.61058
C	-2.30909	1.41834	-1.52433
C	-0.93314	1.06878	-2.08453
C	-2.18195	-0.91806	-2.22794
N	-0.96423	-0.27316	-2.49207
O	0.00875	1.80803	-2.22379
O	-2.42446	-2.06678	-2.49958
C	-3.62538	-0.16836	-0.14787
C	-2.39959	1.8701	-0.02015
C	-3.84628	1.33187	0.24038
O	-4.82359	1.89329	0.6234
C	-2.1333	-3.94535	1.91091
C	-2.56869	-2.82902	1.23082
C	-1.95434	-1.56865	1.41958
C	-0.83863	-1.46442	2.3041
C	-0.43023	-2.62912	2.99319
C	-1.06222	-3.84134	2.81003
C	-2.39261	-0.37709	0.74415
C	-0.12879	-0.1985	2.44033
C	-0.51348	0.92804	1.65148
C	-1.69225	0.80818	0.8355
C	0.26318	2.10872	1.71649
H	0.00462	2.9496	1.09156
C	1.34501	2.20719	2.56403
C	1.69242	1.12343	3.3827
C	0.9734	-0.05083	3.31222
H	-2.6171	-4.90208	1.74419
H	-3.38637	-2.92168	0.5321
H	0.40916	-2.58735	3.67518
H	-0.71807	-4.71617	3.35251
H	1.9214	3.12581	2.59919
H	2.5337	1.20109	4.06375
H	1.27414	-0.87412	3.94704
C	-2.22472	3.34356	0.26064
C	-2.71693	3.87965	1.45887
C	-1.5991	4.2057	-0.64714
C	-2.58787	5.23579	1.73881
H	-3.20681	3.23479	2.17824
C	-1.47048	5.56516	-0.3651
H	-1.16261	3.81173	-1.55681
C	-1.96588	6.08624	0.82628
H	-2.97832	5.62951	2.67182
H	-0.97499	6.21392	-1.08049
H	-1.86708	7.14485	1.04459
C	-4.85098	-1.03432	0.01966
C	-5.55366	-0.99427	1.23189
C	-5.33018	-1.86282	-1.00079
C	-6.69991	-1.75913	1.41732
H	-5.20439	-0.35858	2.03707
C	-6.48033	-2.62892	-0.81409
H	-4.77958	-1.9553	-1.9287
C	-7.17068	-2.579	0.39298
H	-7.22892	-1.71112	2.36378
H	-6.82942	-3.27128	-1.61636
H	-8.06592	-3.17543	0.53728
C	0.10952	-0.90139	-3.1987
C	-0.07209	-1.27743	-4.52676
C	1.33726	-1.13156	-2.56328
C	0.96335	-1.86818	-5.24196
H	-1.03327	-1.09852	-4.99509
C	2.38175	-1.70997	-3.28836
C	2.19032	-2.07519	-4.61683
H	0.81372	-2.15811	-6.2758
H	3.33542	-1.8793	-2.80482
H	3.01006	-2.52972	-5.1637
O	1.42476	-0.80177	-1.2409
C	2.69034	-0.61509	-0.68156
C	3.37047	0.56923	-0.93168
C	3.20365	-1.60462	0.14339
C	4.62103	0.78113	-0.34505
H	2.89517	1.30313	-1.56885
C	4.45336	-1.42184	0.74574
H	2.61088	-2.49599	0.30008
C	5.13503	-0.22807	0.48091
H	6.10434	-0.07366	0.9411
H	-2.73297	2.20453	-2.15419
H	-3.99467	0.20284	-2.26853
C	5.42755	2.07292	-0.57458
C	6.78706	1.72574	-1.22177
H	7.37152	2.63506	-1.39346
H	7.38525	1.06404	-0.59111
H	6.64732	1.22849	-2.18549
C	5.67086	2.77849	0.77867
H	6.23472	2.15146	1.47325
H	6.23991	3.70165	0.63113
H	4.72426	3.03853	1.25979
C	4.69489	3.05888	-1.50149
H	4.52066	2.63631	-2.49457
H	3.72941	3.36699	-1.09234
H	5.29852	3.96113	-1.63222
C	5.07916	-2.47669	1.6772
C	4.20407	-3.73659	1.80199

H	3.21832	-3.51349	2.21825
H	4.05877	-4.2314	0.83779
H	4.68538	-4.45695	2.46907
C	6.45852	-2.90588	1.12903
H	7.15555	-2.06713	1.06816
H	6.90964	-3.66197	1.77904
H	6.36767	-3.3346	0.12726
C	5.25589	-1.87221	3.08854
H	5.69377	-2.60866	3.76967
H	5.91181	-0.99867	3.07945
H	4.29363	-1.55834	3.50209

C/PD

B3LYP+D3/6-311+G(d,p), C1

Atom	Cartesian (Hartree/Bohr)		
	X	Y	Z
C	3.28261	0.03384	1.49163
C	2.48356	1.36162	1.53621
C	1.13352	0.98547	2.13176
C	2.39838	-0.99298	2.17274
N	1.19102	-0.36405	2.49638
O	0.18031	1.70464	2.29673
O	2.66065	-2.14326	2.41623
C	3.52851	-0.22283	-0.0318
C	2.42597	1.87229	0.05365
C	3.78857	1.27045	-0.42443
O	4.73161	1.78136	-0.93853
C	1.43814	-3.9001	-1.67846
C	2.07008	-2.80885	-1.12463
C	1.53491	-1.50874	-1.26652
C	0.30262	-1.32944	-1.96159
C	-0.30036	-2.46807	-2.53698
C	0.25118	-3.72515	-2.40498
C	2.16146	-0.34587	-0.713
C	-0.32442	-0.01782	-2.01683
C	0.26071	1.08617	-1.32757
C	1.53739	0.88172	-0.70845
C	-0.42545	2.32137	-1.29815
H	-0.01051	3.14938	-0.74725
C	-1.61969	2.48573	-1.96178
C	-2.18158	1.41578	-2.67117
C	-1.547	0.19431	-2.68933
H	1.86014	-4.89092	-1.55023
H	2.97926	-2.95045	-0.56064
H	-1.22344	-2.36655	-3.08861
H	-0.24298	-4.57944	-2.8562
H	-2.12279	3.44568	-1.92989
H	-3.12611	1.53848	-3.18909
H	-2.01605	-0.61884	-3.22456
C	2.26478	3.3495	-0.15435
C	2.61123	3.90494	-1.39113
C	1.74856	4.18572	0.83883
C	2.44243	5.26378	-1.62894
H	3.00792	3.26933	-2.17251
C	1.57865	5.5475	0.59904
H	1.41788	3.76713	1.78071
C	1.92527	6.09144	-0.63407
H	2.71468	5.67746	-2.59419
H	1.1648	6.17998	1.3774
H	1.79128	7.15172	-0.82109
C	4.62556	-1.16953	-0.4215
C	5.03095	-1.20134	-1.76062
C	5.25426	-2.01641	0.49306
C	6.0373	-2.06321	-2.17687
H	4.54752	-0.55172	-2.48102
C	6.26421	-2.88119	0.07481
H	4.92063	-2.04963	1.52184
C	6.6593	-2.90772	-1.25858
H	6.33703	-2.07653	-3.21943
H	6.73447	-3.54148	0.79594
H	7.4437	-3.5835	-1.58292
C	0.10997	-1.04521	3.12647
C	0.22377	-1.45877	4.4484
C	-1.06487	-1.28109	2.4072
C	-0.84272	-2.08963	5.07815
H	1.15182	-1.27333	4.97632
C	-2.14435	-1.89147	3.04671
C	-2.02644	-2.29289	4.37318
H	-0.75269	-2.41087	6.10924
H	-3.0648	-2.05339	2.50146
H	-2.8707	-2.77286	4.85651
O	-1.07253	-0.91386	1.08997
C	-2.31829	-0.63421	0.52797
C	-2.86477	0.62476	0.73771
C	-2.96296	-1.60907	-0.20832
C	-4.11466	0.9222	0.20391
H	-2.28915	1.33614	1.3129
C	-4.22854	-1.33974	-0.7483
H	-2.47027	-2.5642	-0.34052
C	-4.77588	-0.07653	-0.52802
H	-5.75503	0.14563	-0.92781
H	2.95754	2.1107	2.17299
H	4.24029	0.09425	2.01152
C	-4.80015	2.27318	0.44482
C	-6.01801	2.04684	1.36501
H	-6.5273	2.99364	1.56903
H	-6.7429	1.36659	0.91172
H	-5.70786	1.61504	2.3199
C	-5.28161	2.88045	-0.88751
H	-5.99879	2.23598	-1.39962
H	-5.774	3.8404	-0.70817
H	-4.44416	3.05179	-1.56534
C	-3.86003	3.28227	1.12215
H	-3.56049	2.95527	2.12033
H	-2.9525	3.44647	0.5376
H	-4.36802	4.24372	1.23255
C	-4.97578	-2.44179	-1.51084
C	-4.12243	-2.92846	-2.6976

H	-3.92291	-2.11027	-3.39479
H	-3.16495	-3.33364	-2.36741
H	-4.64435	-3.71759	-3.24642
C	-5.23283	-3.62427	-0.55397
H	-5.83331	-3.30676	0.30245
H	-5.77127	-4.4259	-1.06837
H	-4.29983	-4.04202	-0.16998
C	-6.32736	-1.96283	-2.0597
H	-6.81457	-2.77669	-2.60226
H	-7.00565	-1.65058	-1.26179
H	-6.21116	-1.12695	-2.75463
