

Supplementary Information for:

Role of Explicit Solvation and Level of Theory in
Predicting the Aqueous Reduction Potential of
Carbonate Radical Anion by DFT

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Table S1

Calculated Reduction Potentials (in Volts) and Errors. Each value is an average of three optimized geometries. Errors reported are standard deviations of replicates. †Only one optimized geometry

Number of Explicit Waters	B3LYP (V)	B3LYP Error (V)	ω 97BX -D (V)	ω 97BX -D Error (V)	M06-2X (V)	M06-2X Error (V)	M06 (V)	M06 Error (V)	M06-L (V)	M06-L Error (V)
0	0.4220 [†]	0								
3	0.6778	0.0612			1.1727	0.1161	0.8764	0.0847	0.3423	0.1068
6	0.9455	0.0594	1.0964	0.0284	1.3790	0.0307	1.1650	0.0632	0.6171	0.0266
9	1.0528	0.0304			1.5012	0.0488	1.2947	0.0164	0.7135	0.0239
12	1.1185	0.0738	1.4245	0.0781	1.6764	0.0205	1.3856	0.0617	0.8415	0.0327
15					1.8950	0.1168	1.7039	0.0434	1.0315	0.0696
18	1.1700	0.0344	1.5381	0.1018						
24	1.1863	0.1052	1.6395	0.1327	2.0503	0.0844	1.6325	0.1483	1.0852	0.1214
27	1.4094	0.0803								
30	1.2044	0.1170								

Table S2

Results of natural bond order (NBO) calculations. All values are the total charge located on the carbonate ion or radical species.

Number of Explicit Waters	B3LYP Ion form	B3LYP Radical Form	ω 97BX-D ion	ω 97BX-D radical	M06-2X ion	M06-2X radical
0	-1.999	-1				
3	-1.850	-0.96467			-1.82767	-0.96267
6	-1.735	-0.931	-1.75667	-0.93067	-1.76067	-0.943
9	-1.722	-0.926			-1.75067	-0.92767
12	-1.684	-0.913	-1.68633	-0.90333	-1.72333	-0.93333
15					-1.712	-0.926
18	-1.668	-0.915	-1.64933	-0.887		
24	-1.663	-0.912	-1.655	-0.89567		
27	-1.666	-0.914				
30	-1.672	-0.916				

Table S3

Calculated Reduction Potentials (in Volts) and Errors for the M06 functional variants with GD3 dispersion corrections applied after the optimization. Each data point is the average of three optimized geometries.

Number of Explicit Water	M06-2X No GD3 (V)	M06-2X With GD3 (V)	Percent Difference	M06 No GD3 (V)	M06 With GD3 (V)	Percent Difference	M06-L No GD3 (V)	M06-L With GD3 (V)	Percent Difference
3	1.1727	1.1721	-0.0510	0.8972	0.8997	0.2769	0.4558	0.4556	-0.0477
6	1.3790	1.3784	-0.0493	1.1634	1.1684	0.4272	0.6758	0.6762	0.0617
9	1.5012	1.5010	-0.0181	1.2845	1.3070	1.7483	0.8567	0.8548	-0.2233
12	1.6764	1.6761	-0.0211	1.4073	1.4095	0.1527	0.9049	0.9044	-0.0501
15	1.8950	1.8962	0.06748	1.7857	1.7945	0.4932	1.1913	1.1936	0.1941

Table S4

Calculated Reduction Potentials (in Volts) and Errors for the B3LYP functional with dispersion corrections applied throughout the optimization. Each data point is the average of three optimized geometries. †Only two optimized geometries were found, data value is average of two geometries.

Number of Explicit Water Molecules	B3LYP with GD2 (V)	B3LYP with GD2 error (V)	B3LYP with GD3 (V)	B3LYP with GD3 error (V)	B3LYP with GD3BJ (V)	B3LYP with GD3BJ error (V)
9	1.138162	0.049394	1.059803	0.053526	1.094824	0.015901
12	1.279	0.035603	1.219207	0.035037	1.207914	0.056232
18	1.368335	0.122178	1.355854	0.082883	1.308823	0.102223
24	1.545957†	0.079308	1.557635	0.099616	1.551948	0.132762
27	1.662227†	0.053171	1.474078	0.03616	1.57632	0.067161

Optimized Geometries and Energies

The nomenclature is as follows: The functional used is listed first, the following number is the number of explicit water molecules included, the s1, s2, and s3, denote the replicate number.

Eopt is the energy of the system in Hartrees/particle. D2, D3, D3BJ indicate the corresponding dispersion correction was applied throughout optimization. Reduction potentials were calculated between matching replicates (e.x. s1 and radical s1).

B3LYP_3_s1 Eopt -493.58888
 O -1.988639 -1.308930 -0.957581
 O -1.037023 -1.053559 0.997368
 O -2.009852 0.667194 -0.001609
 O 0.250694 2.429212 -0.326128
 H 0.506485 2.450934 -1.255316
 H -0.557914 1.886697 -0.300443
 O 1.575393 0.288290 0.997987
 H 0.784745 -0.270965 1.072853
 H 1.247426 1.078645 0.525770
 O 3.373686 -1.000190 -0.702687
 H 4.019407 -1.424927 -0.128350
 H 2.744224 -0.559608 -0.093503
 C -1.676406 -0.556151 0.020029

B3LYP_3_s2 Eopt -493.594596
 C 0.003684 0.000144 -0.047351
 O 0.422909 1.230820 -0.046862
 O -1.271834 -0.251740 -0.087141
 O 0.859365 -0.976392 -0.009710
 O 3.434038 -0.355887 0.033863
 H 2.442601 -0.527655 0.015736
 H 3.521865 0.607005 0.037376
 O -1.416040 3.135299 0.072502
 H -2.283641 2.715289 -0.011048
 H -0.757412 2.376910 0.016934
 O -2.030736 -2.782924 0.047917
 H -1.237080 -3.328547 0.141887
 H -1.690055 -1.837283 -0.001330

B3LYP_3_s3 Eopt -493.587193
 C 2.654323 -0.058632 -0.009988
 O 2.384963 -1.324933 -0.001239
 O 3.885590 0.340768 -0.037596
 O 1.693121 0.808010 0.009276
 O -0.792624 -0.118608 0.078764
 H 0.164762 0.171678 0.053286
 H -0.758771 -1.080562 0.075653
 O -3.203704 1.713467 -0.015874
 H -2.369995 1.237533 -0.011830
 H -3.033389 2.658231 -0.012021
 O -4.267134 -1.445355 -0.031971
 H -3.433425 -1.921289 -0.027927
 H -4.096819 -0.500591 -0.028118

B3LYP_6_s1 Eopt -722.979325

O 1.571023 1.082408 0.173294
 O -0.616449 1.338182 -0.197962
 O 0.382378 -0.594175 -0.734458
 O 2.581379 -2.180098 -0.920495
 O 3.927673 -0.121933 0.581975
 O -0.503689 3.831242 0.786056
 H 3.028914 0.281443 0.438201
 H 3.234505 -1.660087 -0.422379
 H 0.273629 4.271147 0.427391
 H -0.470623 2.907443 0.420206
 H 3.930170 -0.415126 1.499315
 H 1.774998 -1.609858 -0.864882
 O -2.349821 -2.475430 2.015025
 O -1.998821 -1.828502 -0.655254
 O -3.082937 0.778680 -1.110835
 H -1.109672 -1.383293 -0.684009
 H -2.166183 0.970034 -0.776649
 H -2.212865 -2.263654 1.064316
 H -3.674587 1.079112 -0.412820
 H -2.608137 -1.084054 -0.805802
 H -2.012646 -3.370836 2.122435
 C 0.454437 0.605790 -0.250682

B3LYP_6_s2 Eopt -722.979661
 O -0.632819 1.421024 0.143729
 O 1.458602 0.662310 -0.040872
 O -0.253108 -0.786927 0.022424
 O -2.443159 -1.039190 -1.684058
 O -3.282651 1.295405 -0.223232
 O 2.273298 3.215087 0.180190
 H -2.297315 1.321700 -0.079644
 H -2.946243 -0.274281 -1.355138
 H 1.508162 3.790950 0.082802
 H 1.911038 2.293373 0.098983
 H -3.481577 2.066982 -0.764158
 H -1.640469 -1.011779 -1.119013
 O 1.455401 -2.915159 -0.069610
 O 3.601390 -0.983722 -0.136142
 H 0.827931 -2.153217 -0.036654
 H 2.797117 -0.404451 -0.128682
 H 3.921699 -0.961234 -1.044278
 H 2.319629 -2.471697 -0.107649
 C 0.187005 0.438278 0.041937
 O -2.135665 -1.254338 1.957221
 H -1.482342 -1.052720 1.245799
 H -2.889969 -0.689218 1.758805

B3LYP_6_s3 Eopt -722.978069

O	-0.598137	-1.752090	0.014513
O	1.171649	-0.527821	-0.582476
O	-0.879917	0.387186	-0.608539
O	-3.537118	-0.048199	-0.914788
O	-3.061060	-2.200843	0.946747
O	3.564953	-3.530062	0.668998
H	-2.148898	-2.011439	0.588107
H	-3.664248	-0.821594	-0.341235
H	4.203523	-4.208626	0.913539
H	3.743425	-2.801927	1.274773
H	-3.256769	-3.104534	0.677538
H	-2.565491	0.121390	-0.822858
O	0.335800	3.561751	2.208296
O	0.198634	2.837211	-0.459245
O	2.596305	1.585779	-1.354255
H	-0.214252	1.932432	-0.504538
H	2.041714	0.807652	-1.063265
H	0.263047	3.292834	1.264785
H	3.323862	1.629114	-0.725079
H	1.114550	2.660474	-0.740232
H	-0.560611	3.793720	2.471802
C	-0.101455	-0.632133	-0.391225

B3LYP_9_s1 Eopt -952.360202

O	0.366014	0.809133	-1.074786
O	0.751594	-1.392341	-0.947969
O	0.159723	-0.260831	0.889419
O	-1.123083	-2.388885	1.913058
H	-0.585845	-1.658266	1.505489
H	-0.594430	-3.186947	1.808220
O	3.492982	-1.544185	-0.422771
H	2.538137	-1.563088	-0.645857
H	3.520484	-1.050716	0.409298
O	-1.401987	-2.714962	-2.116108
H	-2.062418	-2.724530	-1.400284
H	-0.637026	-2.236810	-1.732661
O	-0.695969	3.052777	-0.032294
H	-0.306224	2.223301	-0.415691
H	-0.908622	2.784938	0.879691
O	2.764627	0.685688	1.676043
H	1.855895	0.353238	1.542801
H	2.982528	1.094570	0.821753
O	-1.041842	1.634908	2.420424
H	-1.971839	1.393159	2.481468
H	-0.631333	0.946048	1.840736
O	3.114610	1.392475	-1.225477
H	3.457688	0.485997	-1.201664
H	2.142656	1.264328	-1.253661
O	-3.231044	-2.682681	0.117858
H	-2.498963	-2.565310	0.765641
H	-3.606023	-1.804773	0.002582
O	-3.150097	3.501306	-1.218590
H	-2.265231	3.339899	-0.819750
H	-2.967505	3.849527	-2.097197
C	0.415640	-0.280629	-0.386897

B3LYP_9_s2 Eopt -952.355072

O	-0.038445	0.196167	-1.036914
O	0.355876	-1.900250	-0.790558
O	0.152703	-0.635977	1.023766
O	-2.212057	-1.746561	2.209629
H	-1.353816	-1.442963	1.863236
H	-2.155021	-2.709256	2.204807
O	3.358996	-2.027802	-0.736086
H	2.413962	-2.174456	-0.892003
H	3.384293	-1.637739	0.154312
O	-2.307456	-2.747599	-1.898333
H	-2.812124	-2.164264	-1.297039

H	-1.385990	-2.594031	-1.645929
O	0.244687	3.051098	-0.268975
H	0.226600	2.192787	-0.717736
H	0.117230	2.809359	0.670339
O	3.097257	-0.183417	1.569733
H	2.144030	-0.355499	1.604634
H	3.195916	0.392470	0.792953
O	-0.073257	1.938076	2.308483
H	-0.984786	2.057032	2.598885
H	-0.051523	1.053492	1.900045
O	3.191252	0.862382	-1.217741
H	3.285205	-0.105033	-1.276344
H	2.239227	1.011357	-1.283045
O	-3.663951	-1.037752	-0.093806
H	-3.183260	-1.282078	0.725062
H	-3.303674	-0.178708	-0.342538
O	-2.055104	4.372896	-1.165834
H	-1.243980	3.911609	-0.866498
H	-1.848736	4.688357	-2.051904
C	0.152072	-0.767086	-0.228026

B3LYP_9_s3 Eopt -952.358058

O	-0.471535	0.700739	-1.015308
O	1.689506	0.268867	-1.381365
O	0.537396	-0.964779	0.098467
O	2.523281	-2.533567	1.082777
H	1.829907	-1.923419	0.726283
H	2.863068	-2.095997	1.870714
O	2.638000	2.778161	-0.820199
H	2.319648	1.871396	-1.046078
H	3.384271	2.641827	-0.226434
O	3.851001	-1.381293	-1.203015
H	3.630755	-1.906949	-0.415633
H	3.068496	-0.783230	-1.281363
O	-2.832219	-0.221733	-0.148535
H	-1.955406	0.145702	-0.451689
H	-2.632479	-1.168246	-0.024424
O	0.334039	0.697657	2.436461
H	0.403693	0.030929	1.724475
H	0.340017	1.542700	1.947823
O	-1.532922	-2.727920	0.219983
H	-1.527840	-3.242311	-0.594400
H	-0.773329	-2.100046	0.137117
O	0.153455	2.937177	0.608260
H	1.054289	3.050521	0.251579
H	-0.213062	2.238867	0.028434
O	-4.712920	0.013794	-2.178665
H	-4.016735	-0.078449	-1.492456
H	-4.246958	-0.065929	-3.017557
C	0.584996	-0.001095	-0.773197
O	-2.524691	0.551223	2.580363
H	-1.550742	0.609107	2.613061
H	-2.706698	0.293484	1.655949

B3LYP_12_s1 Eopt -1181.741917

O	1.117689	-0.714549	-0.734487
O	-0.860036	-0.029876	0.044867
O	0.980741	1.197550	0.412610
O	-1.120179	-0.508383	2.763416
H	-1.099734	-0.325673	1.796797
H	-0.188463	-0.377418	3.024398
O	3.804759	-0.827250	-0.667160
H	2.825735	-0.670208	-0.659131
H	4.215540	0.055599	-0.749367
O	-3.544935	-0.239630	-2.389939
H	-3.187291	-1.005639	-1.898608
H	-3.421240	0.506053	-1.772077
O	1.018336	-3.247334	0.413080
H	0.214392	-3.282524	0.968742
H	1.001141	-2.349499	0.010798

O	-1.838790	4.253399	-0.547804
H	-1.286579	4.280531	-1.336979
H	-1.239740	3.959846	0.176807
O	0.596297	-1.503609	-3.286788
H	-0.141718	-0.994228	-3.680720
H	0.687711	-1.165572	-2.364806
O	5.042008	1.682032	-1.182013
H	4.531451	2.367407	-0.736716
H	4.740814	1.702979	-2.115846
O	-2.978199	1.650055	-0.287927
H	-2.660296	2.552479	-0.484928
H	-2.156135	1.119857	-0.163002
O	-1.470392	-3.216672	1.839186
H	-1.346207	-2.361459	2.292885
H	-1.879082	-2.967800	0.988331
O	-2.277779	-2.204237	-0.749862
H	-1.683342	-1.451497	-0.501654
H	-1.711502	-2.807704	-1.268881
O	1.710031	0.080512	2.942329
H	2.231911	-0.688692	2.637718
H	1.516879	0.568905	2.118395
O	-0.355646	3.253272	1.569019
H	0.089319	2.473568	1.149489
H	-1.126224	2.873195	2.029023
C	0.413568	0.164209	-0.094813

B3LYP_12_s2 Eopt -1181.737134

O	0.729808	-0.122106	0.037672
O	-1.171006	-0.431205	-1.095098
O	0.642683	-1.632153	-1.612496
O	-1.523703	1.893892	-2.517122
H	-1.331048	1.085519	-1.990325
H	-0.650497	2.311200	-2.671681
O	-1.113991	0.624628	3.210231
H	-0.583287	-0.180206	3.052599
H	-0.692836	1.293661	2.638113
O	3.367924	0.538651	0.075589
H	2.434499	0.231533	-0.025522
H	3.863601	0.087179	-0.634485
O	-3.534749	-2.559871	0.577898
H	-3.386369	-1.630077	0.841304
H	-3.452488	-2.531633	-0.394983
O	0.037645	2.279949	1.129338
H	-0.804550	2.589581	0.742964
H	0.204145	1.404144	0.699719
O	0.537902	-1.565577	2.366489
H	-0.022557	-2.322888	2.099574
H	0.608907	-1.035125	1.540216
O	4.727299	-1.071796	-1.852247
H	4.456766	-0.825939	-2.743728
H	4.100664	-1.778978	-1.576702
O	3.384813	-1.822376	1.844172
H	3.487197	-0.977779	1.369284
H	2.450518	-1.826074	2.123057
O	-3.055100	-2.038387	-2.212083
H	-2.657435	-2.775568	-2.713039
H	-2.290824	-1.526376	-1.848878
O	-2.523827	2.897450	-0.026306
H	-2.227734	2.666404	-0.928587
H	-2.802927	2.042704	0.351655
O	-2.862112	0.186169	0.965867
H	-2.189129	-0.003262	0.267321
H	-2.342648	0.297611	1.785812
O	2.252705	3.137838	-0.440673
H	2.760947	2.309017	-0.348639
H	1.467853	2.983798	0.122351
C	0.071483	-0.734884	-0.894542

B3LYP_12_s3 Eopt -1181.739905

O	0.974842	-0.884622	-0.705793
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O	-0.896041	0.034938	0.095314
O	0.869346	1.362478	-0.311274
O	-1.174909	-0.398488	2.819561
H	-1.145777	-0.223271	1.851779
H	-0.230782	-0.379024	3.067765
O	3.629774	-1.318002	-0.672582
H	2.676778	-1.044832	-0.652758
H	4.142115	-0.491015	-0.764894
O	-3.619323	0.138794	-2.303417
H	-3.349333	-0.662628	-1.812587
H	-3.398956	0.866678	-1.691273
O	0.588563	-3.382843	0.456731
H	-0.206250	-3.319373	1.022918
H	0.673521	-2.490967	0.049823
O	-1.363044	4.402274	-0.507965
H	-0.822244	4.360045	-1.304345
H	-0.793719	4.041900	0.210431
O	0.328406	-1.615412	-3.246811
H	0.817428	-2.462243	-3.302066
H	0.472038	-1.287200	-2.327941
O	5.151383	1.023074	-1.217029
H	4.732570	1.766364	-0.768909
H	5.804772	0.670890	-0.574963
O	-2.802220	1.955115	-0.219221
H	-2.381287	2.812214	-0.425221
H	-2.047909	1.330784	-0.102045
O	-1.859155	-3.048902	1.914689
H	-1.627408	-2.212968	2.362083
H	-2.246556	-2.756167	1.067844
O	-2.574401	-1.957067	-0.669183
H	-1.890858	-1.279970	-0.432777
H	-2.091465	-2.625996	-1.192183
O	1.707590	-0.152034	2.958680
H	2.129509	-0.979363	2.651542
H	1.563187	0.352792	2.134665
O	0.448108	3.533401	1.401406
H	0.378151	4.249631	2.082624
H	1.233304	3.774583	0.876858
C	0.389638	0.074585	-0.061867

B3LYP_18_s1 Eopt -1640.494461

O	-0.922097	-0.457077	-0.056004
O	1.270698	-0.061780	0.108989
O	-0.056915	1.388882	-0.969411
O	2.553203	-1.233124	-2.025994
H	2.120864	-0.819087	-1.243728
H	1.876962	-1.140364	-2.726790
O	-0.782090	-3.261660	2.422049
H	-1.183425	-2.383883	2.578262
H	-0.850721	-3.379569	1.456950
O	-3.246988	-0.317370	-1.382538
H	-2.366164	-0.254311	-0.928694
H	-3.468006	0.591527	-1.663816
O	-0.151140	1.105174	4.048857
H	0.766778	0.816877	3.845533
H	-0.258407	1.943085	3.584919
O	-4.679612	2.726059	0.735158
H	-5.624979	2.902299	0.799509
H	-4.573288	1.786218	1.003589
O	2.430273	0.190467	3.516099
H	2.218343	-0.655836	3.074430
H	2.765439	0.748112	2.787740
O	-0.734309	-3.151558	-0.501544
H	0.209676	-3.390538	-0.586168
H	-0.729540	-2.181436	-0.314084
O	2.725500	4.182273	0.329058
H	1.934826	4.500766	0.778317
H	2.402616	3.784114	-0.511665
O	-1.806476	-0.604164	2.526502
H	-1.259086	-0.014208	3.084774

H	-1.424250	-0.519988	1.621796
O	-4.075710	2.342122	-1.968049
H	-3.277479	2.865479	-2.174636
H	-4.276935	2.547785	-1.036660
O	4.276165	1.075001	-1.668773
H	4.105902	1.191649	-0.716858
H	3.774414	0.272081	-1.902571
O	-4.313353	0.026691	1.282037
H	-4.032503	-0.170426	0.367004
H	-3.507862	-0.116159	1.815055
O	3.279475	1.481996	1.089612
H	3.094162	2.430385	0.948864
H	2.506894	1.010323	0.693341
O	2.092575	-3.645885	-0.536777
H	2.304211	-2.920035	-1.154873
H	2.103070	-3.211954	0.337266
O	1.779408	-2.054675	1.872144
H	1.502625	-1.355712	1.225343
H	0.946515	-2.479878	2.153053
O	0.399791	-0.748809	-3.836864
H	-0.379929	-1.264841	-3.535021
H	0.254576	0.137579	-3.484161
O	-1.822861	-2.244174	-2.993649
H	-2.394793	-1.560660	-2.596055
H	-1.431318	-2.689852	-2.217304
O	1.975957	2.838143	-1.978620
H	1.263684	2.264310	-1.592554
H	2.768644	2.271625	-1.989633
C	0.097753	0.305382	-0.313124

B3LYP_18_s2 Eopt -1640.495242

O	0.948978	0.111221	-0.123162
O	-1.266904	0.060550	0.093245
O	-0.117994	-1.786435	-0.136037
O	-2.070619	1.165693	-2.460362
H	-1.862286	0.848355	-1.565333
H	-1.287108	0.890243	-2.984334
O	0.821263	3.452108	2.105566
H	1.146714	2.581844	2.407868
H	1.045748	3.464042	1.157457
O	3.669540	-0.066938	-1.048733
H	2.743301	-0.175773	-0.778183
H	3.986032	-0.973572	-1.248793
O	-0.419608	-0.665521	3.731411
H	-1.276929	-0.224742	3.542518
H	-0.405083	-1.437948	3.154194
O	4.325708	-3.045485	1.359917
H	3.454212	-3.193015	0.976707
H	4.349257	-2.095004	1.606302
O	-2.866872	0.629071	3.242923
H	-2.540502	1.394731	2.734252
H	-3.295553	0.067764	2.572249
O	1.193170	2.996573	-0.761861
H	0.295396	3.303504	-1.010652
H	1.063678	2.068695	-0.504149
O	-3.825610	-3.682335	0.645646
H	-4.571491	-4.232873	0.381875
H	-3.279389	-3.584015	-0.162903
O	1.717550	0.774930	2.615818
H	0.997160	0.293176	3.076820
H	1.529750	0.611745	1.676528
O	4.634696	-2.680566	-1.386764
H	3.936413	-3.173486	-1.832602
H	4.534655	-2.896375	-0.433861
O	-4.114763	-0.902153	-2.083972
H	-4.199351	-0.805284	-1.119667
H	-3.490998	-0.200851	-2.344610
O	4.314669	-0.283737	1.780374
H	4.164487	-0.112783	0.831201
H	3.488189	-0.001165	2.210042

O	-3.850313	-0.860934	0.904706
H	-3.879485	-1.839011	0.929762
H	-2.943218	-0.654746	0.620394
O	-1.486820	3.732983	-1.282238
H	-1.722336	2.941176	-1.802285
H	-1.712549	3.487805	-0.366776
O	-1.785604	2.592433	1.408742
H	-1.550783	1.775393	0.935774
H	-0.926064	2.931893	1.736474
O	0.226855	0.264391	-3.794880
H	1.022026	0.765314	-3.508182
H	0.319421	-0.602583	-3.383461
O	2.484982	1.732934	-3.005254
H	2.999494	1.092701	-2.481027
H	2.062387	2.295625	-2.329294
O	-2.375899	-3.104245	-1.699671
H	-1.587196	-2.705700	-1.304638
H	-2.956014	-2.342850	-1.910518
C	-0.150538	-0.506423	-0.053743

B3LYP_18_s3 Eopt -1640.491791

O	-0.930753	-0.088029	-0.128325
O	1.287911	-0.086345	0.064190
O	0.161076	1.788088	0.038368
O	2.047986	-0.935327	-2.598462
H	1.854009	-0.708287	-1.673255
H	1.262325	-0.598542	-3.081805
O	-0.822173	-3.639781	1.747397
H	-1.132617	-2.800966	2.140687
H	-1.057497	-3.552410	0.805890
O	-3.659001	0.216196	-0.996654
H	-4.557697	-0.004591	-1.290864
H	-3.965682	1.142234	-1.099497
O	0.491490	0.275656	3.767703
H	1.340701	-0.153891	3.524195
H	0.578401	-0.183346	4.611383
O	-4.248347	2.941693	1.710418
H	-3.379358	3.116970	1.333249
H	-4.281713	1.971417	1.859166
O	2.915694	-0.991845	3.119346
H	2.573471	-1.697744	2.539616
H	3.344174	-0.370368	2.503871
O	-1.220390	-2.890200	-1.053945
H	-2.192746	-3.010758	-1.008238
H	-1.075701	-1.995013	-0.704882
O	3.902106	3.549754	0.962006
H	4.652193	4.115267	0.746203
H	3.345526	3.540859	0.154594
O	-1.677055	-1.017875	2.538442
H	-0.945174	-0.594275	3.036927
H	-1.497734	-0.762170	1.618320
O	-4.593171	2.862091	-1.055022
H	-3.893496	3.389402	-1.457192
H	-4.479514	2.978532	-0.086452
O	4.123496	1.058679	-2.039555
H	4.217686	0.863114	-1.091237
H	3.487580	0.395123	-2.362268
O	-4.269182	0.151555	1.847734
H	-4.132018	0.076340	0.884282
H	-3.441718	-0.183230	2.236004
O	3.892318	0.716548	0.932537
H	3.934739	1.686567	1.056536
H	2.979413	0.551319	0.640181
O	1.443546	-3.602016	-1.680204
H	1.683649	-2.764266	-2.119976
H	1.682839	-3.454063	-0.747474
O	1.787823	-2.745078	1.108816
H	1.558528	-1.881357	0.724362
H	0.927616	-3.105768	1.411133
O	-0.252269	0.124775	-3.805391

H	-1.050722	-0.393124	-3.561118
H	-0.328674	0.946403	-3.306825
O	-2.520604	-1.389237	-3.140792
H	-3.020622	-0.799561	-2.547751
H	-2.097895	-2.022879	-2.530919
O	2.418442	3.230975	-1.411490
H	1.629038	2.803805	-1.049124
H	2.181693	4.180733	-1.462713
C	0.177571	0.506051	-0.010321

B3LYP_24_s1 Eopt -2099.251481

O	1.272188	0.084738	-0.844408
O	-0.753530	-0.416274	-0.029241
O	1.082998	-1.245026	0.939721
O	2.423488	0.061113	2.942264
H	2.206837	1.009426	2.833768
H	1.967990	-0.373753	2.186350
O	-0.114359	-0.503951	4.238888
H	0.796622	-0.301367	3.952481
H	-0.311346	-1.344417	3.788013
O	-2.109854	0.976376	-1.871512
H	-1.601546	1.012465	-2.706016
H	-1.546658	0.449178	-1.246623
O	4.663213	-1.334073	1.637794
H	4.142682	-2.028343	1.194568
H	4.015705	-0.850767	2.180429
O	-2.504928	3.021314	-0.022855
H	-2.164510	2.630406	0.793267
H	-2.333046	2.342010	-0.715905
O	-2.824312	-1.789172	1.333800
H	-3.308855	-1.069541	1.789190
H	-2.096697	-1.330782	0.862228
O	-0.444897	-2.870921	2.490777
H	0.087166	-2.260394	1.920183
H	-1.365360	-2.647674	2.264399
O	-0.426808	0.946790	-4.163053
H	-0.025974	0.085269	-3.944754
H	0.147856	1.584559	-3.695215
O	1.181100	2.428292	-2.363631
H	0.635798	3.110395	-1.914844
H	1.115706	1.631918	-1.791046
O	2.080219	4.528176	0.722183
H	2.593116	5.235441	1.135127
H	2.702826	4.063411	0.116954
O	-0.216363	4.442895	-1.008820
H	-0.969243	4.006507	-0.566910
H	0.453841	4.604776	-0.321011
O	1.323405	2.650682	2.672833
H	1.565286	3.281934	1.965934
H	0.452751	2.287163	2.429795
O	2.850016	-3.172748	0.151538
H	2.243213	-2.428255	0.370141
H	3.050118	-3.067880	-0.800355
O	-1.200543	1.251639	2.271805
H	-1.074078	0.704789	1.470897
H	-0.891223	0.673273	3.002367
O	-3.973238	0.485975	2.537647
H	-3.071322	0.858088	2.506217
H	-4.425949	0.873944	1.760406
O	3.995819	0.400394	-0.583483
H	3.027295	0.222217	-0.623473
H	4.314220	-0.119636	0.176563
O	0.251684	-4.539733	0.119218
H	1.166482	-4.207032	0.055122
H	-0.082146	-4.128497	0.936550
O	-1.118202	-2.840144	-1.716481
H	-0.654602	-3.474173	-1.129449
H	-1.132281	-2.016259	-1.197903
O	0.941791	-1.436956	-3.160698
H	1.117511	-0.855102	-2.388714

H	0.244802	-2.035365	-2.827599
O	-4.623745	-0.210103	-1.848235
H	-3.729558	0.181940	-1.946312
H	-4.452423	-1.131687	-1.570843
O	3.313998	-2.903978	-2.639738
H	2.499824	-2.413631	-2.879551
H	4.021722	-2.252840	-2.711246
O	3.609845	3.147863	-1.118108
H	2.819300	2.958683	-1.662407
H	3.876171	2.263886	-0.797040
O	-5.117526	1.655442	0.234542
H	-4.335484	2.224306	0.125517
H	-5.013205	0.965413	-0.452312
O	-3.952584	-2.855722	-0.988524
H	-3.089416	-2.982982	-1.422506
H	-3.691902	-2.514442	-0.106777
C	0.538497	-0.521615	0.021427

B3LYP_24_s2 Eopt -2099.248362

O	1.163194	0.650001	-0.506480
O	-0.715582	-0.443932	0.028446
O	1.253155	-1.149496	0.815735
O	2.353918	-0.229830	3.149379
H	1.938680	0.648796	3.269678
H	1.986226	-0.537143	2.289932
O	-0.005880	-1.660455	4.136016
H	0.832735	-1.197039	3.953326
H	-0.039596	-2.352528	3.449417
O	-2.195439	0.866124	-1.794023
H	-1.622984	1.230873	-2.497387
H	-1.582786	0.412551	-1.158681
O	4.829980	-0.639787	1.643256
H	4.478620	-1.332236	1.053019
H	4.091769	-0.442174	2.247543
O	-3.426072	2.605448	-0.073120
H	-3.106850	2.343768	0.799587
H	-2.962419	2.003079	-0.703292
O	-2.466465	-2.543806	0.845883
H	-2.734429	-2.964668	0.010502
H	-1.885829	-1.805893	0.571387
O	0.071496	-3.393087	1.791880
H	0.479589	-2.563650	1.434734
H	-0.864202	-3.311848	1.525677
O	-0.318816	1.875555	-3.700191
H	0.229104	1.070539	-3.661070
H	0.058852	2.447877	-3.006418
O	0.664306	3.233694	-1.326925
H	-0.179806	3.666473	-1.078545
H	0.653836	2.319639	-0.966774
O	1.237338	4.147296	1.507088
H	1.174949	3.838783	0.587701
H	0.479000	4.733306	1.615772
O	-1.635101	4.691343	-0.662466
H	-2.298093	4.017189	-0.404851
H	-1.398273	5.139740	0.157749
O	0.745906	2.082502	3.370746
H	0.896387	2.759530	2.682017
H	-0.029966	1.569437	3.075086
O	3.442260	-2.450845	-0.192612
H	2.679393	-1.903346	0.103923
H	3.640724	-2.146386	-1.101148
O	-1.448317	0.339223	2.680457
H	-1.255343	0.085889	1.755947
H	-1.040967	-0.372898	3.215587
O	-4.306169	0.120099	2.777836
H	-3.334379	0.170390	2.709950
H	-4.635543	0.155492	1.861246
O	3.863588	1.175322	-0.390605
H	2.912562	0.920683	-0.376930
H	4.275335	0.661389	0.326902

O	1.266754	-4.321595	-0.703554
H	2.083299	-3.794363	-0.614770
H	0.816413	-4.183129	0.150651
O	-0.408859	-2.523238	-2.114942
H	0.186988	-3.163167	-1.667744
H	-0.614572	-1.866428	-1.425922
O	1.362543	-0.430239	-3.099631
H	1.378849	0.004823	-2.220686
H	0.777703	-1.197248	-2.952647
O	-4.329504	-0.920488	-2.109334
H	-3.556750	-0.320001	-2.092995
H	-3.952192	-1.814392	-2.025020
O	3.901755	-1.620141	-2.869070
H	3.018016	-1.221956	-3.018841
H	3.907140	-2.424939	-3.399376
O	3.498419	3.829055	-1.289462
H	2.528699	3.775059	-1.330868
H	3.755085	2.960134	-0.928841
O	-5.412696	0.451376	0.136873
H	-4.889882	1.265754	0.037321
H	-5.081761	-0.128362	-0.578267
O	-3.024395	-3.454277	-1.819323
H	-2.089697	-3.267467	-2.048785
H	-3.224456	-4.327921	-2.172707
C	0.571711	-0.308097	0.115506

B3LYP_24_s3 Eopt -2099.253428

O	1.287140	0.028262	-0.833874
O	-0.759156	-0.385336	-0.021067
O	1.041031	-1.270231	0.966273
O	2.422314	0.010155	2.957694
H	2.242082	0.964489	2.836162
H	1.953580	-0.416943	2.205452
O	-0.139993	-0.441884	4.250536
H	-0.979871	-0.924558	4.371309
H	-0.109258	0.154193	5.020095
O	-2.054846	1.033587	-1.886783
H	-1.542367	1.039667	-2.719492
H	-1.514364	0.493627	-1.252799
O	4.612640	-1.485340	1.680776
H	4.067924	-2.165137	1.244229
H	3.981806	-0.970958	2.214409
O	-2.379359	3.115715	-0.066118
H	-2.057069	2.722819	0.756385
H	-2.230646	2.421501	-0.749688
O	-2.885527	-1.661340	1.350510
H	-2.909711	-2.574418	0.995918
H	-2.139315	-1.236882	0.876245
O	-0.553125	-2.817095	2.531410
H	0.003805	-2.234518	1.955349
H	-1.463622	-2.562203	2.298252
O	-0.365419	0.910856	-4.170519
H	0.001727	0.037711	-3.939513
H	0.231161	1.532471	-3.708408
O	1.290491	2.353744	-2.383294
H	1.879460	1.681241	-1.977234
H	1.838244	2.789177	-3.073733
O	2.256608	4.457913	0.679264
H	1.533104	4.704567	0.088068
H	2.487103	5.275854	1.177051
O	-0.034956	4.437017	-1.060342
H	-0.805470	4.035113	-0.616125
H	0.638268	4.582361	-0.371789
O	1.421946	2.635708	2.650481
H	1.690204	3.248185	1.936618
H	0.539102	2.302205	2.408376
O	2.736896	-3.273317	0.210372
H	2.157844	-2.503683	0.416840
H	2.944438	-3.188395	-0.741916
O	-1.151544	1.327877	2.256540

H	-1.042797	0.766333	1.463235
H	-0.867090	0.747741	2.995753
O	-3.952193	0.670935	2.520249
H	-3.036741	1.008296	2.487936
H	-4.386954	1.065635	1.736180
O	4.019745	0.244218	-0.565324
H	3.045337	0.102230	-0.607188
H	4.315367	-0.277590	0.202663
O	0.088886	-4.541540	0.184377
H	1.015844	-4.244468	0.119960
H	-0.232265	-4.107460	0.994949
O	-1.208779	-2.815325	-1.678747
H	-0.771715	-3.458761	-1.081679
H	-1.193674	-1.984860	-1.170804
O	0.908265	-1.509698	-3.131927
H	1.102919	-0.924959	-2.366694
H	1.711359	-2.063078	-3.192374
O	-4.611864	-0.056743	-1.859130
H	-3.703129	0.299963	-1.958372
H	-4.476560	-0.980473	-1.569253
O	3.221319	-3.058370	-2.582095
H	2.427182	-2.540778	-2.831643
H	2.873137	-3.884229	-2.226154
O	3.739948	2.997157	-1.136662
H	2.944892	2.830934	-1.681885
H	3.579350	3.890934	-0.774998
O	-5.042685	1.852889	0.197503
H	-4.239288	2.390367	0.084573
H	-4.961913	1.150590	-0.480024
O	-4.044472	-2.714475	-0.962814
H	-4.913618	-3.154817	-0.946120
H	-3.700890	-2.969445	-1.845337
C	0.527764	-0.538714	0.036484

B3LYP_27_s1 Eopt -2328.635602

O	-1.177065	-0.471483	-0.237679
O	0.276657	1.515749	-0.204951
O	1.250241	-0.736472	-0.129417
O	4.031674	-0.139395	0.654690
H	4.313759	0.600348	0.069782
H	3.124367	-0.324623	0.365016
O	-5.227346	-1.046601	-0.987928
H	-4.783358	-1.413668	-1.776631
H	-4.735270	-0.232965	-0.767249
O	-1.866238	-3.152743	0.831048
H	-1.193964	-3.819101	0.548239
H	-1.715584	-2.382817	0.261258
O	2.652906	0.217798	-2.731847
H	1.948033	0.453275	-3.377619
H	2.162680	-0.005428	-1.928086
O	4.418779	1.915081	-1.160063
H	3.865415	1.504433	-1.847965
H	3.829727	2.537880	-0.694073
O	-0.353950	2.951895	-2.701291
H	-1.309644	3.107612	-2.538646
H	-0.090224	2.368192	-1.973547
O	2.813389	0.409111	3.139748
H	3.381183	0.327295	2.344870
H	1.912871	0.322494	2.794071
O	-2.962737	3.462518	-1.777578
H	-2.597973	3.968539	-1.034463
H	-3.264146	2.636346	-1.348231
O	-3.932918	-2.090590	-3.302513
H	-4.000625	-3.048565	-3.363090
H	-2.974988	-1.894925	-3.292618
O	2.218455	3.299572	3.110530
H	1.252902	3.262026	3.219976
H	2.521884	2.389265	3.270181
O	-1.126749	-1.746920	2.980000
H	-0.567031	-2.194004	3.624942

H	-1.363323	-2.412406	2.281105
O	0.782915	5.205071	-1.079424
H	0.503040	4.626749	-1.808538
H	1.492544	4.705922	-0.631810
O	-1.225200	-1.282635	-3.120410
H	-0.566593	-1.989798	-2.968003
H	-1.307726	-0.866472	-2.247966
O	3.412955	-2.578125	-2.893653
H	3.293383	-1.615909	-2.986427
H	3.858655	-2.692055	-2.028066
O	4.546022	-2.829971	-0.310617
H	4.635133	-1.903121	-0.028310
H	3.813696	-3.154825	0.244594
O	3.010018	-2.350731	3.867862
H	2.458837	-2.556521	4.629487
H	2.961748	-1.380932	3.758264
O	-3.895141	-0.829393	3.344375
H	-4.246661	-1.396543	2.623808
H	-2.972664	-1.113248	3.437305
O	0.451542	0.770524	-4.348112
H	-0.150494	0.068037	-4.042220
H	0.099425	1.586871	-3.946624
O	-0.774039	2.871886	3.052466
H	-0.914400	3.447700	2.276299
H	-0.546744	2.008529	2.678631
O	2.214352	-3.238166	1.346748
H	2.454195	-3.025356	2.274440
H	1.794607	-2.433138	1.011724
O	-1.220675	4.050390	0.512638
H	-0.554204	4.629691	0.085279
H	-0.943771	3.162135	0.243260
O	-3.584189	1.155211	-0.269321
H	-3.667689	1.432427	0.672417
H	-2.758957	0.643350	-0.293019
O	2.447797	3.358415	0.304888
H	2.474925	3.448809	1.281714
H	1.793387	2.654680	0.162389
O	0.804104	-2.960268	-2.076159
H	1.703029	-2.966674	-2.480067
H	0.881619	-2.272472	-1.396380
O	-4.681449	-2.560990	1.278600
H	-4.896785	-2.059328	0.461576
H	-3.815615	-2.961871	1.101905
O	-3.714642	1.779686	2.427750
H	-3.770419	0.871922	2.802509
H	-2.882873	2.152041	2.753618
O	0.187238	-4.786502	0.032147
H	0.890173	-4.472226	0.628632
H	0.402026	-4.355015	-0.816209
C	0.092469	0.122008	0.214726

B3LYP_27_s2 Eopt -2328.636769

O	-1.103360	-0.342597	-0.723827
O	0.161689	1.408734	-0.149177
O	1.114453	-0.539454	-0.717113
O	3.562252	0.088158	0.388377
H	3.846644	0.906852	-0.057494
H	2.671713	-0.098527	0.003025
O	-5.203287	-1.287342	-0.555191
H	-5.100334	-1.297907	-1.519739
H	-4.627930	-0.528581	-0.300619
O	-1.303893	-2.775909	0.490373
H	-0.692381	-3.417159	0.081826
H	-1.263638	-1.944417	-0.041679
O	2.368890	0.754189	-2.882928
H	1.602336	1.081268	-3.400537
H	1.961288	0.310499	-2.110565
O	3.983899	2.440000	-1.199601
H	3.430389	1.966165	-1.852401
H	3.356555	2.830150	-0.561373

O	-0.637060	3.330978	-2.056109
H	-1.592121	3.366409	-1.841759
H	-0.299291	2.642896	-1.444203
O	2.748249	-0.049743	3.036261
H	3.095215	0.044591	2.114954
H	1.814256	-0.276972	2.918824
O	-3.289440	3.356726	-0.973704
H	-2.829034	3.706228	-0.195667
H	-3.422955	2.419911	-0.717052
O	-4.207069	-1.884687	-3.486549
H	-4.842093	-1.324408	-3.939155
H	-3.376032	-1.394493	-3.466877
O	2.112505	2.672108	3.542808
H	1.159950	2.610440	3.712658
H	2.383278	1.741120	3.415054
O	-0.423203	-1.570841	2.841216
H	0.270093	-2.095854	3.256458
H	-0.682880	-2.074456	2.038821
O	0.378926	5.266228	-0.140609
H	0.058271	4.780771	-0.922497
H	1.099402	4.690906	0.190739
O	-1.727976	-0.545675	-3.428433
H	-1.098134	-1.196901	-3.756724
H	-1.528958	-0.469151	-2.467775
O	4.009109	-1.638630	-3.275238
H	3.487668	-0.826188	-3.169688
H	4.275829	-1.877263	-2.366894
O	4.787913	-2.225459	-0.596589
H	4.529365	-1.336164	-0.274388
H	4.100314	-2.781968	-0.193558
O	3.242060	-2.815763	3.442004
H	4.181668	-3.007056	3.332710
H	3.175273	-1.841262	3.385153
O	-3.272280	-1.799654	3.506942
H	-3.567740	-2.271826	2.701396
H	-2.301406	-1.755956	3.426443
O	0.012711	1.646688	-4.197679
H	-0.573319	0.886809	-4.027624
H	-0.272527	2.309220	-3.536597
O	-0.864604	1.936946	3.521373
H	-1.004794	2.534496	2.756516
H	-0.494449	1.130257	3.143680
O	2.451010	-3.190945	0.773254
H	2.669632	-3.094887	1.724251
H	1.991265	-2.375321	0.529124
O	-1.326085	3.390579	1.217853
H	-0.780585	4.141481	0.918969
H	-0.967716	2.632926	0.709596
O	-3.445158	0.758688	0.050453
H	-3.437311	0.856270	1.024413
H	-2.548818	0.398402	-0.198163
O	2.080201	3.223629	0.745563
H	2.146662	3.098337	1.714520
H	1.458069	2.522964	0.442206
O	0.681790	-2.634398	-2.559330
H	-0.265067	-2.751802	-2.691849
H	0.759472	-1.905080	-1.903810
O	-3.970968	-3.195312	1.123166
H	-4.417103	-2.576346	0.513429
H	-3.031802	-3.147837	0.868721
O	-3.546553	0.932449	2.880733
H	-3.517378	-0.019867	3.104050
H	-2.676055	1.266808	3.157791
O	0.557415	-4.688074	-0.583960
H	1.251962	-4.319431	-0.005087
H	0.603777	-4.111492	-1.368488
C	0.062403	0.178244	-0.521295

B3LYP_27_s3 Eopt -2328.635779

O	-1.149623	-0.780778	-0.244669
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O	0.385939	0.745043	-0.824106
O	1.029121	-1.208215	0.064278
O	3.697723	-0.389392	0.186547
H	3.954944	-0.202311	-0.736693
H	2.730992	-0.573977	0.139638
O	-5.327042	-1.004604	-0.126324
H	-5.062875	-1.906953	-0.412400
H	-4.663950	-0.406464	-0.531722
O	-1.739102	-1.098742	2.412150
H	-1.219467	-1.833126	2.801243
H	-1.523270	-1.092405	1.451449
O	2.205758	-2.082985	-2.403693
H	1.437542	-2.106661	-3.013808
H	1.825569	-1.795350	-1.551045
O	4.008106	0.121987	-2.595451
H	3.346855	-0.594028	-2.676981
H	3.488010	0.935804	-2.443542
O	-0.153463	0.771188	-3.612659
H	-1.066535	1.109355	-3.693949
H	0.019006	0.777610	-2.651930
O	4.478685	1.677929	1.831205
H	4.169440	0.931512	1.272460
H	3.964642	1.614997	2.643397
O	-2.757265	1.844202	-3.658222
H	-2.478309	2.742527	-3.437114
H	-2.958549	1.418434	-2.793973
O	-4.456041	-3.556097	-1.004548
H	-4.979998	-3.768802	-1.784229
H	-3.570274	-3.316731	-1.349804
O	3.341665	3.779015	0.364345
H	2.487901	3.971561	0.801708
H	3.748602	3.070041	0.904071
O	-0.842823	1.446072	2.984896
H	-0.542832	1.806310	2.140332
H	-1.100360	0.514653	2.790095
O	0.450782	4.232935	-2.678131
H	0.792000	5.117011	-2.500347
H	1.185914	3.624885	-2.451915
O	-1.889587	-2.836699	-1.912700
H	-1.366100	-3.620705	-1.711357
H	-1.584792	-2.149146	-1.275352
O	3.556607	-4.297761	-1.147610
H	3.077010	-3.611017	-1.644885
H	3.792518	-3.866207	-0.305390
O	4.325167	-2.893415	1.233085
H	4.197592	-2.013005	0.819166
H	3.671479	-2.900355	1.943723
O	1.510222	0.860382	4.383510
H	0.709668	1.154658	3.898699
H	2.177028	1.530391	4.205279
O	-3.685437	2.067571	2.873419
H	-4.040500	1.162994	2.743544
H	-2.726340	1.933993	2.982783
O	-0.093319	-1.968907	-4.008471
H	-0.739430	-2.302483	-3.357652
H	-0.152320	-0.991377	-3.924580
O	0.827958	4.319656	1.547445
H	0.223633	3.884520	0.906675
H	0.744580	3.809379	2.360322
O	2.029617	-1.458667	2.888375
H	1.888277	-0.622273	3.377881
H	1.669995	-1.302951	1.998353
O	-0.807510	3.168991	-0.366612
H	-0.503916	3.638776	-1.169523
H	-0.479207	2.246650	-0.492994
O	-3.327131	0.638786	-1.211398
H	-3.411755	1.449927	-0.664556
H	-2.510589	0.183900	-0.887586
O	2.399263	2.365374	-1.852962
H	2.780840	2.852916	-1.089001

H	1.761136	1.739584	-1.450058
O	0.189035	-3.802017	0.664458
H	-0.747019	-3.879520	0.447999
H	0.427777	-2.873856	0.431473
O	-4.504905	-0.623517	2.533617
H	-4.812895	-0.777429	1.616384
H	-3.567203	-0.896563	2.527201
O	-3.530704	3.014767	0.229868
H	-3.592503	2.713477	1.161488
H	-2.579042	3.153528	0.060267
O	-0.102904	-3.187594	3.408577
H	0.670896	-2.586973	3.415555
H	-0.055456	-3.564445	2.506958
C	0.090218	-0.408393	-0.335248

B3LYP_30_s1	Eopt -2558.004636		
O	0.618647	-0.326097	1.410664
O	1.783597	-0.063535	-0.481329
O	0.246597	1.452948	0.112390
O	-1.177077	2.277933	3.979870
H	-1.383557	2.702037	3.122604
H	-1.331817	1.334438	3.786060
O	-4.404294	-2.712055	-0.060154
H	-3.972829	-3.083951	-0.839473
H	-3.913160	-1.878738	0.113438
O	-5.429965	1.330661	-0.010549
H	-4.969806	2.126278	-0.330980
H	-4.696430	0.765787	0.303318
O	-1.689045	-0.244876	2.776531
H	-1.719685	-1.156690	3.133496
H	-0.831387	-0.204608	2.281284
O	1.924544	3.485382	1.190727
H	1.824287	3.298682	2.149353
H	1.342841	2.822572	0.766071
O	5.415619	1.384450	-1.763246
H	5.551269	0.414560	-1.795185
H	5.035022	1.541755	-0.880005
O	-0.393603	-4.474554	0.218555
H	-0.789878	-3.821666	-0.391416
H	0.076081	-3.942140	0.894624
O	0.900777	-1.826286	-2.516434
H	-0.738741	-2.280968	-1.997103
H	1.191428	-1.205590	-1.817248
O	-1.580963	-2.540933	-1.565133
H	-2.914906	-1.738334	-2.769474
H	-1.741411	-1.854462	-0.903865
O	5.699723	-1.427277	-1.796547
H	5.492966	-1.690689	-2.700200
H	4.921874	-1.708080	-1.265437
O	-3.477642	3.363821	-0.868091
H	-2.954017	3.302579	-0.043531
H	-3.176281	2.586666	-1.380480
O	-1.686992	3.120579	1.340912
H	-1.219421	3.969066	1.202345
H	-1.073633	2.450485	0.970223
O	1.619602	2.695396	3.894865
H	0.656806	2.517790	3.946775
H	2.028954	1.825630	3.731438
O	-1.154979	4.852464	-1.909603
H	-0.631241	4.057684	-2.139587
H	-2.004018	4.483782	-1.605533
O	3.562894	-2.158322	-0.169180
H	3.093343	-2.925439	-0.554567
H	2.907417	-1.423657	-0.207435
O	-2.388488	1.067898	-2.035240
H	-1.523745	1.350015	-2.377477
O	-5.903715	-0.883860	-1.812299
H	-5.601243	-1.569743	-1.192266
H	-5.798774	-0.052945	-1.310322
O	3.697775	-2.554529	2.616195

H	3.491925	-1.648071	2.908802
H	3.729532	-2.473727	1.639581
O	0.114396	2.403725	-2.383902
H	0.972937	2.250301	-2.805191
H	0.236697	2.058948	-1.458846
O	-3.158331	-0.282371	0.423999
H	-2.619296	-0.230553	1.244322
H	-2.671502	0.187976	-0.276869
O	3.965755	1.484456	0.725460
H	3.427539	2.284877	0.878951
H	3.345241	0.885902	0.269343
O	-2.889004	-4.459724	1.684926
H	-3.436797	-3.866968	1.137031
H	-2.060090	-4.559910	1.180315
O	-1.536393	-2.932868	3.657523
H	-0.637869	-2.980798	3.276761
H	-2.085021	-3.438740	3.024338
O	-0.142524	5.421116	0.678835
H	0.645221	4.861654	0.818714
H	-0.410753	5.268683	-0.250949
O	2.753481	1.241454	-2.752620
H	3.701952	1.353664	-2.539557
H	2.374923	0.818165	-1.949534
O	2.020197	-4.171221	-1.469576
H	1.295130	-4.427374	-0.872235
H	1.648497	-3.412927	-1.964689
O	2.819844	0.182045	3.093453
H	3.380423	0.623789	2.430186
H	2.019095	-0.051075	2.580164
O	2.059280	-0.550355	-4.724785
H	2.346763	0.146167	-4.092150
H	1.216155	-1.434226	-3.357358
O	0.880457	-2.921996	2.174040
H	1.819162	-3.006538	2.427948
H	0.818479	-2.004813	1.818150
O	-3.479590	-1.167239	-3.321698
H	-4.321232	-1.081236	-2.830289
H	-2.721427	0.355260	-2.617712
H	1.401729	-0.128937	-5.289230
C	0.871939	0.351425	0.343683

B3LYP_30_s2 Eopt -2558.004475

O	0.282940	-0.093918	1.002766
O	1.677458	-0.651503	-0.645344
O	1.241704	1.501993	-0.245737
O	0.530658	3.416323	3.935404
H	0.259645	3.336744	2.991356
H	-0.012219	2.782183	4.419798
O	-5.358681	-0.842593	-0.125832
H	-4.984480	-1.098733	-0.977717
H	-4.632682	-0.368257	0.327680
O	-4.196555	3.442933	0.233716
H	-3.381815	3.832225	-0.146915
H	-3.883224	2.608056	0.637165
O	-1.339873	0.844820	2.946633
H	-1.476922	1.800218	2.908374
H	-0.706204	0.651795	2.220777
O	3.508897	2.514729	1.066963
H	3.397110	2.375338	2.034768
H	2.706093	2.156845	0.652229
O	5.780683	-1.324516	-1.218551
H	5.456660	-2.247803	-1.178276
H	5.367826	-0.919411	-0.433148
O	-2.317240	-3.834927	0.025834
H	-2.378502	-3.054015	-0.560351
H	-1.937582	-3.500961	0.856986
O	0.225130	-1.910570	-2.658224
H	-1.539101	-1.754028	-2.184897
H	0.700671	-1.425395	-1.949422
O	-2.432908	-1.573193	-1.834044

H	-3.433689	-0.257962	-2.945629
H	-2.284899	-0.926217	-1.132827
O	4.708162	-3.883846	-0.838178
H	4.661384	-4.573234	-1.508625
H	3.779251	-3.710340	-0.569609
O	-1.682019	4.304067	-0.865659
H	-1.154790	4.047941	-0.080199
H	-1.708019	3.492604	-1.415900
O	0.061640	3.525198	1.210400
H	0.779895	4.186302	1.121479
H	0.435965	2.720795	0.768136
O	2.983305	2.058322	3.764035
H	2.107051	2.493779	3.834162
H	2.799849	1.119508	3.587558
O	0.919399	5.219725	-1.859177
H	1.201953	4.450569	-2.368375
H	0.034418	4.974437	-1.524903
O	2.156102	-3.289110	0.071861
H	1.472896	-3.787503	-0.417459
H	1.950356	-2.342944	-0.114421
O	-1.672903	1.941391	-2.252294
H	-0.816724	1.874601	-2.712119
O	-5.605089	1.757707	-1.629076
H	-5.736834	0.960329	-1.091349
H	-5.117377	2.374466	-1.049731
O	1.517931	-3.704436	2.729044
H	1.849542	-2.915481	3.169589
H	1.762454	-3.565026	1.783798
O	1.019328	1.837094	-2.995386
H	1.547419	2.556040	-3.356621
H	1.232277	1.786197	-2.040278
O	-3.358536	0.777981	0.979035
H	-2.792885	0.698062	1.774713
H	-2.717805	0.832859	0.257084
O	4.140291	-0.313944	0.928368
H	4.146835	0.668493	0.947552
H	3.388171	-0.528605	0.342555
O	-5.030061	-3.522075	0.852295
H	-5.165467	-2.613284	0.536621
H	-4.133383	-3.745828	0.539885
O	-4.033881	-3.638879	3.492314
H	-3.104954	-3.785116	3.289963
H	-4.457528	-3.567791	2.611780
O	2.322903	5.172686	0.619473
H	2.839125	4.354335	0.743327
H	1.971179	5.144787	-0.292851
O	3.538400	-0.298061	-2.672135
H	4.359262	-0.610462	-2.247262
H	2.863554	-0.328576	-1.959249
O	0.121377	-4.426738	-1.486507
H	-0.679732	-4.364062	-0.933568
H	0.163989	-3.550722	-1.934470
O	2.533104	-0.901522	3.243496
H	3.077259	-0.702582	2.459649
H	1.617570	-0.744072	2.946841
O	2.281605	-1.839331	-4.573098
H	2.804159	-1.290713	-3.945175
H	0.864585	-1.939601	-3.401808
O	-1.128459	-2.890519	2.423651
H	-0.225272	-3.236776	2.584152
H	-1.428740	-2.508102	3.252728
O	-3.806153	0.493997	-3.437581
H	-4.435355	0.922275	-2.823706
H	-2.351347	1.528152	-2.816435
H	2.066434	-1.248683	-5.303793
C	1.050568	0.254674	0.051443

B3LYP_30_s3 Eopt -2558.012254

O	0.305624	0.453538	-0.943285
O	1.699649	-0.218116	0.678791

O	0.070959	-1.574043	-0.030270
O	-0.659499	-2.497557	-4.138162
H	-1.146713	-2.569899	-3.291080
H	-0.116837	-1.693463	-4.024282
O	-2.943233	3.413509	0.277532
H	-2.516237	3.092270	1.097444
H	-2.668202	2.767823	-0.408222
O	-4.754356	0.534679	-1.792745
H	-4.610810	-0.299330	-1.303439
H	-3.860912	0.920547	-1.862531
O	0.930888	-0.226967	-3.556341
H	0.753446	0.571059	-4.068421
H	0.659403	-0.005499	-2.636177
O	1.643657	-3.762615	-0.641127
H	1.593442	-4.418706	0.063244
H	1.058108	-3.022013	-0.359230
O	5.093969	-2.189369	1.934421
H	5.347270	-1.267970	2.147772
H	4.734671	-2.136004	1.028322
O	1.277519	4.924220	-0.129954
H	1.849174	5.622528	-0.469859
H	1.393379	4.162952	-0.748049
O	0.974874	1.556750	2.821339
H	-2.094719	2.509111	3.381450
H	1.183256	0.944655	2.089735
O	-1.743426	2.223558	2.530129
H	-5.625764	1.035997	3.414121
H	-2.172055	1.354981	2.345779
O	5.705589	0.514444	2.471282
H	5.382772	0.670906	3.365835
H	5.027192	0.911935	1.880705
O	-4.100734	-1.742554	-0.227238
H	-3.326396	-2.024471	-0.765797
H	-3.719024	-1.159069	0.459133
O	-1.869205	-2.606398	-1.617697
H	-1.863201	-3.518589	-1.261000
H	-1.166344	-2.140083	-1.099442
O	1.191180	-4.513709	-3.359828
H	0.569293	-3.826803	-3.671271
H	1.334010	-4.300100	-2.419989
O	-4.132785	-4.199978	1.145768
H	-3.961149	-4.036157	2.080035
H	-4.173219	-3.312362	0.730179
O	3.845524	1.588954	0.713070
H	3.488041	2.392223	1.148969
H	3.073661	0.986107	0.646210
O	-2.971760	-0.133562	1.843303
H	-2.475984	-0.903807	2.190070
O	-5.514238	2.168605	0.397377
H	-4.683073	2.679311	0.456456
H	-5.351291	1.569560	-0.360562
O	4.197852	2.048542	-2.048672
H	4.074313	1.155199	-2.433453
H	4.166115	1.904887	-1.081191
O	-1.274086	-2.310880	2.286738
H	-1.813786	-3.048715	1.976904
H	-0.736606	-2.052296	1.504803
O	-2.114842	1.632136	-1.753853
H	-1.722420	2.328395	-2.320946
H	-1.348516	1.116263	-1.427783
O	3.733408	-1.848773	-0.569491
H	3.176569	-2.648412	-0.643429
H	3.131367	-1.214325	-0.133357
O	-1.407704	5.472919	-0.925194
H	-1.937859	4.808374	-0.441365
H	-0.495567	5.351872	-0.597368
O	-0.825105	3.739496	-3.124539
H	0.045445	3.416514	-2.824018
H	-1.074040	4.396297	-2.443672
O	-1.929404	-5.122000	-0.317851

H	-1.117879	-5.053758	0.198510
H	-2.647909	-4.842618	0.288622
O	2.317198	-2.071763	2.654834
H	3.284340	-2.139136	2.546295
H	2.035279	-1.438057	1.956909
O	2.585766	3.703854	2.072156
H	2.129227	4.169045	1.344386
H	1.951031	3.019022	2.374919
O	3.720206	-0.530035	-3.088297
H	3.728210	-1.031145	-2.248160
H	2.772507	-0.430016	-3.305171
O	1.088692	-1.728817	5.110991
H	1.538955	-1.826700	4.244733
H	0.027923	1.775586	2.717462
O	1.491487	2.767833	-1.810280
H	2.434527	2.570768	-1.992628
H	1.128580	1.944300	-1.407103
O	-5.574921	0.489027	2.622599
H	-5.575852	1.120733	1.868153
H	-3.826631	-0.065986	2.314555
H	0.152411	-1.830527	4.908807
C	0.689189	-0.442105	-0.100932

B3LYP_Radical_3_s1 Eopt -493.401197

O	2.093524	0.180446	-0.501878
O	0.939435	-0.597907	1.366338
O	0.587314	-1.596618	-0.538734
O	-2.266557	-1.138347	-0.576790
H	-2.614130	-0.944026	-1.450307
H	-1.327476	-1.327118	-0.640763
O	-1.494834	1.002131	1.048840
H	-0.715764	0.548471	1.378755
H	-2.004402	0.403509	0.497847
O	0.110184	2.218721	-0.785995
H	0.434771	3.086943	-0.536127
H	-0.544388	1.925916	-0.147716
C	1.169809	-0.706851	0.134011

B3LYP_Radical_3_s2 Eopt -493.402828

C	-0.001557	-0.000060	0.060680
O	-0.395487	-1.233254	0.046500
O	-0.872698	0.957051	0.097460
O	1.262772	0.276150	0.037678
O	2.961781	-1.760499	-0.050678
H	2.274381	-1.033914	-0.018126
H	2.455472	-2.579132	-0.050141
O	-3.007409	-1.676072	-0.077838
H	-3.458846	-0.828471	-0.013191
H	-2.033427	-1.451121	-0.027345
O	0.051234	3.438107	-0.067398
H	1.010541	3.398568	-0.134009
H	-0.240324	2.482564	-0.007062

B3LYP_Radical_3_s3 Eopt -493.399098

C	2.654323	-0.058632	-0.009988
O	2.384963	-1.324933	-0.001239
O	3.885590	0.340768	-0.037596
O	1.693121	0.808010	0.009276
O	-0.792624	-0.118608	0.078764
H	0.164762	0.171678	0.053286
H	-0.758771	-1.080562	0.075653
O	-3.203704	1.713467	-0.015874
H	-2.369995	1.237533	-0.011830
H	-3.033389	2.658231	-0.012021
O	-4.267134	-1.445355	-0.031971
H	-3.433425	-1.921289	-0.027927
H	-4.096819	-0.500591	-0.028118

B3LYP_Radical_6_s1 Eopt -722.779444

O	-2.013434	0.831865	-0.941285
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O	-1.236962	-1.166465	-0.346190
O	-0.071803	0.248845	-1.623795
O	1.146356	2.668543	-0.223881
O	-1.448831	2.984099	0.962391
O	-3.403720	-1.693676	1.443587
H	-1.735846	2.243669	0.402135
H	0.315970	2.857137	0.251369
H	-4.236205	-1.610678	0.966296
H	-2.718220	-1.463141	0.791180
H	-1.422482	2.622351	1.855615
H	0.934355	1.876849	-0.738448
O	3.856371	0.150757	1.507593
O	2.610683	-0.932195	-0.756619
O	0.889589	-3.001707	0.069223
H	1.917939	-0.320642	-1.043728
H	0.132854	-2.396216	-0.049299
H	3.417794	-0.196274	0.703147
H	0.971445	-3.116090	1.022825
H	2.107557	-1.708277	-0.434563
H	4.318112	0.943810	1.215721
C	-1.104878	-0.075504	-0.945074

B3LYP_Radical_6_s2 Eopt -722.779034

O	-2.010749	0.826426	-0.904429
O	-1.227541	-1.168429	-0.306457
O	-0.072469	0.244033	-1.596465
O	1.160594	2.671587	-0.223036
O	-1.445956	3.046270	0.917030
O	-3.466426	-1.750545	1.378308
H	-1.728961	2.272948	0.400922
H	0.325452	2.884235	0.233345
H	-4.265767	-1.375358	0.993491
H	-2.752193	-1.491712	0.768800
H	-1.432412	2.743473	1.832121
H	0.943963	1.872654	-0.724326
O	3.870282	0.137150	1.500093
O	2.615493	-0.939417	-0.761748
O	0.899700	-3.012468	0.065777
H	1.920516	-0.326860	-1.041306
H	0.142484	-2.404518	-0.036248
H	3.428541	-0.208059	0.696576
H	0.992823	-3.138883	1.016824
H	2.114777	-1.717241	-0.440112
H	4.332426	0.929821	1.207818
C	-1.100847	-0.079559	-0.910080

B3LYP_Radical_6_s3 Eopt -722.781541

O	-0.785476	-0.327655	-1.262608
O	-0.299017	1.299162	0.150848
O	0.057765	-0.823728	0.676459
O	-2.486745	-2.194925	1.545405
O	-3.493128	-1.429921	-1.034538
O	-2.734361	2.830253	-0.075636
H	-2.643291	-0.986111	-1.193121
H	-2.930745	-1.974024	0.705704
H	-2.843284	3.072571	-1.001541
H	-1.922364	2.295936	-0.053280
H	-4.126917	-0.714334	-0.909323
H	-1.601869	-1.817953	1.435933
O	4.347954	-1.488891	-1.232039
O	3.002259	-0.394454	0.958306
O	2.390091	2.326607	0.467829
H	2.093743	-0.728216	0.904813
H	1.463362	2.073464	0.311913
H	3.886145	-1.112304	-0.453646
H	2.730488	2.572368	-0.399967
H	2.902696	0.563265	0.785299
H	5.043195	-2.044210	-0.863894
C	-0.340985	0.071328	-0.136851

B3LYP_Radical_9_s1 Eopt -952.155952

O	-0.624235	-1.333320	-0.924753
O	-0.620084	0.767387	-1.307962
O	-0.408411	0.067352	0.799254
O	0.585403	2.518168	1.839671
H	0.204268	1.721268	1.425111
H	-0.053051	3.219586	1.666962
O	-3.674918	1.323928	-0.985071
H	-2.758988	1.334657	-1.295734
H	-3.598983	1.076379	-0.046666
O	1.933931	2.057739	-2.103977
H	2.263961	2.439367	-1.266698
H	1.116971	1.599434	-1.858046
O	1.693509	-3.027486	-0.043393
H	1.027616	-2.549042	-0.558911
H	1.578544	-2.667093	0.859125
O	-3.311080	-0.045208	1.592584
H	-2.345780	0.031572	1.548923
H	-3.511811	-0.768885	0.975855
O	1.089765	-1.772156	2.415806
H	1.861761	-1.293376	2.738579
H	0.573612	-1.112726	1.916962
O	-3.704632	-1.665265	-0.883916
H	-3.824397	-0.738511	-1.150504
H	-2.748541	-1.800138	-0.950261
O	2.831528	3.186454	0.332265
H	2.065110	2.938431	0.893152
H	3.557058	2.629588	0.635819
O	4.227656	-2.116680	-0.812168
H	3.328873	-2.432735	-0.582848
H	4.352425	-2.367689	-1.733472
C	-0.539350	-0.157898	-0.427346

B3LYP_Radical_9_s2 Eopt -952.152797

O	-0.059153	-0.456484	-1.136894
O	-1.111775	1.398163	-0.974611
O	-0.290314	0.467610	0.881103
O	0.906207	2.779779	2.059714
H	0.415130	2.018580	1.691627
H	0.412541	3.556525	1.751275
O	-3.960363	0.402579	-0.631532
H	-3.149741	0.853248	-0.903844
H	-3.746145	0.071723	0.256130
O	0.612398	3.730296	-1.603849
H	1.424534	3.439677	-1.149215
H	0.003405	2.988549	-1.483108
O	1.424699	-3.277896	-0.249037
H	0.896974	-2.807192	-0.907289
H	1.299952	-2.759163	0.573218
O	-2.802700	-1.094501	1.659822
H	-1.982180	-0.583396	1.643269
H	-2.713709	-1.695908	0.899203
O	1.012777	-1.765729	2.069777
H	1.878114	-1.471967	2.378971
H	0.609463	-0.977861	1.659877
O	-2.622112	-2.253596	-1.057902
H	-3.162864	-1.449518	-1.163025
H	-1.710074	-1.931934	-1.175147
O	2.798395	2.707790	-0.034856
H	2.196219	2.711541	0.741582
H	2.758580	1.808456	-0.371956
O	4.090883	-2.708517	-0.948341
H	3.163955	-2.938718	-0.736668
H	4.257962	-3.108020	-1.808918
C	-0.473942	0.473238	-0.360522

B3LYP_Radical_9_s3 Eopt -952.155702

O	0.735010	-0.365102	-1.851927
O	1.732489	1.194064	-0.776981
O	1.668764	-0.857159	0.106050

O	4.469260	-1.157420	0.713916
H	3.506468	-1.084854	0.586859
H	4.617614	-0.911185	1.634022
O	-0.449685	3.015413	-0.193302
H	0.322267	2.460582	-0.398955
H	-0.143828	3.620988	0.491955
O	4.744482	1.213505	-0.867491
H	4.770269	0.413436	-0.309680
H	3.796764	1.383154	-0.966206
O	-1.942624	-1.164250	-0.699235
H	-1.306791	-0.816700	-1.341136
H	-1.450424	-1.878806	-0.242207
O	0.341419	0.094148	2.603411
H	0.881687	-0.239406	1.871333
H	-0.467190	0.419454	2.162286
O	-0.229719	-2.972662	0.578369
H	-0.053707	-3.708457	-0.019200
H	0.487318	-2.334418	0.409088
O	-1.928064	1.003664	1.126940
H	-1.452243	1.726945	0.669235
H	-1.912008	0.253002	0.497937
O	-4.704669	-1.014381	-1.195350
H	-3.749372	-1.159149	-1.047261
H	-5.141984	-1.748927	-0.750670
C	1.389421	-0.036634	-0.802810
O	-4.740409	1.266684	0.555528
H	-3.799342	1.274706	0.809620
H	-4.812052	0.497403	-0.039576

B3LYP_Radical_12_s1 Eopt -1181.534612

O	0.332772	-0.491408	1.369166
O	0.390483	0.456905	-0.655163
O	-1.248860	-0.975868	-0.144039
O	1.231025	-1.118255	-2.795434
H	0.903587	-0.488340	-2.117183
H	0.696940	-1.914849	-2.620686
O	-0.824256	-2.145422	3.237675
H	-0.394920	-1.559249	2.572854
H	-1.665808	-2.368188	2.805103
O	1.419175	3.776223	0.772868
H	2.039024	3.083914	0.478048
H	0.642066	3.642466	0.193678
O	2.637730	-2.134429	1.071528
H	3.031768	-1.827733	0.234333
H	1.854516	-1.563574	1.193597
O	-3.419824	2.737649	-0.761192
H	-3.654074	2.643587	0.168727
H	-3.332024	1.817928	-1.098978
O	0.545451	1.907801	2.803930
H	0.825613	2.585248	2.162232
H	0.497667	1.080517	2.281855
O	-3.007968	-2.413161	1.377623
H	-2.370924	-1.863713	0.860753
H	-3.706790	-1.805683	1.642733
O	-0.611575	3.028353	-1.039749
H	-1.574439	3.015256	-0.876287
H	-0.328544	2.095680	-0.934461
O	3.701733	-1.047845	-1.390400
H	2.897723	-1.179887	-1.931923
H	3.565750	-0.167247	-0.994901
O	2.849901	1.393983	-0.065637
H	1.935753	1.030244	-0.220164
H	3.082617	1.096204	0.821849
O	-0.667765	-3.079033	-1.897445
H	-0.237908	-3.773192	-1.385831
H	-0.890787	-2.381679	-1.243600
O	-3.049448	0.190104	-1.792139
H	-2.328477	-0.212287	-1.245029
H	-2.657481	0.340939	-2.659366

C	-0.176573	-0.335191	0.196651
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B3LYP_Radical_12_s2 Eopt -1181.534863

O	-0.757504	0.178827	0.131728
O	1.249739	0.991054	-0.430862
O	-0.549897	2.310036	-0.539842
O	1.825892	0.387743	-3.069841
H	1.596170	0.665088	-2.153864
H	1.003820	0.462935	-3.567162
O	0.690076	-2.878404	1.745574
H	0.232878	-2.162581	2.226017
H	0.272930	-2.860395	0.862435
O	-3.437972	0.221481	-0.130581
H	-2.449240	0.224345	-0.030269
H	-3.613801	1.119311	-0.467613
O	4.248761	0.796316	1.874364
H	3.746836	0.049210	1.498741
H	3.859511	1.576942	1.436492
O	-0.439634	-2.359312	-0.846726
H	0.383726	-2.394016	-1.371845
H	-0.487194	-1.427877	-0.522022
O	-0.737368	-0.606251	2.747263
H	-0.212266	-0.014180	3.297542
O	-0.670590	-0.245562	1.830538
H	-3.143143	2.919907	-0.979109
H	-3.234857	2.976474	-1.936275
H	-2.196462	2.667495	-0.822888
O	-3.574766	-0.011196	2.720272
H	-3.644182	0.109391	1.754235
H	-2.631570	-0.210406	2.856734
O	2.961290	2.909880	0.426995
H	2.502435	3.489248	1.044810
H	2.271206	2.282541	0.095414
O	2.148398	-2.263101	-2.085689
H	2.034377	-1.409552	-2.548550
H	2.447677	-1.994348	-1.195525
O	2.643004	-1.150484	0.519234
H	2.062447	-0.410117	0.209191
H	2.052152	-1.738349	1.027672
O	-3.085118	-1.993763	-1.930957
H	-3.310024	-1.216708	-1.386464
H	-2.172510	-2.205565	-1.663021
C	-0.029588	1.174137	-0.281484

B3LYP_Radical_12_s3 Eopt -1181.533356

O	0.974842	-0.884622	-0.705793
O	-0.896041	0.034938	0.095314
O	0.869346	1.362478	-0.311274
O	-1.174909	-0.398488	2.819561
H	-1.145777	-0.223271	1.851779
H	-0.230782	-0.379024	3.067765
O	3.629774	-1.318002	-0.672582
H	2.676778	-1.044832	-0.652758
H	4.142115	-0.491015	-0.764894
O	-3.619323	0.138794	-2.303417
H	-3.349333	-0.662628	-1.812587
H	-3.398956	0.866678	-1.691273
O	0.588563	-3.382843	0.456731
H	-0.206250	-3.319373	1.022918
H	0.673521	-2.490967	0.049823
O	-1.363044	4.402274	-0.507965
H	-0.822244	4.360045	-1.304345
H	-0.793719	4.041900	0.210431
O	0.328406	-1.615412	-3.246811
H	0.817428	-2.462243	-3.302066
H	0.472038	-1.287200	-2.327941
O	5.151383	1.023074	-1.217029
H	4.732570	1.766364	-0.768909
H	5.804772	0.670890	-0.574963
O	-2.802220	1.955115	-0.219221

H	-2.381287	2.812214	-0.425221
H	-2.047909	1.330784	-0.102045
O	-1.859155	-3.048902	1.914689
H	-1.627408	-2.212968	2.362083
H	-2.246556	-2.756167	1.067844
O	-2.574401	-1.957067	-0.669183
H	-1.890858	-1.279970	-0.432777
H	-2.091465	-2.625996	-1.192183
O	1.707590	-0.152034	2.958680
H	2.129509	-0.979363	2.651542
H	1.563187	0.352792	2.134665
O	0.448108	3.533401	1.401406
H	0.378151	4.249631	2.082624
H	1.233304	3.774583	0.876858
C	0.389638	0.074585	-0.061867

B3LYP_Radical_18_s1

Eopt -1640.287721

O	-0.954397	-0.224892	-0.096358
O	1.263422	-0.092748	0.082234
O	0.010252	1.689394	0.261973
O	2.060503	-0.903228	-2.572134
H	1.851411	-0.721926	-1.639874
H	1.278742	-0.543682	-3.045534
O	-0.655950	-3.740281	1.685037
H	-1.019235	-2.937588	2.107334
H	-0.902744	-3.639142	0.748167
O	-3.688967	0.074299	-0.987717
H	-2.762086	0.108495	-0.698157
H	-3.944331	1.012706	-1.115694
O	0.484771	0.115123	3.791462
H	1.362000	-0.236643	3.524969
H	0.423024	0.975629	3.362608
O	-3.872049	2.856201	1.601176
H	-4.519135	3.353018	2.112345
H	-4.044625	1.909473	1.801236
O	3.003585	-0.918204	3.073071
H	2.700486	-1.625263	2.474115
H	3.361188	-0.236094	2.478518
O	-1.137840	-2.964188	-1.108668
H	-0.239401	-3.235799	-1.390772
H	-1.014665	-2.077018	-0.738024
O	3.573993	3.824763	0.848934
H	3.053096	4.214011	1.562394
H	2.959617	3.751568	0.090549
O	-1.679590	-1.201158	2.558730
H	-0.944296	-0.769367	3.044716
H	-1.525793	-0.932354	1.637885
O	-4.397510	2.802628	-1.126113
H	-3.616590	3.184101	-1.569681
H	-4.218991	2.914514	-0.168598
O	3.848405	1.334318	-2.056774
H	4.004706	1.166736	-1.112257
H	3.300965	0.582242	-2.348317
O	-4.267468	0.101618	1.878836
H	-4.163849	-0.016035	0.915626
H	-3.464990	-0.294460	2.259319
O	3.770173	0.998542	0.939553
H	3.731360	1.971468	1.036105
H	2.871764	0.745609	0.665673
O	1.547993	-3.618015	-1.713696
H	1.758572	-2.770140	-2.147833
H	1.788843	-3.467093	-0.781558
O	1.922152	-2.734711	1.067880
H	1.655297	-1.881282	0.685277
H	1.078033	-3.129242	1.372509
O	-0.220606	0.272929	-3.688480
H	-1.001973	-0.289387	-3.492988
H	-0.281014	1.008400	-3.058799
O	-2.427477	-1.387443	-3.186059
H	-2.973268	-0.852631	-2.581256

H	-2.008564	-2.043355	-2.598760
O	1.938558	3.317622	-1.400644
H	1.234577	2.824227	-0.956559
H	2.564443	2.630395	-1.709626
C	0.115300	0.420894	0.076168

B3LYP_Radical_18_s2

Eopt -1640.286481

O	0.948978	0.111221	-0.123162
O	-1.266904	0.060550	0.093245
O	-0.117994	-1.786435	-0.136037
O	-2.070619	1.165693	-2.460362
H	-1.862286	0.848355	-1.565333
H	-1.287108	0.890243	-2.984334
O	0.821263	3.452108	2.105566
H	1.146714	2.581844	2.407868
H	1.045748	3.464042	1.157457
O	3.669540	-0.066938	-1.048733
H	2.743301	-0.175773	-0.778183
H	3.986032	-0.973572	-1.248793
O	-0.419608	-0.665521	3.731411
H	-1.276929	-0.224742	3.542518
H	-0.405083	-1.437948	3.154194
O	4.325708	-3.045485	1.359917
H	3.454212	-3.193015	0.976707
H	4.349257	-2.095004	1.606302
O	-2.866872	0.629071	3.242923
H	-2.540502	1.394731	2.734252
H	-3.295553	0.067764	2.572249
O	1.193170	2.996573	-0.761861
H	0.295396	3.303504	-1.010652
H	1.063678	2.068695	-0.504149
O	-3.825610	-3.682335	0.645646
H	-4.571491	-4.232873	0.381875
H	-3.279389	-3.584015	-0.162903
O	1.717550	0.774930	2.615818
H	0.997160	0.293176	3.076820
H	1.529750	0.611745	1.676528
O	4.634696	-2.680566	-1.386764
H	3.936413	-3.173486	-1.832602
H	4.534655	-2.896375	-0.433861
O	-4.114763	-0.902153	-2.083972
H	-4.199351	-0.805284	-1.119667
H	-3.490998	-0.200851	-2.344610
O	4.314669	-0.283737	1.780374
H	4.164487	-0.112783	0.831201
H	3.488189	-0.001165	2.210042
O	-3.850313	-0.860934	0.904706
H	-3.879485	-1.839011	0.929762
H	-2.943218	-0.654746	0.620394
O	-1.486820	3.732983	-1.282238
H	-1.722336	2.941176	-1.802285
H	-1.712549	3.487805	-0.366776
O	-1.785604	2.592433	1.408742
H	-1.550783	1.775393	0.935774
H	-0.926064	2.931893	1.736474
O	0.226855	0.264391	-3.794880
H	1.022026	0.765314	-3.508182
H	0.319421	-0.602583	-3.383461
O	2.484982	1.732934	-3.005254
H	2.999494	1.092701	-2.481027
H	2.062387	2.295625	-2.329294
O	-2.375899	-3.104245	-1.699671
H	-1.587196	-2.705700	-1.304638
H	-2.956014	-2.342850	-1.910518
C	-0.150538	-0.506423	-0.053743

B3LYP_Radical_18_s3

Eopt -1640.285527

O	-1.062780	-0.087246	0.215028
O	1.067260	-0.293132	-0.344391
O	-0.168044	1.392780	-1.081114

O	1.078038	-1.936946	-2.716967
H	1.173005	-1.444989	-1.884596
H	0.205578	-1.641172	-3.046353
O	-0.509037	-2.716464	3.114959
H	-0.599152	-1.751639	3.243655
H	-1.113639	-2.901926	2.374440
O	-4.408850	0.304790	-0.083706
H	-5.370548	0.290934	-0.019668
H	-4.196199	1.050040	-0.690019
O	1.740447	1.132216	3.598636
H	2.383417	0.542034	3.154560
H	1.946129	1.072144	4.539746
O	-2.035220	3.406440	0.368324
H	-1.254151	2.918337	0.072872
H	-2.440209	2.831904	1.052398
O	3.542166	-0.554038	2.287870
H	2.963210	-1.300897	2.066666
H	3.732842	-0.133119	1.424591
O	-2.142694	-2.804511	0.701436
H	-3.000712	-2.624207	1.099578
H	-1.753943	-1.914995	0.560887
O	4.095534	3.251038	-0.436186
H	4.594124	3.489649	-1.226394
H	3.167141	3.507597	-0.621557
O	-0.834270	0.128401	3.107107
H	0.051214	0.493739	3.317513
H	-0.843734	0.066964	2.138418
O	-3.613307	2.387025	-1.727134
H	-2.999216	1.959445	-2.336098
H	-3.045247	2.807292	-1.046190
O	3.699182	-0.573980	-3.163475
H	3.795216	-0.197780	-2.270303
H	2.828832	-1.003477	-3.152935
O	-3.308852	1.689764	2.205295
H	-3.675589	1.111950	1.509189
H	-2.571383	1.194292	2.593382
O	3.802175	0.475399	-0.421893
H	3.935453	1.446706	-0.437359
H	2.837533	0.351705	-0.433926
O	1.282587	-4.269212	-0.975334
H	1.159039	-3.571731	-1.642376
H	1.417707	-3.781174	-0.143892
O	1.684497	-2.549135	1.349133
H	1.379340	-1.819800	0.781407
H	0.966171	-2.650623	2.009461
O	-1.466541	-0.818275	-3.404036
H	-2.171346	-1.158202	-2.809335
H	-1.262796	0.062176	-3.064109
O	-3.510309	-1.824232	-1.771531
H	-3.859856	-1.091793	-1.224640
H	-3.040866	-2.383029	-1.132384
O	1.424414	3.857729	-0.966728
H	0.929808	3.021989	-0.925790
H	1.049267	4.416900	-0.275263
C	-0.027934	0.324576	-0.399654

B3LYP_Radical_24_s1

Eopt -2099.043196

O	-0.810330	0.899795	0.929281
O	0.994857	-0.096681	0.114311
O	-1.009724	-1.021970	-0.034785
O	-3.199142	-1.816579	-1.827297
H	-3.204160	-1.119396	-2.519608
H	-2.476667	-1.544497	-1.240964
O	-1.140561	-3.387722	-3.138125
H	-1.942916	-2.974749	-2.767290
H	-0.651101	-3.688549	-2.351716
O	2.789576	1.990038	0.966378
H	2.646410	2.303853	1.885731
H	2.154498	1.263589	0.846616
O	-4.690597	-1.708821	0.663683

H	-3.996515	-2.084717	1.233814
H	-4.322033	-1.764713	-0.236623
O	1.940434	2.922065	-1.547461
H	1.230367	2.289101	-1.705523
H	2.243024	2.723011	-0.636470
O	2.461174	-2.337744	-1.053395
H	2.658108	-2.042330	-1.970563
H	1.967615	-1.592365	-0.668782
O	0.160046	-3.853609	-0.571649
H	-0.386520	-3.092957	-0.327776
H	1.018751	-3.444888	-0.809843
O	2.280321	2.641171	3.642737
H	1.565677	1.956313	3.741550
H	1.847733	3.469345	3.741274
O	-1.284990	3.913706	0.999337
H	-0.715559	4.358671	0.334467
H	-1.010573	2.987856	0.982783
O	-2.702840	2.640484	-2.620479
H	-2.853672	3.393042	-3.225978
H	-3.141574	2.884034	-1.783605
O	0.375959	5.181569	-0.862385
H	0.924237	4.422470	-1.169085
H	-0.163393	5.422111	-1.611758
O	-2.806247	0.116393	-3.811734
H	-2.824600	1.004281	-3.400214
H	-1.863371	-0.125011	-3.840206
O	-2.292916	-2.474211	2.222007
H	-1.860467	-1.978554	1.506793
H	-2.244641	-1.879589	3.000913
O	-0.024139	-0.832584	-3.545236
H	0.002246	-0.481715	-2.662262
H	-0.353347	-1.761669	-3.433012
O	2.838126	-1.232342	-3.578889
H	1.883763	-1.054074	-3.669065
H	3.229469	-0.399796	-3.237806
O	-3.846768	0.907367	1.358906
H	-2.884460	0.821961	1.294316
H	-4.190032	0.034107	1.079149
O	0.291130	-3.795868	2.402836
H	-0.605740	-3.414466	2.456143
H	0.394412	-3.999335	1.457739
O	1.932983	-1.515117	2.628849
H	1.379647	-2.325508	2.589140
H	1.781585	-1.086304	1.772390
O	0.302645	0.569256	3.696436
H	-0.109453	0.834180	2.859448
H	0.878271	-0.182744	3.444767
O	5.051292	0.544702	0.087549
H	4.338432	1.082564	0.484610
H	4.868173	-0.365336	0.395650
O	-2.060905	-0.832058	4.475795
H	-1.241211	-0.320602	4.269152
H	-2.761409	-0.190381	4.473965
O	-3.780523	3.301290	-0.162765
H	-2.939349	3.610982	0.234050
H	-3.944156	2.449772	0.287413
O	4.040075	1.076182	-2.515941
H	3.345114	1.718707	-2.290351
H	4.423313	0.823586	-1.650573
O	4.410232	-2.087836	0.956949
H	3.785678	-1.964092	1.689681
H	3.826095	-2.254636	0.190112
C	-0.243174	-0.067930	0.326350

B3LYP_Radical_24_s2

Eopt -2099.036896

O	1.270978	0.105077	-0.856006
O	-0.740107	-0.417732	-0.018600
O	1.116362	-1.215919	0.937941
O	2.458067	0.120412	2.919642
H	2.227757	1.065064	2.807407

H	2.001327	-0.325185	2.170760
O	-0.059694	-0.470247	4.243727
H	0.845765	-0.257358	3.947453
H	-0.249669	-1.316058	3.799893
O	-2.132187	0.945226	-1.856401
H	-1.632280	0.982860	-2.695897
H	-1.556144	0.429477	-1.233672
O	4.703857	-1.252981	1.602534
H	4.188499	-1.956867	1.168524
H	4.055085	-0.774951	2.148323
O	-2.537131	2.996232	-0.016624
H	-2.183858	2.614990	0.798607
H	-2.362719	2.314960	-0.707105
O	-2.779449	-1.809511	1.372408
H	-2.761974	-2.720317	1.011633
H	-2.062492	-1.344438	0.891156
O	-0.375016	-2.852274	2.513347
H	0.143452	-2.238299	1.934004
H	-1.300469	-2.642706	2.294353
O	-0.470530	0.923718	-4.163589
H	-0.056188	0.068984	-3.943837
H	0.099939	1.571982	-3.705137
O	1.134303	2.437681	-2.388606
H	0.584185	3.115260	-1.938846
H	1.084943	1.644098	-1.810565
O	2.034285	4.568565	0.675630
H	1.291020	4.781774	0.096053
H	2.229667	5.393969	1.176111
O	-0.277138	4.441940	-1.032944
H	-1.019930	3.998345	-0.581247
H	0.397285	4.617012	-0.352530
O	1.321004	2.693388	2.644825
H	1.547770	3.323375	1.931814
H	0.453036	2.316811	2.412290
O	2.901480	-3.124853	0.144831
H	2.286869	-2.387146	0.364625
H	3.091198	-3.023279	-0.809542
O	-1.187691	1.258424	2.276337
H	-1.061474	0.708314	1.477626
H	-0.863813	0.688796	3.007456
O	-3.947287	0.457627	2.573163
H	-3.050758	0.841499	2.530898
H	-4.412433	0.834680	1.797894
O	3.992484	0.458552	-0.622879
H	3.026093	0.267264	-0.652584
H	4.324940	-0.052441	0.137278
O	0.321451	-4.526450	0.145538
H	1.231079	-4.182018	0.070728
H	-0.010138	-4.114594	0.963470
O	-1.088227	-2.856726	-1.687441
H	-0.610696	-3.480855	-1.100967
H	-1.108431	-2.029879	-1.173803
O	0.939159	-1.435310	-3.159703
H	1.114346	-0.846361	-2.392995
H	0.253391	-2.040844	-2.816348
O	-4.629674	-0.274414	-1.802007
H	-3.741766	0.128867	-1.910963
H	-4.443454	-1.191888	-1.520620
O	3.335547	-2.867371	-2.652315
H	2.512676	-2.389403	-2.887385
H	3.034884	-3.712220	-2.297634
O	3.564830	3.197253	-1.170616
H	2.771797	2.994181	-1.706220
H	3.845950	2.318918	-0.846688
O	-5.128713	1.597368	0.273910
H	-4.355400	2.175891	0.153989
H	-5.021651	0.904512	-0.409669
O	-3.915174	-2.905453	-0.932534
H	-3.054504	-3.023929	-1.373902
H	-3.650789	-2.555237	-0.055406

C	0.553631	-0.505562	0.020447
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B3LYP_Radical_24_s3

Eopt -2099.049633

O	-1.174257	-1.665510	-0.317814
O	-0.333086	0.360847	0.122546
O	-1.894035	-0.540049	1.381605
O	-0.820092	-2.294278	3.606429
H	0.154217	-2.209142	3.527284
H	-1.170873	-1.735909	2.901140
O	2.546405	2.517867	2.600669
H	1.615480	2.724436	2.361261
H	2.596941	2.580935	3.561563
O	1.226084	0.471422	-2.346982
H	0.892184	-0.236757	-2.940806
H	0.667711	0.417685	-1.553318
O	-5.747778	-2.385666	0.903472
H	-5.425450	-1.463918	0.813211
H	-5.779848	-2.548834	1.854211
O	3.675498	0.081613	-0.988548
H	3.312691	0.040184	-0.079557
H	2.875221	0.136381	-1.552623
O	-0.032063	2.890306	1.665839
H	0.040437	3.495489	0.898703
H	-0.199714	2.019310	1.266358
O	-2.487059	3.709407	2.736074
H	-2.703078	3.155146	3.494010
H	-1.614826	3.391480	2.421149
O	0.234305	-1.640907	-3.885365
H	-0.718683	-1.520019	-3.721907
H	0.485181	-2.330402	-3.241011
O	0.735677	-3.466905	-1.721793
H	0.169013	-2.939453	-1.136634
H	0.231161	-4.269731	-1.901011
O	3.033769	-4.421080	2.292107
H	3.930799	-4.558281	2.621236
H	2.532435	-5.184698	2.602638
O	4.991627	-2.408853	-1.307458
H	4.513230	-1.564069	-1.210100
H	4.349927	-3.093531	-1.035277
O	1.966310	-2.044851	3.461685
H	2.326745	-2.859177	3.063756
H	2.113231	-1.349454	2.788473
O	-4.632459	0.194257	0.515296
H	-3.745373	-0.073986	0.798979
H	-4.573408	0.242814	-0.465470
O	2.335839	-0.041378	1.502103
H	1.460603	0.030494	1.090335
H	2.470070	0.819774	1.952209
O	4.312736	4.111243	0.993490
H	3.712214	3.599064	1.563076
H	4.279925	3.662621	0.124399
O	-3.435912	-3.693097	-0.110895
H	-2.758770	-3.003466	-0.112087
H	-4.227237	-3.256898	0.258965
O	-4.061911	3.001623	0.530329
H	-4.311586	2.064059	0.622974
H	-3.550667	3.217455	1.337871
O	-2.044998	2.603846	-1.341350
H	-2.759906	2.762081	-0.683984
H	-1.557591	1.844876	-0.990204
O	-2.475924	-1.430439	-2.909657
H	-2.106846	-1.579206	-2.021460
H	-2.926121	-2.253937	-3.134750
O	1.752776	3.247132	-2.727306
H	1.511696	2.301970	-2.675546
H	1.181852	3.685539	-2.067928
O	-4.453790	0.450538	-2.253323
H	-3.791847	-0.225856	-2.507978
H	-3.959089	1.279295	-2.279081
O	3.152388	-4.411933	-0.563711

H	2.299006	-4.071146	-0.891340
H	3.082601	-4.411841	0.409025
O	4.259012	2.821185	-1.506917
H	4.150331	1.876859	-1.279788
H	3.407372	3.056081	-1.929925
O	0.015622	4.337252	-0.748204
H	-0.218931	5.271620	-0.780967
H	-0.792593	3.842147	-1.015139
C	-1.104549	-0.601137	0.369414

B3LYP_Radical_27_s1

Eopt -2328.419727

O	0.551066	1.032798	-0.522125
O	0.613660	-1.065392	-0.000756
O	-1.345679	-0.097561	-0.329363
O	-2.957820	-2.294798	0.712754
H	-2.703371	-3.067451	0.167065
H	-2.444568	-1.564128	0.329241
O	3.005988	4.248771	-0.748520
H	2.404259	4.285265	-1.518192
H	3.210584	3.300877	-0.627856
O	-0.806371	3.115426	1.073534
H	-1.688689	3.318813	0.694444
H	-0.371645	2.550567	0.415860
O	-1.924964	-1.881321	-2.739006
H	-1.166732	-1.598341	-3.297513
H	-1.815386	-1.359080	-1.930085
O	-2.055228	-4.276287	-1.102436
H	-1.931115	-3.564482	-1.757085
H	-1.203676	-4.334083	-0.630390
O	2.259157	-1.919260	-2.363456
H	3.087073	-1.393466	-2.287411
H	1.733272	-1.656165	-1.591728
O	-1.629997	-1.536716	3.150926
H	-2.053207	-1.849369	3.328304
H	-1.194259	-0.693708	2.924655
O	4.588475	-0.439898	-2.029047
H	5.162937	-1.012356	-1.507644
H	4.251590	0.232104	-1.396498
O	1.290485	4.406985	-3.020288
H	0.618456	5.064857	-2.809238
H	0.800025	3.568370	-3.134162
O	0.583023	-3.382041	3.040797
H	1.343921	-2.806051	2.835885
H	-0.170298	-2.766241	3.127558
O	-0.479137	1.137340	3.082463
H	-1.021274	1.368220	3.846682
H	-0.726868	1.789173	2.394414
O	2.935432	-4.353303	-1.016671
H	2.779771	-3.571191	-1.581552
H	2.116253	-4.412611	-0.489352
O	0.039049	1.864714	-3.276212
H	-0.923061	1.936990	-3.125301
H	0.373512	1.588282	-2.407014
O	-4.345817	-0.273189	-2.937188
H	-3.580842	-0.869847	-3.026402
H	-4.692400	-0.461286	-2.039931
O	-5.242581	-0.845284	-0.302242
H	-4.603133	-1.535587	-0.048857
H	-4.946310	-0.088528	0.238937
O	-3.914796	0.014816	3.927591
H	-3.614112	0.692747	4.543839
H	-3.136210	-0.558202	3.781427
O	2.009273	2.632062	3.465983
H	1.890856	3.358310	2.818842
H	1.191267	2.106863	3.398665
O	0.283660	-0.909334	-4.153760
H	0.201415	0.035783	-3.929919
H	1.019776	-1.234096	-3.598834
O	2.650018	-1.585304	2.135947
H	3.332980	-2.130560	1.683975

H	2.035380	-1.322820	1.433854
O	-3.899120	1.062298	1.332786
H	-3.937387	0.756478	2.264971
H	-3.043013	0.751285	1.006860
O	4.578996	-3.125325	0.859795
H	4.039550	-3.586541	0.178313
H	5.139079	-2.515532	0.365470
O	3.457662	1.468328	-0.350727
H	3.664556	1.306792	0.600717
H	2.519957	1.232625	-0.435767
O	0.421021	-4.062532	0.314815
H	0.425732	-3.952348	1.290975
H	0.446437	-3.149764	-0.007046
O	-2.619467	1.825359	-2.193240
H	-3.289962	1.199398	-2.542224
H	-2.156900	1.294416	-1.523665
O	1.497700	4.684366	1.582917
H	2.026534	4.550476	0.767812
H	0.632951	4.281377	1.380865
O	3.918766	0.950164	2.317044
H	3.258492	1.540933	2.740181
H	3.507356	0.063395	2.327605
O	-3.377992	3.511588	0.003144
H	-3.714964	2.801480	0.580085
H	-3.215127	3.051686	-0.842402
C	-0.090857	-0.038916	-0.284186

B3LYP_Radical_27_s2

Eopt -2328.423567

O	-1.004478	-0.464234	-0.295507
O	0.481849	1.161999	-0.388855
O	1.202839	-0.889888	-0.263938
O	4.141041	-0.349731	0.330559
H	4.353057	0.278062	-0.394476
H	3.225017	-0.636619	0.119785
O	-5.243659	-0.671555	-0.543841
H	-5.156105	-1.055072	-1.444782
H	-4.584902	0.055244	-0.503106
O	-1.842000	-2.641526	1.498550
H	-1.305656	-3.467388	1.344332
H	-1.588133	-2.015015	0.823220
O	2.472827	-0.510406	-2.966973
H	1.686848	-0.303358	-3.474434
H	2.180322	-0.622273	-2.052152
O	4.361870	1.432032	-1.835746
H	3.736346	0.835239	-2.363495
H	3.843795	2.058618	-1.385207
O	-0.317534	2.552171	-2.929828
H	-1.229568	2.830653	-2.722586
H	-0.012521	2.054722	-2.142696
O	2.996266	0.659823	2.705391
H	3.498005	0.399007	1.914551
H	2.063827	0.593715	2.459107
O	-2.833555	3.487369	-2.036217
H	-2.420120	4.151173	-1.495806
H	-3.004339	2.749305	-1.456400
O	-4.503158	-2.053271	-2.940713
H	-4.815589	-1.847807	-3.816185
H	-3.539658	-1.903300	-2.964662
O	2.997279	3.534720	2.366881
H	2.066939	3.783208	2.568976
H	3.049130	2.573401	2.537960
O	-1.070591	-1.059800	3.641948
H	-0.885412	-1.600637	4.455691
H	-1.321889	-1.728327	3.000456
O	0.870240	4.850998	-1.666762
H	0.506534	4.143381	-2.261093
H	1.603305	4.419072	-1.230404
O	-1.732720	-1.604494	-2.928434
H	-1.324839	-2.474531	-2.715039
H	-1.625461	-1.113639	-2.093614

O	3.181548	-3.350970	-2.636769
H	3.019283	-2.375247	-2.794413
H	3.652678	-3.332614	-1.766726
O	4.491892	-3.234763	-0.058668
H	4.609390	-2.255132	-0.035908
H	3.687183	-3.337067	0.513585
O	2.992903	-1.938916	3.895860
H	3.911348	-2.241856	3.971224
H	3.063531	-1.008878	3.573987
O	-3.749617	-0.116683	3.610362
H	-4.134280	-0.751652	2.981806
H	-2.831857	-0.421176	3.730500
O	0.139408	0.081352	-4.323631
H	-0.494583	-0.538680	-3.887415
H	-0.085117	0.943144	-3.923599
O	0.317197	4.278918	2.895396
H	-0.130129	4.291633	2.022160
H	-0.536869	4.035834	3.698398
O	2.138966	-3.117767	1.534174
H	2.394546	-2.737191	2.386188
H	1.764430	-2.371921	1.018950
O	-0.959573	4.315210	0.402982
H	-0.318986	4.518297	-0.302037
H	-1.169017	3.374523	0.289695
O	-3.281875	1.340243	-0.345203
H	-3.349674	1.689376	0.571109
H	-2.470441	0.786697	-0.344491
O	2.715550	3.135643	-0.386919
H	2.878968	3.358943	0.580247
H	1.998949	2.486414	-0.340208
O	-0.630049	-3.920238	-1.861876
H	-1.164192	-3.767508	-1.034471
H	0.268801	-3.658671	-1.591444
O	-4.618438	-2.084881	1.763335
H	-4.824818	-1.637373	0.924183
H	-3.698287	-2.412221	1.670419
O	-3.537069	2.273828	2.241580
H	-3.576414	1.432620	2.760684
H	-2.715337	2.703392	2.507582
O	-0.233002	-4.936895	1.301528
H	0.576695	-4.415819	1.442747
H	-0.210051	-5.210795	0.385620
C	0.221746	-0.095039	-0.324275

B3LYP_Radical_27_s3

Eopt -2328.416706

O	1.096303	1.123159	0.674085
O	-0.314432	-0.287408	-0.102894
O	1.661552	-1.042317	0.552215
O	0.274426	-3.595370	-0.505717
H	-0.423730	-3.914787	0.110638
H	0.640577	-2.797192	-0.094821
O	0.632181	5.223112	0.691151
H	1.212297	5.019480	1.452326
H	-0.049550	4.522472	0.704772
O	2.892571	2.016946	-1.457202
H	3.712372	1.485755	-1.340735
H	2.371599	1.833086	-0.659179
O	1.328885	-2.881951	2.810017
H	1.418027	-2.225603	2.099220
H	0.521292	-3.362056	2.590535
O	-1.768387	-4.501475	1.127121
H	-1.481825	-4.552884	2.046141
H	-2.439423	-3.783994	1.102184
O	-2.209818	-0.389069	2.214783
H	-2.680670	0.473704	2.227580
H	-1.574725	-0.309628	1.486085
O	-0.916766	-2.607508	-2.819198
H	-0.488139	-2.944957	-2.002021
H	-0.466971	-1.776222	-3.009774
O	-3.447547	2.133340	2.176728

H	-4.089389	1.895247	1.486458
H	-2.700962	2.533308	1.685379
O	2.282233	4.601848	2.902874
H	1.950990	5.123893	3.642212
H	2.042845	3.677222	3.116208
O	-3.530591	-2.148329	-1.877238
H	-3.886295	-1.321372	-2.253875
H	-2.622945	-2.244742	-2.230336
O	1.018402	0.811677	-3.136177
H	0.396009	0.420120	-2.509675
H	1.730162	1.191353	-2.572597
O	-6.187401	-1.214687	1.077437
H	-6.786935	-1.617864	0.439156
H	-5.366595	-1.747994	1.030979
O	1.595321	1.901107	3.391257
H	2.397986	1.460426	3.697521
H	1.468794	1.590823	2.476865
O	3.401231	-4.673524	1.919173
H	2.699718	-4.082427	2.248754
H	3.271418	-4.690049	0.951025
O	2.876357	-4.679051	-0.889026
H	1.929023	-4.486356	-0.753175
H	3.230660	-3.820056	-1.186371
O	2.274317	-1.517540	-4.070944
H	1.804263	-0.698890	-3.806769
H	1.579610	-2.177697	-4.180689
O	-0.106885	3.454502	-3.390901
H	0.531095	3.942799	-2.828267
H	0.231635	2.539880	-3.393443
O	-0.528362	0.225771	4.483622
H	0.175833	0.797629	4.132593
H	-1.081532	0.004305	3.712528
O	-4.778240	0.243549	-2.832998
H	-4.881044	0.588720	-1.923903
H	-4.155584	0.843541	-3.258774
O	3.517893	-1.979890	-1.615522
H	3.080274	-1.850394	-2.485499
H	2.871106	-1.670024	-0.961317
O	-4.826887	0.929110	-0.092624
H	-5.394741	0.228685	0.298768
H	-3.942840	0.540415	-0.078013
O	-1.253537	3.110101	0.691572
H	-1.642104	3.127923	-0.213474
H	-0.618301	2.377976	0.682213
O	-3.655348	-2.438239	0.879263
H	-3.565830	-2.272087	-0.086351
H	-3.189198	-1.701372	1.323234
O	4.227340	-0.121822	1.717229
H	4.060043	0.707616	2.179967
H	3.353224	-0.410572	1.404262
O	1.848954	4.692945	-1.771156
H	1.457320	4.874013	-0.889538
H	2.349194	3.866723	-1.658988
O	-2.372933	3.254367	-1.829013
H	-1.583987	3.300998	-2.417574
H	-2.812711	2.424935	-2.049729
O	5.063009	0.335550	-0.976368
H	4.639930	-0.470264	-1.330707
H	4.897431	0.264640	-0.015681
C	0.858427	-0.093240	0.388547

B3LYP_Radical_30_s1

Eopt -2557.792218

O	-0.440206	0.582074	1.196041
O	-1.713282	-0.249199	-0.386501
O	0.148852	-1.271851	0.205601
O	1.839997	-1.222914	4.234709
H	2.115510	-1.654673	3.401335
H	1.824967	-0.274434	4.019595
O	3.580849	3.327787	-0.797399
H	2.881172	3.237558	-1.459085

H	3.443164	2.558159	-0.202009
O	5.509927	-0.399810	-0.193671
H	5.116328	-1.268877	-0.396459
H	4.807103	0.079277	0.277608
O	1.715956	1.421469	3.052815
H	1.565999	2.390171	3.134784
H	0.939187	1.100513	2.571791
O	-1.128210	-3.465146	1.925189
H	-0.995275	-3.048073	2.807118
H	-0.683544	-2.858878	1.314165
O	-5.015554	-2.635401	-1.160723
H	-5.396348	-1.741411	-1.298545
H	-4.627010	-2.596119	-0.271506
O	-0.545143	4.441931	-0.634083
H	-0.047344	3.723483	-1.066204
H	-0.866592	4.059128	0.206246
O	-1.463374	1.216013	-2.941028
H	0.129858	1.923788	-2.416563
H	-1.584709	0.698410	-2.128694
O	0.926193	2.277747	-1.968797
H	2.226352	1.340102	-3.078090
H	1.037252	1.719673	-1.188520
O	-6.059292	-0.044941	-1.549200
H	-6.049383	0.113269	-2.499823
H	-5.383957	0.562733	-1.179586
O	4.056176	-2.875898	-0.656025
H	3.540852	-2.679643	0.150419
H	3.565853	-2.454019	-1.395816
O	2.478690	-2.405588	1.716566
H	2.139182	-3.324003	1.802941
H	1.765448	-1.935519	1.257006
O	-0.823867	-2.145098	4.366810
H	0.085328	-1.776990	4.339516
H	-1.410255	-1.403201	4.136146
O	2.050004	-5.052612	-0.995104
H	1.362083	-4.492534	-1.401728
H	2.816081	-4.460043	-0.911977
O	-4.111751	1.565546	-0.324041
H	-3.753717	2.288734	-0.888372
H	-3.381652	0.929103	-0.267656
O	2.708836	-1.856963	-2.840323
H	1.792157	-2.175762	-2.816453
O	5.302265	1.507295	-2.307013
H	4.859922	2.221215	-1.811737
H	5.422201	0.796633	-1.644869
O	-3.928863	2.386057	2.398395
H	-3.588066	1.569095	2.805179
H	-4.074986	2.143490	1.461619
O	0.216772	-3.122699	-2.034275
H	-0.708298	-3.144458	-2.335073
H	0.198964	-2.523001	-1.275279
O	3.235892	1.048941	0.759478
H	2.792813	1.210635	1.621381
H	2.597534	0.530128	0.255162
O	-3.533883	-1.961825	1.379803
H	-2.816191	-2.595997	1.574662
H	-3.141560	-1.371906	0.718566
O	1.975735	5.242047	0.641727
H	2.588301	4.626886	0.194619
H	1.122105	5.092051	0.197227
O	1.083082	4.135162	3.087700
H	0.166612	3.942821	2.818182
H	1.483139	4.520233	2.281477
O	1.351646	-4.973924	1.750355
H	0.447100	-4.609768	1.819403
H	1.523068	-5.070039	0.787236
O	-2.559478	-2.278939	-2.462414
H	-3.445722	-2.485054	-2.090977
H	-2.203391	-1.621511	-1.841543
O	-2.915736	3.444039	-2.022809

H	-2.197563	3.897186	-1.543680
H	-2.459709	2.711463	-2.479701
O	-2.595365	-0.052449	3.323673
H	-3.018554	-0.702807	2.730607
H	-1.848310	0.279271	2.804341
O	-2.382482	-0.693829	-4.750068
H	-2.488593	-1.329569	-4.010493
H	-1.717755	0.608469	-3.666861
O	-1.332926	3.291392	1.829689
H	-2.265421	3.108153	2.073121
H	-0.969595	2.415141	1.629599
O	2.871996	0.824478	-3.594013
H	3.738805	1.038780	-3.189591
H	2.681459	-0.913383	-3.108175
H	-1.672633	-1.052975	-5.294249
C	-0.667908	-0.315706	0.326625

B3LYP_Radical_30_s2

Eopt -2557.800585

O	0.920647	0.936908	0.593128
O	2.698157	0.624765	-0.692202
O	1.459046	2.470766	-0.811903
O	-2.571126	2.071981	3.437244
H	-3.021600	2.363383	2.616648
H	-3.253517	1.995557	4.113693
O	-3.749514	-3.687307	-0.131681
H	-3.139051	-4.127661	-0.736112
H	-3.402262	-2.777480	-0.061388
O	-5.533431	-0.250566	-0.679380
H	-5.378926	0.602800	-1.118734
H	-4.664813	-0.479367	-0.302943
O	-1.329438	-0.095625	2.158847
H	-1.776694	0.588123	2.698443
H	-0.623642	0.370593	1.687736
O	0.581018	4.573585	1.141362
H	0.253348	4.183270	1.982431
H	0.757450	3.822212	0.554443
O	6.732905	-0.176688	-2.478568
H	6.683843	-0.558473	-1.574303
H	7.326052	0.578942	-2.402028
O	0.265918	-4.050713	1.036244
H	-0.124404	-3.617569	0.250498
H	0.300658	-3.358431	1.731151
O	1.705229	-1.819553	-2.060188
H	0.014626	-2.370639	-1.607572
H	1.978948	-1.023034	-1.577722
O	-0.811227	-2.809052	-1.318533
H	-2.020749	-2.429307	-2.863197
H	-1.330833	-2.135391	-0.846219
O	6.605039	-1.290423	0.058083
H	6.931853	-2.194078	-0.015377
H	5.676338	-1.374978	0.366129
O	-4.492454	2.282793	-1.840174
H	-4.266831	2.486613	-0.914393
H	-3.801272	1.644746	-2.115399
O	-3.415193	2.642584	0.846047
H	-2.904409	3.457024	0.619797
H	-2.849859	1.906370	0.578725
O	-0.173716	3.558052	3.631090
H	-1.017034	3.067386	3.610680
H	0.521841	2.873463	3.630593
O	-2.444068	4.279943	-2.596207
H	-1.713373	3.662176	-2.790525
H	-3.208231	3.700988	-2.426454
O	3.971625	-1.421271	0.959446
H	3.578585	-2.247440	0.596160
H	3.533558	-0.706648	0.465354
O	-2.423632	0.499897	-2.406947
H	-1.651002	1.021129	-2.696624
O	-5.208958	-2.510113	-2.385240
H	-4.854990	-3.070411	-1.672910

H	-5.399665	-1.668518	-1.925332
O	2.847785	-1.030653	3.527651
H	2.636213	-0.079249	3.523734
H	3.258618	-1.191583	2.653929
O	-0.401310	2.353802	-3.036373
H	0.057946	2.346177	-3.884146
H	0.294003	2.403248	-2.358487
O	-2.762196	-0.988997	-0.047121
H	-2.306363	-0.632545	0.744697
H	-2.561482	-0.377903	-0.785305
O	3.295718	3.934160	2.121471
H	2.453264	4.283069	1.778146
H	3.740970	3.570901	1.346654
O	-2.232392	-5.105537	1.929040
H	-2.843436	-4.621950	1.345538
H	-1.346690	-4.833898	1.615810
O	-1.684520	-3.797378	4.409281
H	-0.947868	-3.238013	4.107682
H	-1.970167	-4.259371	3.598333
O	-2.097864	4.944283	0.118326
H	-1.165643	4.866560	0.394746
H	-2.116086	4.767502	-0.845251
O	4.218313	0.803810	-3.177886
H	5.101037	0.468464	-2.910592
H	3.700701	0.834060	-2.356498
O	2.810526	-3.656692	-0.218584
H	2.004407	-3.872859	0.289216
H	2.477889	-3.108147	-0.956622
O	1.962588	1.695135	3.233957
H	2.546415	2.421490	2.931462
H	1.547446	1.385200	2.412533
O	2.957842	-1.285518	-4.485236
H	3.423172	-0.515331	-4.085736
H	2.071392	-1.699445	-2.963460
O	0.318367	-2.180825	3.132395
H	1.202039	-1.787065	3.300383
H	-0.256047	-1.436812	2.867517
O	-2.631317	-2.062488	-3.527134
H	-3.525858	-2.226950	-3.163957
H	-2.449146	-0.321083	-2.941494
H	2.342825	-0.908178	-5.124003
C	1.728263	1.325641	-0.318687

B3LYP_Radical_30_s3 Eopt -2557.803042

O	-0.066727	0.144367	-0.227184
O	1.796172	-0.529016	0.692343
O	0.317780	-1.998899	-0.102220
O	-0.729164	-1.019408	-4.254451
H	-1.137919	-1.556405	-3.547097
H	-0.583720	-0.148080	-3.840040
O	-3.351022	3.025451	1.155874
H	-2.729219	2.532678	1.728781
H	-3.343576	2.549868	0.299413
O	-5.607776	0.077666	-0.772948
H	-5.072657	-0.717035	-0.571780
H	-4.951744	0.715531	-1.106667
O	-0.248205	1.436429	-2.872733
H	-1.075351	1.932970	-2.911617
H	-0.232808	1.035979	-1.987358
O	2.084259	-3.529113	-1.856337
H	2.017540	-4.483460	-1.736998
H	1.423509	-3.138368	-1.259524
O	5.562377	-2.112698	1.552576
H	5.774601	-1.172605	1.728307
H	5.147372	-2.104966	0.669868
O	0.924953	4.773744	-0.177799
H	1.244414	5.681134	-0.246240
H	1.200775	4.334965	-1.019587
O	1.169821	1.367031	2.963828
H	-1.908366	1.705130	3.719506

H	1.418552	0.733812	2.273633
O	-1.620870	1.535446	2.814419
H	-4.890403	-0.170195	4.383145
H	-1.952635	0.632413	2.601455
O	6.054498	0.628788	1.998860
H	5.894017	0.793429	2.934781
H	5.279049	1.011066	1.534558
O	-3.900053	-2.077039	-0.135616
H	-3.209445	-2.115060	-0.829482
H	-3.463308	-1.657633	0.635745
O	-1.833225	-2.415721	-2.044165
H	-1.951926	-3.388371	-2.111603
H	-1.098109	-2.287278	-1.420913
O	1.879438	-2.037459	-4.308620
H	0.968598	-1.673408	-4.301735
H	1.919922	-2.618473	-3.528207
O	-3.885600	-4.850585	0.256926
H	-3.346093	-5.058004	1.028493
H	-3.906433	-3.870217	0.211706
O	3.889520	1.622744	0.541950
H	3.449163	2.381144	0.991389
H	3.221187	0.920177	0.554273
O	-2.678140	-0.913795	2.118979
H	-2.129869	-1.694406	2.337217
O	-5.731521	1.409654	1.720386
H	-4.962223	2.001743	1.631924
H	-5.748247	0.915440	0.873827
O	4.055149	2.211249	-2.216797
H	3.967227	1.341556	-2.655984
H	4.024153	2.012585	-1.259406
O	-0.958909	-3.131089	2.282010
H	-1.510446	-3.864710	1.984573
H	-0.486703	-2.837191	1.484744
O	-3.409482	1.785113	-1.375904
H	-3.158875	2.566287	-1.919313
H	-2.647856	1.193887	-1.396515
O	4.074341	-1.799882	-0.866670
H	3.535213	-2.543868	-1.200330
H	3.433819	-1.270654	-0.365981
O	-1.888883	5.121095	-0.184892
H	-2.305831	4.429926	0.364261
H	-0.926121	4.954395	-0.147560
O	-2.757277	4.153450	-2.630920
H	-2.014266	4.080116	-3.240525
H	-2.384771	4.545927	-1.808103
O	-2.398437	-5.146071	-2.093027
H	-1.610009	-5.676014	-1.930933
H	-2.885508	-5.136154	-1.240935
O	3.053407	-2.258999	2.802002
H	3.953677	-2.229868	2.411921
H	2.515831	-1.721318	2.200983
O	2.477800	3.592772	1.872327
H	1.921706	3.996203	1.176388
H	1.925808	2.893060	2.279944
O	3.968408	-0.380824	-3.340445
H	4.092735	-0.844815	-2.490110
H	3.201431	-0.837191	-3.741376
O	3.244653	-1.073781	5.319649
H	3.168161	-1.498430	4.439204
H	0.193442	1.421549	2.909212
O	1.637808	3.538635	-2.513958
H	2.498278	3.072989	-2.418413
H	0.985193	2.826479	-2.653360
O	-5.047453	-0.579963	3.525127
H	-5.309060	0.158518	2.928627
H	-3.456217	-0.917202	2.717385
H	3.168133	-1.796195	5.951742
C	0.704180	-0.816288	0.126687

D2_B3LYP_9_sl Eopt -952.384173

O	-1.126239	0.334043	-1.603782
O	1.101706	0.539785	-1.573249
O	0.048604	-0.466493	0.126865
O	2.209039	-0.073153	1.630508
H	1.431821	-0.210521	1.021223
H	2.629842	0.730291	1.303417
O	1.623718	2.635578	0.151013
H	1.564287	1.868458	-0.462285
H	1.133310	2.343993	0.930926
O	3.031795	-1.397955	-1.780529
H	3.334240	-1.663239	-0.893065
H	2.342009	-0.714255	-1.624471
O	-3.201474	0.435345	0.091017
H	-2.442107	0.330526	-0.543557
H	-2.766628	0.762353	0.892632
O	-1.026494	1.555799	1.755645
H	-0.632548	0.791204	1.286702
H	-1.161225	2.201719	1.039662
O	-1.313836	-2.832685	0.334085
H	-2.263004	-2.628180	0.425108
H	-0.876122	-1.957189	0.241022
O	-1.126803	3.098533	-0.710073
H	-0.166311	3.137859	-0.559923
H	-1.260427	2.222869	-1.117457
O	3.869645	-2.084229	0.855553
H	3.264635	-1.373951	1.179345
H	3.382439	-2.905520	0.981953
O	-4.047389	-2.092602	0.587385
H	-3.766005	-1.162034	0.404806
H	-4.394113	-2.416283	-0.251132
C	0.008206	0.127430	-1.029291

D2_B3LYP_9_s2 Eopt -952.384627

O	-1.288641	0.164574	-1.237115
O	0.912962	0.369568	-1.558562
O	0.150467	-0.669288	0.270143
O	2.490916	-0.045965	1.435371
H	1.659099	-0.325143	0.969795
H	2.629069	0.854696	1.106768
O	1.763411	2.483714	0.069145
H	1.548348	1.771378	-0.569817
H	1.105539	2.348997	0.773708
O	2.869593	-1.490065	-2.005480
H	3.436796	-1.555381	-1.215566
H	2.180377	-0.827296	-1.770794
O	-3.261915	0.012027	0.570218
H	-2.522233	0.090239	-0.089276
H	-2.888492	-0.611371	1.219636
O	-0.435688	1.704370	1.827324
H	-0.265596	0.815287	1.466345
H	-0.962184	2.134154	1.130640
O	-1.600945	-1.805209	1.949178
H	-1.919697	-2.614342	1.535222
H	-0.982204	-1.402261	1.284535
O	-1.383839	2.877978	-0.654629
H	-0.440549	3.079350	-0.712207
H	-1.438759	1.943976	-0.952872
O	4.454597	-1.568608	0.359482
H	3.747523	-1.023971	0.785632
H	4.306330	-2.465581	0.677780
O	-4.941572	-1.622223	-0.866390
H	-4.327477	-1.041874	-0.359551
H	-4.434880	-1.906290	-1.634516
C	-0.076522	-0.052711	-0.851184

D2_B3LYP_9_s3 Eopt -952.385216

O	-0.471665	0.700808	-1.014904
O	1.689461	0.269477	-1.381102
O	0.537597	-0.964851	0.098357
O	2.524063	-2.532929	1.082629

H	1.830477	-1.922998	0.726170
H	2.864114	-2.095010	1.870257
O	2.637053	2.779093	-0.819747
H	2.319032	1.872234	-1.045717
H	3.383511	2.642973	-0.226169
O	3.850781	-1.381037	-1.203970
H	3.630896	-1.906596	-0.416423
H	3.068341	-0.782833	-1.281890
O	-2.832175	-0.222372	-0.148581
H	-1.955393	0.145308	-0.451540
H	-2.632311	-1.168908	-0.024849
O	0.333911	0.697060	2.436747
H	0.403702	0.030451	1.724669
H	0.339659	1.542177	1.948233
O	-1.532447	-2.728433	0.219210
H	-1.527179	-3.242624	-0.595300
H	-0.772961	-2.100402	0.136582
O	0.152686	2.936966	0.609102
H	1.053442	3.050735	0.252360
H	-0.213622	2.238691	0.029095
O	-4.712209	0.014666	-2.179118
H	-4.016278	-0.078164	-1.492729
H	-4.246033	-0.064974	-3.017897
C	0.585009	-0.000896	-0.773011
O	-2.524790	0.549707	2.580600
H	-1.550859	0.607870	2.613319
H	-2.706726	0.292206	1.656105

D2_B3LYP_12_sl Eopt -1181.777618

O	0.332772	-0.491408	1.369166
O	0.390483	0.456905	-0.655163
O	-1.248860	-0.975868	-0.144039
O	1.231025	-1.118255	-2.795434
H	0.903587	-0.488340	-2.117183
H	0.696940	-1.914849	-2.620686
O	-0.824256	-2.145422	3.237675
H	-0.394920	-1.559249	2.572854
H	-1.665808	-2.368188	2.805103
O	1.419175	3.776223	0.772868
H	2.039024	3.083914	0.478048
H	0.642066	3.642466	0.193678
O	2.637730	-2.134429	1.071528
H	3.031768	-1.827733	0.234333
H	1.854516	-1.563574	1.193597
O	-3.419824	2.737649	-0.761192
H	-3.654074	2.643587	0.168727
H	-3.332024	1.817928	-1.098978
O	0.545451	1.907801	2.803930
H	0.825613	2.585248	2.162232
H	0.497667	1.080517	2.281855
O	-3.007968	-2.413161	1.377623
H	-2.370924	-1.863713	0.860753
H	-3.706790	-1.805683	1.642733
O	-0.611575	3.028353	-1.039749
H	-1.574439	3.015256	-0.876287
H	-0.328544	2.095680	-0.934461
O	3.701733	-1.047845	-1.390400
H	2.897723	-1.179887	-1.931923
H	3.565750	-0.167247	-0.994901
O	2.849901	1.393983	-0.065637
H	1.935753	1.030244	-0.220164
H	3.082617	1.096204	0.821849
O	-0.667765	-3.079033	-1.897445
H	-0.237908	-3.773192	-1.385831
H	-0.890787	-2.381679	-1.243600
O	-3.049448	0.190104	-1.792139
H	-2.328477	-0.212287	-1.245029
H	-2.657481	0.340939	-2.659366
C	-0.176573	-0.335191	0.196651

D2_B3LYP_12_s2 Eopt -1181.776357

O	-0.757504	0.178827	0.131728
O	1.249739	0.991054	-0.430862
O	-0.549897	2.310036	-0.539842
O	1.825892	0.387743	-3.069841
H	1.596170	0.665088	-2.153864
H	1.003820	0.462935	-3.567162
O	0.690076	-2.878404	1.745574
H	0.232878	-2.162581	2.226017
H	0.272930	-2.860395	0.862435
O	-3.437972	0.221481	-0.130581
H	-2.449240	0.224345	-0.030269
H	-3.613801	1.119311	-0.467613
O	4.248761	0.796316	1.874364
H	3.746836	0.049210	1.498741
H	3.859511	1.576942	1.436492
O	-0.439634	-2.359312	-0.846726
H	0.383726	-2.394016	-1.371845
H	-0.487194	-1.427877	-0.522022
O	-0.737368	-0.606251	2.747263
H	-0.212266	-0.014180	3.297542
H	-0.670590	-0.245562	1.830538
O	-3.143143	2.919907	-0.979109
H	-3.234857	2.976474	-1.936275
H	-2.196462	2.667495	-0.822888
O	-3.574766	-0.011196	2.720272
H	-3.644182	0.109391	1.754235
H	-2.631570	-0.210406	2.856734
O	2.961290	2.909880	0.426995
H	2.502435	3.489248	1.044810
H	2.271206	2.282541	0.095414
O	2.148398	-2.263101	-2.085689
H	2.034377	-1.409552	-2.548550
H	2.447677	-1.994348	-1.195525
O	2.643004	-1.150484	0.519234
H	2.062447	-0.410117	0.209191
H	2.052152	-1.738349	1.027672
O	-3.085118	-1.993763	-1.930957
H	-3.310024	-1.216708	-1.386464
H	-2.172510	-2.205565	-1.663021
C	-0.029588	1.174137	-0.281484

D2_B3LYP_12_s3 Eopt -1181.780159

O	0.271374	-0.996173	0.830129
O	0.386532	0.618543	-0.724102
O	-0.988072	-1.112508	-1.023206
O	2.636721	0.192396	-2.362471
H	1.816026	0.329250	-1.844261
H	2.846783	-0.753014	-2.237981
O	-1.020476	-3.188788	1.837446
H	-0.530120	-2.415332	1.469416
H	-1.826775	-3.201532	1.298077
O	-0.210003	4.251750	0.317410
H	0.474999	3.636559	0.639933
H	-0.752618	3.694482	-0.275313
O	2.999360	-1.507223	0.878959
H	3.427718	-0.656671	0.661535
H	2.037373	-1.302787	0.875202
O	-3.987120	1.824742	0.023101
H	-3.739185	1.822927	0.954247
H	-4.333927	0.922869	-0.152052
O	0.807530	0.472435	3.088882
H	1.566556	0.036939	3.492041
H	0.618583	-0.051574	2.274420
O	-3.045099	-2.549045	-0.161604
H	-2.240511	-2.042860	-0.467570
H	-3.156491	-3.264791	-0.797429
O	-1.602705	2.441195	-1.375670
H	-2.407310	2.174706	-0.889241
H	-0.937797	1.741054	-1.189776

O	4.062697	1.020656	-0.008295
H	3.691276	0.789214	-0.882402
H	3.335798	1.514433	0.421287
O	1.695055	2.223923	0.999946
H	1.220711	1.614362	0.371809
H	1.512786	1.819400	1.867266
O	3.309010	-2.509631	-1.697822
H	3.172673	-2.251582	-0.758506
H	2.559844	-3.074552	-1.917171
O	-5.065667	-0.687032	-0.519970
H	-4.355644	-1.362443	-0.435879
H	-5.277676	-0.658025	-1.459682
C	-0.119363	-0.503826	-0.306638

D2_B3LYP_18_s1 Eopt -1640.563559

O	-0.948536	0.156731	0.354576
O	1.256812	0.111621	0.005334
O	0.024166	-1.729363	-0.343427
O	2.604424	-1.146838	2.075931
H	2.190793	-0.675430	1.317751
H	1.925517	-1.807924	2.311322
O	-0.812549	3.714599	1.567382
H	-1.196055	3.400411	0.723763
H	-0.893682	2.945508	2.160018
O	-3.298544	-1.008219	0.952855
H	-2.407033	-0.678946	0.670006
H	-3.536925	-1.711124	0.317229
O	-0.073496	3.222691	-2.936123
H	0.841649	3.084473	-2.604039
H	-0.187464	2.576256	-3.641601
O	-4.592731	-0.734978	-2.788919
H	-5.520363	-0.737279	-3.050088
H	-4.513346	-0.021164	-2.117005
O	2.497327	2.950434	-1.887606
H	2.263327	2.982325	-0.938758
H	2.796740	2.030448	-2.018275
O	-0.808058	1.128235	2.958079
H	0.137923	1.164719	3.203260
H	-0.809828	0.804388	2.028910
O	2.623882	-1.855730	-3.725124
H	1.793980	-1.630319	-4.159776
H	2.366292	-2.381331	-2.932984
O	-1.764133	2.479891	-0.805784
H	-1.199094	2.722965	-1.567994
H	-1.374860	1.649555	-0.442900
O	-4.161959	-2.862923	-1.023744
H	-3.392943	-3.354694	-1.332730
H	-4.307708	-2.164028	-1.697171
O	4.389247	-1.928367	-0.091395
H	4.168332	-1.180274	-0.675777
H	3.885864	-1.749515	0.723787
O	-4.288193	1.116254	-0.740556
H	-4.029128	0.430209	-0.094543
H	-3.474283	1.638038	-0.875355
O	3.271424	0.174171	-1.826867
H	3.067230	-0.428952	-2.567669
H	2.509575	0.073754	-1.208799
O	2.015119	1.332999	3.423080
H	2.261023	0.443633	3.104939
H	2.041545	1.880947	2.615631
O	1.758373	2.641153	0.853472
H	1.481804	1.735998	0.560583
H	0.922476	3.100808	1.063747
O	0.304376	-2.898357	2.251578
H	-0.427289	-2.444546	2.715845
H	0.196545	-2.617933	1.321827
O	-1.894656	-1.499966	3.442195
H	-2.468942	-1.485875	2.653816
H	-1.494626	-0.609550	3.440627
O	2.080087	-3.180183	-1.352147

H	1.363127	-2.614168	-0.968046
H	2.892331	-2.876260	-0.907464
C	0.111408	-0.494328	-0.005735

D2_B3LYP_18_s2			Eopt -1640.56444
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O	1.092520	0.133692	0.282492
O	-1.103155	0.375873	-0.052413
O	-0.132243	-1.605358	-0.415037
O	-1.298998	2.039550	-2.231047
H	-1.157382	1.439768	-1.464037
H	-0.490648	1.948980	-2.777757
O	1.074108	2.573832	3.122865
H	1.218411	1.612350	3.217641
H	1.396420	2.767206	2.222300
O	3.565312	-0.485501	-0.665976
H	2.631350	-0.355116	-0.371797
H	3.554421	-1.307093	-1.193799
O	-0.974458	-1.621065	3.445246
H	-1.711411	-0.996748	3.262572
H	-0.931874	-2.185359	2.664309
O	1.760531	-3.440718	0.253191
H	1.098481	-2.739328	0.032805
H	2.368498	-3.014705	0.885349
O	-3.066396	0.174440	2.951339
H	-2.547480	0.968596	2.714785
H	-3.396274	-0.141446	2.087940
O	1.685771	2.796110	0.299227
H	0.896580	3.313429	0.046231
H	1.382733	1.854102	0.288339
O	-3.794974	-3.226637	-0.596157
H	-4.634905	-3.355204	-1.050789
H	-3.159863	-2.959867	-1.298170
O	1.470191	-0.264918	2.973644
H	0.649441	-0.730667	3.235033
H	1.344224	-0.109467	2.009738
O	3.431010	-3.044476	-1.927565
H	2.899351	-2.994354	-2.729562
H	2.796747	-3.269795	-1.209481
O	-3.496574	0.206880	-2.679230
H	-3.718266	0.065365	-1.742034
H	-2.775536	0.863586	-2.655801
O	3.608615	-1.920709	1.911023
H	3.752181	-1.406906	1.095706
H	2.925374	-1.417577	2.391375
O	-3.670607	-0.471890	0.212144
H	-3.763916	-1.423757	0.017791
H	-2.709239	-0.273178	0.091832
O	-0.804394	4.103972	-0.306192
H	-1.000111	3.496847	-1.046637
H	-1.142943	3.630863	0.476684
O	-1.497153	2.293345	1.859819
H	-1.272236	1.615231	1.176935
H	-0.674493	2.408500	2.374155
O	1.044267	1.818189	-3.779042
H	1.810446	1.844723	-3.162857
H	1.044230	0.925782	-4.142747
O	3.180632	2.031859	-2.000492
H	3.403369	1.138026	-1.676184
H	2.699151	2.430336	-1.248090
O	-1.922911	-2.220368	-2.392130
H	-1.290770	-1.966165	-1.676849
H	-2.416126	-1.401897	-2.588083
C	-0.047783	-0.373983	-0.063752

D2_B3LYP_18_s3			Eopt -1640.556657
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O	-0.984386	0.292968	-0.114673
O	1.194634	0.061310	0.351038
O	0.185565	-1.368767	-1.039971
O	1.179569	-0.246294	3.049052
H	1.152176	-0.101377	2.073340

H	0.370692	-0.766000	3.217761
O	-0.654331	4.032865	-0.506982
H	-0.876283	3.404227	-1.223128
H	-1.085547	3.637238	0.270696
O	-4.506496	-0.484461	0.256859
H	-5.467162	-0.544606	0.311769
H	-4.187670	-1.413600	0.189508
O	1.077783	1.477162	-3.695814
H	1.831633	1.627621	-3.083549
H	1.187890	2.131286	-4.394767
O	-2.081263	-2.186079	-2.244071
H	-1.260573	-1.838268	-1.806063
H	-2.632574	-1.396739	-2.402736
O	3.211161	1.922396	-1.936442
H	2.733694	2.345332	-1.194888
H	3.493627	1.068187	-1.558194
O	-1.845032	2.272959	1.504795
H	-2.703145	2.470307	1.110385
H	-1.456639	1.563074	0.929028
O	4.022237	-3.007019	-1.582931
H	4.700756	-3.452178	-1.063310
H	3.166663	-3.295556	-1.190531
O	-1.342603	1.911517	-2.290826
H	-0.537079	1.775297	-2.830997
H	-1.210527	1.320664	-1.512948
O	-3.420223	-3.019312	0.013472
H	-2.778429	-3.046567	0.733031
H	-2.899195	-2.780115	-0.790043
O	3.895787	-1.189397	2.467112
H	3.918282	-0.955231	1.521769
H	2.995805	-0.954449	2.751269
O	-3.729719	0.176663	-2.470841
H	-3.983661	0.069282	-1.535415
H	-2.985566	0.803287	-2.470522
O	3.745196	-0.448558	-0.372023
H	3.859667	-1.309422	-0.820046
H	2.778041	-0.371462	-0.175553
O	1.636477	2.601747	3.245015
H	1.419944	1.655193	3.317024
H	1.679678	2.755679	2.283250
O	1.734952	2.744300	0.354292
H	1.456150	1.796642	0.369223
H	0.949016	3.233326	0.038661
O	-1.249508	-1.791328	3.028761
H	-1.971426	-1.134058	2.916252
H	-1.063340	-2.104189	2.135445
O	-3.282648	0.104368	2.771382
H	-3.761741	-0.123336	1.950233
H	-2.751680	0.880348	2.515031
O	1.580614	-3.592383	-0.458109
H	1.090514	-2.752038	-0.653900
H	1.124803	-4.275184	-0.962511
C	0.126844	-0.339976	-0.266224

D2_B3LYP_24_sl			Eopt -2099.349747
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O	1.221770	0.195054	-0.865412
O	-0.783143	-0.350722	-0.027208
O	1.074868	-1.229323	0.849619
O	2.479181	-0.139495	2.940615
H	2.230314	0.806839	2.974556
H	1.995930	-0.483571	2.155933
O	0.033521	-0.954023	4.274892
H	0.924857	-0.694992	3.973168
H	-0.170029	-1.739421	3.734186
O	-2.136518	1.041669	-1.888653
H	-1.623349	1.122759	-2.716301
H	-1.566638	0.516949	-1.268961
O	4.700682	-1.335545	1.468983
H	4.177074	-2.013125	1.003876
H	4.064453	-0.904229	2.067096

O	-2.538725	3.053753	-0.022641
H	-2.186505	2.648388	0.780038
H	-2.364846	2.393178	-0.730777
O	-2.794478	-1.857423	1.277192
H	-3.284754	-1.185239	1.793497
H	-2.085362	-1.347792	0.829124
O	-0.386245	-3.026843	2.264664
H	0.118531	-2.350772	1.744606
H	-1.316070	-2.793651	2.092539
O	-0.453163	1.197952	-4.194607
H	-0.056627	0.321825	-4.035366
H	0.104897	1.798048	-3.660961
O	1.104591	2.592159	-2.286254
H	0.572545	3.267629	-1.814580
H	1.035136	1.778078	-1.741604
O	1.924636	4.269875	1.029002
H	2.321404	5.078836	1.371425
H	2.575577	3.899529	0.388094
O	-0.232413	4.580184	-0.808161
H	-1.015900	4.108247	-0.468227
H	0.438192	4.530673	-0.100253
O	1.313812	2.431413	3.063273
H	1.536481	3.057696	2.346285
H	0.452040	2.045827	2.819514
O	2.867807	-3.072714	-0.070760
H	2.250341	-2.355739	0.204410
H	3.073184	-2.881468	-1.008072
O	-1.149341	0.987836	2.548019
H	-1.047752	0.574388	1.669126
H	-0.812487	0.311531	3.173547
O	-3.942303	0.331763	2.648731
H	-3.026817	0.670888	2.673256
H	-4.353559	0.765653	1.872498
O	3.956036	0.435615	-0.686918
H	2.984777	0.268001	-0.703296
H	4.290105	-0.095376	0.058955
O	0.319998	-4.504493	-0.175635
H	1.224679	-4.142734	-0.226592
H	-0.014183	-4.155724	0.671000
O	-1.114994	-2.723643	-1.861564
H	-0.623489	-3.377371	-1.319403
H	-1.143748	-1.930384	-1.298995
O	0.896399	-1.206658	-3.254312
H	1.042148	-0.651137	-2.457014
H	0.216318	-1.839479	-2.952923
O	-4.636012	-0.188899	-1.825322
H	-3.751974	0.217739	-1.941997
H	-4.444792	-1.117350	-1.585162
O	3.368372	-2.509260	-2.814255
H	2.514783	-2.075637	-3.024516
H	3.996498	-1.782133	-2.730974
O	3.535885	3.199681	-0.937154
H	2.757242	3.074643	-1.515622
H	3.804107	2.282332	-0.725580
O	-5.062998	1.570732	0.369574
H	-4.312986	2.174810	0.229801
H	-4.977760	0.911731	-0.349653
O	-3.923229	-2.848423	-1.072755
H	-3.064961	-2.946167	-1.521647
H	-3.658533	-2.539080	-0.181313
C	0.508257	-0.457572	-0.015064

D2_B3LYP_24_s2

O	1.167617	0.640746	-0.513867
O	-0.707048	-0.454367	0.032945
O	1.264491	-1.143088	0.828310
O	2.364451	-0.154174	3.132205
H	1.941805	0.723310	3.230313
H	1.998018	-0.487738	2.282029
O	0.023048	-1.591719	4.156754

Eopt -2099.343698

H	0.856467	-1.124809	3.959732
H	-0.011047	-2.296548	3.483394
O	-2.190705	0.842161	-1.794942
H	-1.616711	1.213956	-2.493182
H	-1.577637	0.394046	-1.156095
O	4.841701	-0.607723	1.634970
H	4.490682	-1.311549	1.058429
H	4.102781	-0.395747	2.233270
O	-3.464595	2.570482	-0.094076
H	-3.135218	2.335832	0.782527
H	-2.986772	1.968320	-0.714089
O	-2.452088	-2.552251	0.871054
H	-2.717120	-2.983013	0.039833
H	-1.874050	-1.815151	0.589323
O	0.089532	-3.371692	1.840639
H	0.494332	-2.547183	1.468672
H	-0.846611	-3.298784	1.574194
O	-0.301220	1.861574	-3.688680
H	0.242054	1.053297	-3.650060
H	0.080068	2.432656	-2.997502
O	0.660789	3.235226	-1.279202
H	-0.217837	3.634082	-1.104917
H	0.650913	2.312991	-0.940179
O	1.148115	4.242535	1.461593
H	1.077718	3.915643	0.546706
H	0.380150	4.815335	1.573946
O	-1.702267	4.649753	-0.777861
H	-2.357773	3.984274	-0.482235
H	-1.460794	5.137832	0.017854
O	0.734362	2.148849	3.315032
H	0.856799	2.838923	2.633471
H	-0.039355	1.626122	3.030825
O	3.453518	-2.452629	-0.169618
H	2.690548	-1.903074	0.122586
H	3.647278	-2.159942	-1.083002
O	-1.444578	0.368458	2.669149
H	-1.250548	0.097618	1.749751
H	-1.027368	-0.327201	3.218193
O	-4.298233	0.095618	2.778420
H	-3.327668	0.162863	2.707274
H	-4.630728	0.120538	1.862587
O	3.872327	1.159077	-0.437105
H	2.920363	0.909223	-0.408901
H	4.285830	0.664390	0.292965
O	1.275053	-4.327941	-0.654100
H	2.091917	-3.799862	-0.574166
H	0.828177	-4.180317	0.200346
O	-0.398533	-2.547185	-2.090869
H	0.196661	-3.182074	-1.635760
H	-0.605956	-1.883849	-1.408568
O	1.365809	-0.456418	-3.096139
H	1.384317	-0.016626	-2.219384
H	0.781456	-1.222559	-2.943255
O	-4.317789	-0.958090	-2.109666
H	-3.548113	-0.353807	-2.093894
H	-3.936992	-1.849620	-2.015270
O	3.901458	-1.655613	-2.859490
H	3.019456	-1.254301	-3.010639
H	3.902298	-2.463841	-3.384610
O	3.507524	3.828289	-1.269412
H	2.537744	3.787449	-1.301893
H	3.756752	2.946933	-0.932241
O	-5.415228	0.397973	0.137254
H	-4.902504	1.218826	0.036391
H	-5.078041	-0.176741	-0.579017
O	-3.010106	-3.484330	-1.787934
H	-2.076564	-3.293508	-2.019459
H	-3.206427	-4.359091	-2.140769
C	0.579669	-0.312616	0.118591

D2_B3LYP_24_s3 Eopt -2099.344016

O 0.542731 -1.151822 -0.778454
O -1.134992 0.274360 -0.420774
O -0.925293 -1.551015 0.859462
O 0.524271 -1.684725 3.239413
H 0.768214 -0.759439 3.446916
H 0.023779 -1.620218 2.400017
O -3.040113 0.783549 3.470914
H -3.266809 0.050012 2.858669
H -3.792854 1.384287 3.433619
O 0.264517 1.865634 -2.092531
H 0.992280 1.368353 -2.519400
H -0.228656 1.211994 -1.531742
O 1.914060 -3.896630 2.143157
H 1.171234 -4.158972 1.568966
H 1.562715 -3.121549 2.623541
O 1.148041 3.348381 0.058216
H 0.602619 3.016166 0.785409
H 0.875592 2.807399 -0.720458
O -3.825045 0.333612 -0.754352
H -4.053713 -0.315640 -1.429993
H -2.841584 0.271558 -0.652491
O -3.472990 -1.294561 1.638427
H -2.512109 -1.336439 1.380411
H -3.869189 -0.788289 0.908168
O 2.412261 0.441980 -3.280940
H 1.981367 -0.421637 -3.395614
H 2.999278 0.320547 -2.506191
O 4.112423 0.083798 -1.033408
H 3.950639 0.857983 -0.447697
H 3.752822 -0.694333 -0.566450
O 3.723919 1.658149 3.246765
H 4.293321 0.912918 3.473798
H 4.015677 2.381234 3.815070
O 3.751799 2.355638 0.499916
H 2.844515 2.694770 0.358586
H 3.784402 2.109472 1.442969
O 0.985757 1.038842 3.742558
H 1.900575 1.284023 3.514498
H 0.415903 1.379038 3.026316
O -0.515590 -4.225681 0.543651
H -0.588972 -3.244751 0.644582
H -0.457227 -4.362812 -0.422336
O -1.008230 1.888482 1.865651
H -1.066126 1.323057 1.063703
H -1.712403 1.545445 2.457237
O -2.297966 4.393062 1.302439
H -1.852252 3.542238 1.473665
H -1.802255 4.780243 0.555741
O 2.880453 -2.267573 -0.016295
H 1.984321 -1.918295 -0.232477
H 2.730799 -2.823423 0.770568
O -3.420303 -4.013507 0.602916
H -2.462490 -4.191464 0.666204
H -3.531930 -3.134525 1.011574
O -3.144778 -3.156716 -2.058457
H -3.301017 -3.444907 -1.133008
H -2.819357 -2.251976 -1.979072
O 1.053590 -2.216339 -3.206226
H 0.820264 -1.828621 -2.329867
H 1.892337 -2.669681 -3.058885
O -1.668313 3.745788 -2.937853
H -1.009465 3.052202 -2.740211
H -2.523193 3.386063 -2.625673
O -0.630536 -4.454448 -2.326126
H -0.041789 -3.759173 -2.670026
H -1.512196 -4.031172 -2.296781
O 6.869366 -0.208794 -1.366587
H 5.899221 -0.114437 -1.262899
H 7.018108 -0.207083 -2.318003

O -0.700872 5.379978 -0.851929
H 0.016506 4.804500 -0.528119
H -1.085809 4.872588 -1.597232
O -4.173161 2.804428 -2.035972
H -4.696121 2.631586 -2.826809
H -4.062026 1.929310 -1.606769
C -0.501167 -0.818183 -0.118446

D2_B3LYP_27_s1 Eopt -2328.735583

O -1.060668 -0.952904 -0.131299
O -0.496128 1.114207 -0.777213
O 1.064592 -0.482790 -0.615848
O 3.327982 0.942670 -0.209255
H 3.352847 1.544546 -0.979116
H 2.487016 0.440472 -0.345722
O -4.121209 -3.206298 1.019727
H -3.574339 -3.803339 0.471019
H -4.040305 -2.328806 0.590706
O -0.095323 -1.937360 2.255079
H 0.735563 -2.445723 2.131794
H -0.400429 -1.687009 1.353105
O 1.894619 -0.254788 -3.283876
H 1.071963 -0.531419 -3.737558
H 1.640148 -0.283801 -2.336798
O 3.004412 2.377734 -2.685681
H 2.628508 1.554324 -3.044468
H 2.234570 2.842250 -2.295057
O -1.951313 1.209326 -3.174220
H -2.865712 0.895160 -3.010178
H -1.496505 1.138746 -2.308082
O 2.363155 2.088838 2.172051
H 2.703304 1.706038 1.335657
H 1.543353 1.596254 2.378130
O -4.522517 0.227273 -2.655000
H -5.111639 0.979508 -2.529893
H -4.303216 -0.084935 -1.746685
O -2.545051 -4.908206 -0.624866
H -1.976888 -5.412576 -0.031895
H -1.943335 -4.283531 -1.084454
O 1.370495 4.527008 1.080051
H 0.457611 4.608381 1.425823
H 1.718527 3.708794 1.486385
O 0.094093 0.669531 3.165643
H 0.444888 0.649815 4.064365
H 0.122175 -0.267349 2.862639
O -1.929419 4.022830 -2.394226
H -2.054126 3.141322 -2.790889
H -1.001810 3.999867 -2.089802
O -0.930404 -3.026305 -1.938197
H -0.005075 -3.294948 -1.793422
H -1.040944 -2.296720 -1.284105
O 3.778193 -2.342526 -2.817111
H 3.140210 -1.658418 -3.101484
H 4.384119 -1.861815 -2.218671
O 5.382902 -0.755289 -1.102549
H 4.683438 -0.194441 -0.703520
H 5.792884 -1.225527 -0.368321
O 3.784161 0.585459 4.079642
H 3.106184 0.302229 4.703994
H 3.310818 1.155577 3.436990
O -2.748261 0.231364 3.734616
H -2.787250 -0.737367 3.591457
H -1.819770 0.462741 3.551545
O -0.652495 -1.137836 -4.165848
H -0.761085 -1.792635 -3.451028
H -1.137908 -0.346329 -3.857699
O -1.291893 4.705260 1.958607
H -1.680099 4.015005 1.376234
H -1.336208 4.339456 2.849103
O 4.393056 -1.588747 2.431090

H	4.157328	-0.838970	3.019059
H	4.548508	-1.184477	1.569466
O	-2.383526	2.845410	0.215496
H	-2.457675	3.358845	-0.610494
H	-1.745668	2.134376	-0.024406
O	-3.763501	-0.693633	-0.175414
H	-4.005763	-0.005724	0.481384
H	-2.774070	-0.696860	-0.187566
O	0.741147	3.474190	-1.452453
H	0.982507	3.886759	-0.595318
H	0.394590	2.585624	-1.207753
O	1.774447	-3.098364	-0.926494
H	2.515885	-2.988861	-1.554190
H	1.467763	-2.171500	-0.769863
O	-2.629120	-2.570200	3.314389
H	-3.153365	-2.815206	2.522419
H	-1.714830	-2.474468	2.983987
O	-4.283653	1.346665	1.671464
H	-3.739092	0.983434	2.402303
H	-3.685501	1.943086	1.181549
O	2.276768	-3.362080	1.833784
H	2.996124	-2.737635	2.057624
H	2.209369	-3.334016	0.857723
C	-0.163653	-0.098621	-0.507121

D2_B3LYP_27_s2

Eopt -2328.737791

O	-1.104434	-0.746459	-0.655976
O	-0.597339	1.361608	-0.096176
O	0.942533	0.047180	-1.044839
O	3.223851	0.974337	0.059076
H	3.282764	1.898081	-0.251653
H	2.345676	0.674215	-0.282752
O	-4.107183	-3.318031	-0.502339
H	-3.690383	-3.502872	-1.367326
H	-4.058652	-2.342823	-0.415664
O	0.010004	-2.630858	1.069281
H	0.808420	-3.061071	0.692491
H	-0.332370	-2.023484	0.377740
O	1.556222	1.849785	-3.054151
H	0.709539	1.842043	-3.542907
H	1.382835	1.234520	-2.307975
O	2.837466	3.589298	-1.094449
H	2.405041	3.143458	-1.843982
H	2.119707	3.695452	-0.435366
O	-2.206522	2.865254	-1.830887
H	-3.107774	2.481526	-1.784606
H	-1.669752	2.310432	-1.226606
O	2.867176	0.512585	2.772417
H	2.971016	0.693749	1.812244
H	2.034749	0.008033	2.861535
O	-4.726318	1.637303	-1.689499
H	-5.274842	2.157509	-1.091818
H	-4.432161	0.861495	-1.159430
O	-2.906854	-3.717543	-3.048297
H	-3.641511	-3.680603	-3.671202
H	-2.417743	-2.878815	-3.180852
O	1.499468	2.970230	3.363839
H	0.662092	2.543376	3.643767
H	2.083028	2.209389	3.181021
O	0.427009	-0.963559	3.214603
H	0.696848	-1.529355	3.947771
H	0.324813	-1.567243	2.440405
O	-1.933613	4.702874	0.462785
H	-2.147291	4.222005	-0.356631
H	-0.997455	4.471882	0.621282
O	-1.413672	-1.329955	-3.309404
H	-0.576943	-1.683653	-3.634189
H	-1.262387	-1.167325	-2.346617
O	4.052252	0.804714	-3.946135
H	3.176369	1.164041	-3.708503

H	4.283154	0.224573	-3.201027
O	4.476850	-0.942669	-1.591876
H	4.135954	-0.224993	-1.018370
H	3.668544	-1.401928	-1.895781
O	4.776920	-1.493732	3.070103
H	5.633482	-1.060831	3.157727
H	4.126611	-0.761954	2.988276
O	-2.539394	-1.822485	3.571948
H	-2.553191	-2.552349	2.916986
H	-1.639847	-1.463599	3.519976
O	-1.091328	1.513362	-4.088784
H	-1.201882	0.572483	-3.861750
H	-1.517808	1.997010	-3.352985
O	-0.823516	1.528334	4.033544
H	-1.397779	1.788984	3.283670
H	-0.460144	0.663827	3.774060
O	4.764983	-2.833388	0.596717
H	4.767801	-2.330702	1.437063
H	4.746597	-2.162289	-0.111029
O	-2.391898	2.167723	1.807121
H	-2.414992	3.103940	1.538836
H	-1.820710	1.748295	1.122680
O	-3.798287	-0.546016	-0.269311
H	-3.971422	-0.345081	0.675720
H	-2.814303	-0.533974	-0.365745
O	0.714143	3.635596	0.737383
H	1.008138	3.448392	1.654548
H	0.341701	2.782827	0.415829
O	1.972818	-2.111312	-2.260078
H	1.678271	-2.195550	-3.173442
H	1.469924	-1.352425	-1.865022
O	-2.413432	-3.910881	1.668717
H	-2.990731	-3.729535	0.897403
H	-1.531266	-3.582214	1.404095
O	-4.210182	0.118269	2.420728
H	-3.626657	-0.542865	2.849300
H	-3.647045	0.905078	2.293297
O	2.226201	-3.864219	-0.091755
H	3.086130	-3.538073	0.245879
H	2.106596	-3.376053	-0.929138
C	-0.255024	0.227714	-0.594282

D2_B3LYP_27_s3

Eopt -2328.734329

O	1.041672	-0.937553	-0.094224
O	-0.349758	0.389808	1.043726
O	-1.144969	-0.949222	-0.567799
O	-3.833536	-0.190209	-0.494683
H	-4.082664	-0.259223	0.449161
H	-2.871450	-0.395227	-0.503550
O	5.232719	-1.597007	-0.198294
H	4.850855	-2.483847	-0.354331
H	4.576680	-1.147278	0.375296
O	1.886474	-0.033953	-2.539093
H	1.320033	-0.428913	-3.235060
H	1.578257	-0.434021	-1.693738
O	-2.435060	-2.641420	1.425488
H	-1.671175	-2.954542	1.958238
H	-2.034331	-2.105404	0.715922
O	-4.128032	-0.528428	2.314886
H	-3.517662	-1.276566	2.164632
H	-3.548203	0.248366	2.443659
O	0.167827	-0.703279	3.614869
H	1.126990	-0.654199	3.801953
H	0.053113	-0.293756	2.733865
O	-4.188436	2.388623	-1.435037
H	-4.058663	1.469571	-1.110525
H	-3.552950	2.484007	-2.154359
O	2.950140	-0.693321	4.055934
H	3.181731	0.133319	4.493665
H	3.117791	-0.533787	3.098768

O	4.020592	-4.126789	-0.582134
H	4.457622	-4.735603	0.023841
H	3.141391	-3.955650	-0.183164
O	-3.155668	3.788010	0.763546
H	-2.276552	4.122724	0.494003
H	-3.509739	3.329326	-0.026396
O	1.455515	2.638183	-1.948170
H	1.255061	2.669213	-1.003451
H	1.545465	1.680541	-2.163524
O	-0.364932	3.122019	3.813812
H	-0.660708	4.033506	3.916511
H	-1.119623	2.651876	3.397654
O	1.486464	-3.565052	0.491847
H	0.897560	-4.136240	-0.015158
H	1.278535	-2.643874	0.200264
O	-4.194706	-4.319047	-0.041990
H	-3.556946	-3.811696	0.494487
H	-4.554796	-3.660953	-0.666425
O	-5.189494	-2.273603	-1.770064
H	-4.691995	-1.534150	-1.358078
H	-4.773276	-2.409987	-2.628411
O	-0.969702	3.183493	-3.237797
H	-0.132653	3.074800	-2.737873
H	-1.549018	3.699814	-2.665733
O	4.333255	2.686203	-1.574808
H	4.539187	1.767314	-1.846145
H	3.386336	2.785657	-1.782973
O	-0.156886	-3.365256	2.858696
H	0.443782	-3.475391	2.097980
H	-0.007838	-2.442242	3.161034
O	-0.573871	4.728891	0.097542
H	-0.010379	4.024267	0.484116
H	-0.438062	4.662184	-0.854641
O	-1.777336	0.496152	-3.124401
H	-1.506631	1.436760	-3.113861
H	-1.518266	0.133122	-2.260550
O	0.975989	2.770141	1.351692
H	0.639274	2.993688	2.244362
H	0.593359	1.877684	1.179650
O	3.299632	-0.309161	1.354295
H	3.479652	0.653412	1.273174
H	2.447880	-0.467733	0.881905
O	-2.348911	1.687748	2.421571
H	-2.680550	2.408769	1.841496
H	-1.707110	1.193363	1.864429
O	-0.695265	-2.990545	-2.350245
H	0.089864	-3.484807	-2.090911
H	-0.786582	-2.273250	-1.675702
O	4.696594	0.011691	-2.439543
H	4.914266	-0.568207	-1.679429
H	3.729063	-0.079873	-2.546856
O	3.754724	2.429901	1.184170
H	3.986130	2.542035	0.239313
H	2.796325	2.623616	1.242056
O	0.082028	-1.179906	-4.371631
H	-0.579832	-0.509146	-4.105028
H	-0.123523	-1.923093	-3.768434
C	-0.153589	-0.492860	0.129262

D2_B3LYP_Radical_9_s1

Eopt -952.180314

O	0.645571	2.050473	-0.458451
O	0.477782	0.046491	-1.259765
O	0.324759	0.403912	0.945787
O	-0.501137	-2.275314	1.424641
H	-0.154712	-1.372427	1.319788
H	-0.374704	-2.664160	0.540917
O	3.062441	-1.361350	-0.841119
H	2.179303	-1.094468	-1.133330
H	3.035005	-1.231123	0.124428
O	-0.528877	-2.628398	-1.410021

H	-1.467918	-2.431062	-1.287340
H	-0.102009	-1.756853	-1.352927
O	-2.426401	2.527065	-0.423189
H	-1.485173	2.690794	-0.568705
H	-2.454366	2.073889	0.447436
O	3.005211	-0.240989	1.835065
H	2.051852	-0.114579	1.701294
H	3.399765	0.462148	1.293016
O	-2.322136	1.055584	1.941190
H	-2.694570	0.243387	1.534256
H	-1.367337	0.942301	1.808093
O	3.757900	1.450612	-0.449543
H	3.585994	0.555457	-0.796967
H	2.897242	1.886836	-0.483929
O	-3.054978	-1.277346	0.596312
H	-2.213386	-1.693131	0.865775
H	-2.868165	-0.857086	-0.268371
O	-2.526532	0.093208	-1.783502
H	-2.515387	0.973884	-1.350654
H	-1.590673	-0.127185	-1.877774
C	0.471736	0.793633	-0.242372

D2_B3LYP_Radical_9_s2

Eopt -952.176322

O	0.249566	0.072992	-1.035687
O	0.964201	-1.953756	-0.910212
O	0.481172	-0.905076	0.964979
O	-1.984692	-2.416599	1.365141
H	-1.103821	-2.019520	1.446421
H	-2.009137	-2.728890	0.444894
O	3.932117	-0.956296	-0.188209
H	3.202658	-1.512008	-0.490978
H	3.563654	-0.463029	0.566472
O	-2.061149	-2.486803	-1.584751
H	-2.273786	-1.575146	-1.315142
H	-1.096751	-2.506852	-1.633198
O	-0.429552	2.556940	0.257737
H	-0.050774	1.816960	-0.243052
H	-0.754530	2.122387	1.071957
O	2.622791	0.978087	1.552777
H	1.818440	0.435721	1.541478
H	2.618122	1.417609	0.686701
O	-1.169239	0.913520	2.400624
H	-2.096959	0.759807	2.187210
H	-0.685409	0.233448	1.897442
O	2.821532	1.452268	-1.371561
H	3.327867	0.644123	-1.177129
H	1.904652	1.139471	-1.392466
O	-2.805134	-0.077614	-0.139734
H	-2.573373	-0.722090	0.552356
H	-2.038098	0.507062	-0.193922
O	-2.711102	2.994045	-1.259601
H	-1.907501	2.834474	-0.718619
H	-2.449767	3.671773	-1.894195
C	0.553400	-0.904827	-0.291378

D2_B3LYP_Radical_9_s3

Eopt -952.179372

O	0.735010	-0.365102	-1.851927
O	1.732489	1.194064	-0.776981
O	1.668764	-0.857159	0.106050
O	4.469260	-1.157420	0.713916
H	3.506468	-1.084854	0.586859
H	4.617614	-0.911185	1.634022
O	-0.449685	3.015413	-0.193302
H	0.322267	2.460582	-0.398955
H	-0.143828	3.620988	0.491955
O	4.744482	1.213505	-0.867491
H	4.770269	0.413436	-0.309680
H	3.796764	1.383154	-0.966206
O	-1.942624	-1.164250	-0.699235
H	-1.306791	-0.816700	-1.341136

H	-1.450424	-1.878806	-0.242207
O	0.341419	0.094148	2.603411
H	0.881687	-0.239406	1.871333
H	-0.467190	0.419454	2.162286
O	-0.229719	-2.972662	0.578369
H	-0.053707	-3.708457	-0.019200
H	0.487318	-2.334418	0.409088
O	-1.928064	1.003664	1.126940
H	-1.452243	1.726945	0.669235
H	-1.912008	0.253002	0.497937
O	-4.704669	-1.014381	-1.195350
H	-3.749372	-1.159149	-1.047261
H	-5.141984	-1.748927	-0.750670
C	1.389421	-0.036634	-0.802810
O	-4.740409	1.266684	0.555528
H	-3.799342	1.274706	0.809620
H	-4.812052	0.497403	-0.039576

D2_B3LYP_Radical_12_s1

Eopt -1181.564982

O	-0.174764	0.301114	0.999499
O	0.018616	-0.676089	-0.950101
O	-0.174997	1.525438	-0.815857
O	-2.632416	-0.967134	-2.379705
H	-1.702802	-1.020467	-2.113168
H	-2.861153	-0.031291	-2.210421
O	-0.890380	2.601325	2.963268
H	-0.729814	1.729282	2.580724
H	-0.799126	3.202733	2.199991
O	2.440258	-3.326590	0.576969
H	1.481626	-3.472186	0.504574
H	2.645661	-2.723017	-0.167411
O	-2.967996	-0.612007	1.810816
H	-3.124554	-1.303463	1.137196
H	-2.084319	-0.275087	1.607914
O	4.352387	0.699838	-0.762170
H	4.555727	0.611309	0.175732
H	3.704124	1.434080	-0.817268
O	2.021799	-1.199328	2.435888
H	2.197076	-1.944995	1.828963
H	1.337336	-0.681978	1.988595
O	-0.615788	4.098297	0.550259
H	-0.454633	3.271416	0.066905
H	0.241197	4.540131	0.568470
O	2.801456	-1.494921	-1.533521
H	3.360365	-0.743133	-1.242854
H	1.891612	-1.174332	-1.434394
O	-3.311994	-2.617809	-0.173869
H	-3.178260	-2.042963	-0.954310
H	-2.425811	-2.978918	0.004373
O	-0.507498	-3.223429	0.408625
H	-0.336269	-2.355335	0.003285
H	-0.595056	-3.031532	1.350877
O	-2.971014	1.800701	-1.861674
H	-3.601232	1.937604	-1.144887
H	-2.098313	1.859327	-1.442090
O	2.491244	2.768790	-1.013851
H	1.604792	2.372893	-0.986973
H	2.589233	3.098481	-1.914754
C	-0.108120	0.382648	-0.270944

D2_B3LYP_Radical_12_s2

Eopt -1181.564685

O	0.582072	-0.451002	0.199529
O	-1.220890	-1.041763	-0.968875
O	0.522938	-2.347350	-0.886263
O	-1.436982	0.658924	-3.347387
H	-1.303161	0.029103	-2.619493
H	-0.570280	0.750273	-3.759672
O	-0.869330	2.199362	2.331599
H	-0.399099	1.425198	2.691763
H	-0.338686	2.454129	1.553647

O	3.474407	-0.216349	-0.056972
H	2.506813	-0.233027	0.041962
H	3.646231	-0.983292	-0.637593
O	-4.644207	-0.901077	1.399838
H	-4.054879	-0.152068	1.196754
H	-4.238285	-1.647873	0.920974
O	0.564894	2.482916	-0.168793
H	-0.222678	2.681971	-0.717882
H	0.584030	1.512667	-0.124198
O	0.679552	-0.140501	3.042198
H	0.228476	-0.803339	3.578102
H	0.565427	-0.431785	2.120720
O	3.432188	-2.534761	-1.699431
H	3.565084	-2.283044	-2.620767
H	2.470668	-2.531160	-1.577978
O	3.562374	-0.546954	2.826611
H	3.645431	-0.483503	1.858609
H	2.610720	-0.429189	2.990278
O	-3.300252	-2.931830	-0.117140
H	-2.916937	-3.577902	0.486888
H	-2.553512	-2.375060	-0.393851
O	-1.855571	2.836705	-1.571105
H	-1.712615	2.155924	-2.258491
H	-2.292529	2.347252	-0.848891
O	-2.753776	1.083622	0.544122
H	-2.244166	0.387941	0.098206
H	-2.145742	1.432819	1.230866
O	3.226122	2.381106	-1.282615
H	3.429530	1.492305	-0.938449
H	2.317817	2.543052	-0.971910
C	-0.047664	-1.254965	-0.543686

D2_B3LYP_Radical_12_s3

Eopt -1181.570652

O	-0.441726	0.581440	1.462006
O	0.695875	-0.007421	-0.358169
O	1.664501	0.991716	1.374214
O	-1.577717	-0.029318	-2.240788
H	-0.851590	0.043317	-1.599808
H	-2.356838	0.357356	-1.785904
O	-2.533812	2.550428	0.968795
H	-1.757417	1.989894	1.125536
H	-2.203562	3.319377	0.463064
O	2.914810	-3.436651	0.135764
H	1.947934	-3.385062	0.231335
H	3.136088	-2.629372	-0.367716
O	-4.225500	-1.693921	0.200597
H	-3.523436	-2.098655	-0.355744
H	-3.867546	-1.695029	1.095677
O	5.319982	0.736899	-0.650152
H	5.747098	0.359687	0.127090
H	4.771150	1.474343	-0.307955
O	-1.080323	-2.056467	2.604237
H	-2.033381	-2.190389	2.541288
H	-0.940316	-1.134005	2.333449
O	-1.645420	4.818391	-0.461617
H	-1.235772	4.495727	-1.273151
H	-2.439223	5.280052	-0.757185
O	3.257634	-1.042201	-1.365246
H	3.982093	-0.440063	-1.097857
H	2.447574	-0.630850	-1.021280
O	-2.253840	-2.685390	-1.512520
H	-2.028455	-1.797851	-1.860791
H	-1.498642	-2.899349	-0.931913
O	0.061992	-2.896116	0.158551
H	0.306224	-2.005567	-0.142815
H	-0.331636	-2.734604	1.040504
O	-3.850769	0.909179	-0.889431
H	-4.018405	0.057415	-0.439891
H	-3.427058	1.483340	-0.217913
O	3.618628	2.787072	0.194398

H	4.021557	3.254443	0.935380
H	2.905571	2.259156	0.590663
C	0.642242	0.507596	0.785138

D2_B3LYP_Radical_18_s1

O	0.931688	0.142806	-0.122639
O	-1.281680	0.026375	0.094111
O	-0.096779	-1.766668	-0.312001
O	-2.119516	1.351150	-2.341296
H	-1.900622	0.954996	-1.480872
H	-1.333065	1.142615	-2.891129
O	0.746956	3.254776	2.412431
H	1.091334	2.366712	2.630168
H	0.966707	3.360871	1.469086
O	3.650926	0.108874	-1.068406
H	2.728353	-0.044058	-0.806811
H	3.984727	-0.768098	-1.354192
O	-0.402846	-1.022708	3.644944
H	-1.269772	-0.583765	3.500952
H	-0.375425	-1.736664	2.997219
O	4.378413	-3.069857	1.045910
H	5.175074	-3.479604	1.400252
H	4.383911	-2.146632	1.381023
O	-2.878026	0.261679	3.287839
H	-2.569578	1.078530	2.852969
H	-3.298419	-0.242425	2.568265
O	1.114545	3.080012	-0.486241
H	0.209598	3.390563	-0.702411
H	1.005034	2.129467	-0.317090
O	-3.761634	-3.803761	0.297073
H	-3.169280	-4.262765	0.903240
H	-3.221307	-3.618262	-0.500054
O	1.699525	0.560349	2.664709
H	0.991182	0.022478	3.080062
H	1.510659	0.482838	1.714716
O	4.667089	-2.440717	-1.654784
H	3.976824	-2.903545	-2.143319
H	4.575896	-2.747627	-0.726293
O	-4.119683	-0.784589	-2.156544
H	-4.201690	-0.781046	-1.187170
H	-3.511441	-0.049121	-2.351400
O	4.313556	-0.361018	1.725724
H	4.155504	-0.104249	0.797393
H	3.483559	-0.137365	2.182469
O	-3.842114	-1.020578	0.821894
H	-3.851404	-1.997037	0.754409
H	-2.940712	-0.769842	0.555860
O	-1.582184	3.807064	-0.927246
H	-1.804091	3.063276	-1.519201
H	-1.798621	3.471878	-0.038459
O	-1.845250	2.411404	1.644608
H	-1.596191	1.647719	1.095837
H	-0.991216	2.735967	2.000607
O	0.189416	0.627417	-3.761406
H	0.975641	1.115241	-3.430807
H	0.301405	-0.272472	-3.434088
O	2.421092	2.060865	-2.842647
H	2.950884	1.384666	-2.382745
H	1.990389	2.548349	-2.115334
O	-2.334906	-2.976936	-1.987039
H	-1.552572	-2.601381	-1.558257
H	-2.931266	-2.211107	-2.123327
C	-0.154789	-0.501103	-0.108920

D2_B3LYP_Radical_18_s2

O	0.879883	0.115987	-0.167837
O	-1.326694	-0.022585	0.101865
O	-0.197336	-1.679468	-0.768205
O	-2.160211	1.902731	-1.889275
H	-1.915059	1.289355	-1.175820

Eopt -1640.344155

Eopt -1640.34876

H	-1.393053	1.857917	-2.500313
O	0.831106	2.450773	3.097953
H	1.153068	1.528703	3.061873
H	1.022195	2.795102	2.206327
O	3.574459	0.302463	-1.135786
H	2.657531	0.063301	-0.924514
H	3.953561	-0.482182	-1.586889
O	-0.390479	-1.980701	3.232142
H	-1.245992	-1.498048	3.240510
H	-0.411618	-2.509493	2.426106
O	5.211014	-2.976319	0.389387
H	4.576663	-3.675345	0.583421
H	4.874210	-2.182502	0.860168
O	-2.828573	-0.587810	3.316184
H	-2.514539	0.308702	3.094418
H	-3.291267	-0.878597	2.510084
O	1.111495	3.031999	0.258891
H	0.212117	3.409267	0.155807
H	0.978683	2.073471	0.167486
O	-3.884331	-3.726590	-0.515144
H	-4.768675	-3.961571	-0.817643
H	-3.437151	-3.344648	-1.300571
O	1.709709	-0.228841	2.619045
H	1.002447	-0.848281	2.902272
H	1.507970	-0.071387	1.681885
O	4.792090	-1.982002	-2.190225
H	4.140100	-2.525013	-2.647169
H	4.922507	-2.413394	-1.317903
O	-4.197573	-0.152987	-2.200326
H	-4.277818	-0.377114	-1.257630
H	-3.571667	0.594087	-2.219704
O	4.391119	-0.556296	1.492284
H	4.146978	-0.182409	0.623087
H	3.555080	-0.582140	1.988419
O	-3.913145	-1.136155	0.635160
H	-3.970855	-2.063218	0.326485
H	-3.007272	-0.863489	0.409882
O	-1.576259	3.900938	0.093627
H	-1.822992	3.329478	-0.658903
H	-1.781206	3.358603	0.876359
O	-1.806980	1.896051	2.232741
H	-1.596246	1.298970	1.494518
H	-0.933071	2.100168	2.627941
O	0.099900	1.621203	-3.525962
H	0.906774	1.972001	-3.088763
H	0.199861	0.662616	-3.498749
O	2.387338	2.683174	-2.290768
H	2.902847	1.896212	-2.036191
H	1.971799	2.965574	-1.454032
O	-2.535223	-2.407958	-2.599213
H	-1.725102	-2.194248	-2.114305
H	-3.081115	-1.596330	-2.534605
C	-0.218359	-0.499162	-0.265941

D2_B3LYP_Radical_18_s3

O	-1.066535	-0.089525	0.193777
O	1.061124	-0.270425	-0.385307
O	-0.201091	1.388798	-1.125625
O	1.131804	-2.056772	-2.651263
H	1.200686	-1.512525	-1.848924
H	0.249920	-1.814243	-3.000589
O	-0.496117	-2.652189	3.166591
H	-0.607170	-1.686188	3.269945
H	-1.099916	-2.870709	2.434313
O	-4.395863	0.302385	-0.149042
H	-5.357187	0.274976	-0.078867
H	-4.197771	1.053768	-0.753037
O	1.687203	1.219172	3.641542
H	2.344706	0.638268	3.197626
H	1.870152	1.134277	4.583906

Eopt -1640.348077

O	-2.054352	3.430213	0.307760
H	-1.276828	2.941019	0.004878
H	-2.454516	2.854020	0.993917
O	3.513492	-0.443900	2.337054
H	2.939076	-1.202406	2.116871
H	3.716266	-0.045984	1.469819
O	-2.131929	-2.791462	0.765732
H	-2.983959	-2.612631	1.182094
H	-1.751565	-1.913340	0.596853
O	4.103355	3.262634	-0.618885
H	4.540202	3.440402	-1.459308
H	3.162347	3.501213	-0.763575
O	-0.856465	0.185379	3.072103
H	0.017682	0.566846	3.304804
H	-0.834001	0.100148	2.104766
O	-3.656220	2.425902	-1.770379
H	-3.040244	2.020372	-2.392153
H	-3.086355	2.844746	-1.089771
O	3.743278	-0.629290	-3.104895
H	3.819045	-0.242033	-2.214588
H	2.892396	-1.094849	-3.096298
O	-3.309065	1.701774	2.148160
H	-3.665316	1.123392	1.447170
H	-2.564120	1.216405	2.537142
O	3.801116	0.497382	-0.397890
H	3.935365	1.466303	-0.479352
H	2.836609	0.375333	-0.422945
O	1.321010	-4.301938	-0.816383
H	1.205846	-3.634945	-1.516095
H	1.446844	-3.773499	-0.008053
O	1.692392	-2.462066	1.409920
H	1.380514	-1.760079	0.812708
H	0.966034	-2.567624	2.061446
O	-1.425703	-1.061996	-3.417231
H	-2.140636	-1.343041	-2.805169
H	-1.248517	-0.143760	-3.180295
O	-3.502893	-1.905630	-1.730812
H	-3.840203	-1.133845	-1.233175
H	-3.042525	-2.427104	-1.054490
O	1.409552	3.860383	-0.987706
H	0.912634	3.027082	-0.976197
H	1.078353	4.355636	-0.228898
C	-0.044768	0.328997	-0.435710

D2_B3LYP_Radical_24_s1

Eopt -2099.125814

O	1.148479	0.633576	0.059106
O	-0.995879	0.143926	0.028245
O	0.548796	-1.438399	0.231858
O	1.897584	-1.922215	2.691394
H	1.805494	-1.010035	3.058684
H	1.442628	-1.854338	1.834539
O	-0.778085	-2.538322	3.552628
H	0.176250	-2.397409	3.404279
H	-1.069417	-2.989675	2.740670
O	-1.640800	2.230262	-1.805798
H	-0.965078	2.429332	-2.489852
H	-1.311936	1.439836	-1.344844
O	4.054933	-2.573606	0.914599
H	3.489190	-3.006183	0.249282
H	3.437873	-2.333134	1.630231
O	-1.599668	3.141043	0.818945
H	-1.213609	2.308889	1.123278
H	-1.607997	3.036618	-0.154841
O	-3.213944	-1.623424	0.435632
H	-3.684713	-1.170244	1.169647
H	-2.449210	-1.046597	0.264238
O	-1.276232	-3.540174	0.886532
H	-0.571149	-2.890448	0.727558
H	-2.088513	-3.001628	0.786817
O	0.416633	2.666976	-3.609372

H	0.636990	1.714559	-3.614205
H	0.986039	3.021119	-2.899420
O	1.978275	3.130318	-1.301829
H	1.564813	3.687298	-0.602780
H	1.677514	2.236756	-1.080952
O	2.466938	2.729801	2.387799
H	2.918452	3.206664	3.093070
H	3.148092	2.571598	1.691479
O	0.907733	4.469976	0.861641
H	0.016846	4.068787	0.866917
H	1.435783	3.905861	1.464092
O	1.302184	0.560309	3.673978
H	1.700488	1.290998	3.158915
H	0.363258	0.517104	3.409097
O	2.122785	-3.352828	-1.125717
H	1.653193	-2.645239	-0.654520
H	2.605082	-2.872806	-1.833172
O	-1.439926	0.096069	3.023698
H	-1.415595	0.181857	2.060391
H	-1.261587	-0.857366	3.194706
O	-4.247362	-0.058030	2.472718
H	-3.346875	-0.006833	2.841994
H	-4.296345	0.714188	1.863308
O	3.905862	-0.236201	-0.567964
H	2.959750	-0.038436	-0.496384
H	4.030850	-1.019040	0.013411
O	-0.587068	-3.890152	-1.926744
H	0.373141	-3.792956	-1.782867
H	-0.953390	-3.904104	-1.024480
O	-1.291830	-1.323152	-2.659432
H	-1.034227	-2.237016	-2.391897
H	-1.429945	-0.854620	-1.825044
O	1.119910	-0.039463	-3.163300
H	1.411407	0.237939	-2.285501
H	0.279292	-0.524523	-3.005115
O	-4.283270	1.358750	-1.954891
H	-3.356280	1.656209	-2.041139
H	-4.248231	0.383486	-2.037618
O	3.426551	-1.690102	-2.941427
H	2.611867	-1.223575	-3.205161
H	3.736675	-1.168669	-2.173887
O	4.224248	2.437745	0.310029
H	3.561035	2.777996	-0.321656
H	4.263353	1.483530	0.108524
O	-4.295430	2.083751	0.743802
H	-3.399405	2.452320	0.840682
H	-4.332685	1.765442	-0.183574
O	-4.155299	-1.439783	-2.158923
H	-3.282851	-1.483430	-2.584688
H	-3.938541	-1.537272	-1.207546
C	0.207212	-0.226004	0.104611

D2_B3LYP_Radical_24_s2

Eopt -2099.125594

O	1.161507	0.591814	0.053717
O	-0.989457	0.150637	0.026219
O	0.512031	-1.463037	0.261247
O	1.877273	-1.947025	2.702423
H	1.803020	-1.032449	3.063182
H	1.432410	-1.876839	1.841515
O	-0.816093	-2.529493	3.540951
H	0.141186	-2.413594	3.393247
H	-1.130433	-2.953310	2.722321
O	-1.601965	2.239287	-1.820449
H	-0.922588	2.433448	-2.501273
H	-1.277993	1.450928	-1.354561
O	4.035015	-2.616642	0.920716
H	3.459045	-3.039572	0.257456
H	3.424437	-2.365686	1.637948
O	-1.552102	3.150102	0.805307
H	-1.173130	2.313170	1.106928

H	-1.562688	3.046794	-0.168469
O	-3.273870	-1.560679	0.423994
H	-3.727203	-1.106172	1.166270
H	-2.514871	-0.984064	0.228814
O	-1.413450	-3.477869	0.880400
H	-0.687379	-2.851390	0.723393
H	-2.206538	-2.905885	0.782040
O	0.471697	2.652226	-3.618929
H	0.671755	1.696051	-3.622543
H	1.036894	2.991989	-2.897854
O	2.017628	3.086437	-1.299654
H	1.608800	3.656879	-0.608308
H	1.704027	2.199162	-1.071900
O	2.497194	2.712580	2.380778
H	2.951144	3.186347	3.086257
H	3.180169	2.539645	1.690184
O	0.962345	4.460442	0.845901
H	0.066893	4.070660	0.855950
H	1.483132	3.897261	1.456214
O	1.314309	0.549302	3.672355
H	1.721247	1.274788	3.157411
H	0.375132	0.517596	3.410045
O	2.088860	-3.362777	-1.098867
H	1.616291	-2.651562	-0.635131
H	2.565415	-2.893623	-1.816724
O	-1.421585	0.115078	3.029321
H	-1.409024	0.195479	2.065466
H	-1.267759	-0.843077	3.200557
O	-4.242139	0.011475	2.495186
H	-3.339333	0.047109	2.859149
H	-4.279473	0.779752	1.880546
O	3.917674	-0.276467	-0.563792
H	2.972581	-0.074204	-0.494788
H	4.035707	-1.062010	0.015635
O	-0.635346	-3.884225	-1.910302
H	0.321459	-3.793942	-1.745956
H	-1.029156	-3.886671	-1.021048
O	-1.309352	-1.313341	-2.656634
H	-1.061248	-2.227491	-2.384216
H	-1.431254	-0.834192	-1.825157
O	1.125779	-0.066148	-3.165243
H	1.414910	0.207495	-2.285824
H	0.277920	-0.539366	-3.011111
O	-4.254203	1.402806	-1.953343
H	-3.323570	1.686270	-2.043620
H	-4.235841	0.429092	-2.047833
O	3.420823	-1.731984	-2.935720
H	2.609467	-1.260487	-3.199394
H	3.733802	-1.214648	-2.166886
O	4.260241	2.392129	0.307877
H	3.597039	2.732373	-0.323211
H	4.291277	1.436733	0.112745
O	-4.258948	2.136792	0.745603
H	-3.358786	2.497223	0.836600
H	-4.301863	1.813425	-0.179853
O	-4.169998	-1.404240	-2.193225
H	-3.282548	-1.450179	-2.587546
H	-3.987703	-1.498786	-1.235951
C	0.204046	-0.246322	0.112098

D2_B3LYP_Radical_27_s2

O	-0.699592	-0.669925	-0.343855
O	0.152542	1.330006	-0.088892
O	1.482498	-0.398470	-0.044639
O	4.014161	0.792320	1.068356
H	4.147464	1.522884	0.427332
H	3.260025	0.307687	0.699811
O	-4.468598	-1.947260	-1.619752
H	-3.832930	-2.353603	-2.243128
H	-4.088129	-1.078035	-1.385990

Eopt -2328.51439

O	-1.354036	-2.827542	1.480645
H	-0.652939	-3.513992	1.438888
H	-1.064717	-2.117414	0.883633
O	3.046652	0.476425	-2.411880
H	2.342764	0.456420	-3.098539
H	2.574554	0.239100	-1.597768
O	4.108394	2.750616	-0.957595
H	3.749834	2.099113	-1.587670
H	3.325672	3.225393	-0.618427
O	-0.505372	2.412143	-2.869068
H	-1.478981	2.326630	-2.978502
H	-0.324574	2.045134	-1.989907
O	2.130596	1.273292	3.134300
H	2.851715	1.235368	2.472371
H	1.348995	0.989316	2.642336
O	-3.266093	2.160418	-3.070465
H	-3.611819	3.037341	-2.868481
H	-3.359954	1.648541	-2.238247
O	-2.677758	-3.221419	-3.395566
H	-2.923751	-2.970817	-4.293021
H	-1.788102	-2.833030	-3.256753
O	1.219852	4.017712	2.796056
H	0.245747	3.913148	2.780630
H	1.564262	3.128398	2.995545
O	-1.892824	-1.625289	3.935902
H	-1.924211	-2.304502	4.618972
H	-1.630895	-2.096834	3.116140
O	-0.479589	4.928323	-1.478313
H	-0.488514	4.178248	-2.102336
H	0.283135	4.728061	-0.901886
O	-0.201122	-2.022440	-2.895372
H	0.551956	-2.612511	-2.665753
H	-0.430075	-1.585646	-2.058461
O	4.239375	-2.111313	-2.201872
H	3.876191	-1.220978	-2.373929
H	4.556401	-2.068788	-1.275982
O	5.069618	-1.923938	0.505884
H	5.009283	-0.963590	0.637477
H	4.249005	-2.255198	0.922509
O	2.590862	-1.379859	4.123083
H	3.490767	-1.438456	4.463993
H	2.478229	-0.444481	3.862223
O	-4.503062	-1.244334	2.884528
H	-4.455130	-1.894806	2.152197
H	-3.643479	-1.344889	3.340017
O	0.886159	0.302146	-4.165172
H	0.508506	-0.510203	-3.774258
H	0.354265	1.030981	-3.788898
O	-1.590179	3.767369	2.718342
H	-1.910569	3.748450	1.789613
H	-1.841839	2.913852	3.089002
O	2.545390	-2.600662	1.611628
H	2.564894	-2.208460	2.513040
H	2.088462	-1.939777	1.066272
O	-2.525075	3.828697	0.101278
H	-1.811469	4.215232	-0.451709
H	-2.639565	2.927091	-0.225424
O	-3.332725	0.534782	-0.831180
H	-3.698699	0.790606	0.046916
H	-2.424120	0.237130	-0.659087
O	1.675926	3.870338	0.053944
H	1.570651	4.002786	1.023414
H	1.253831	3.011669	-0.101273
O	1.931986	-3.656488	-2.172376
H	1.759818	-3.882541	-1.250781
H	2.752122	-3.111666	-2.154288
O	-4.102851	-3.177372	0.868228
H	-4.231505	-2.773262	-0.016226
H	-3.138856	-3.150298	1.019976
O	-4.378781	1.205657	1.630569

H	-4.395757	0.344868	2.110978
H	-3.720170	1.743378	2.085655
O	0.715973	-4.680032	1.458500
H	1.420545	-3.997410	1.507270
H	0.808187	-5.079553	0.585898
C	0.310812	0.065450	-0.156228

D2_B3LYP_Radical_27_s3

Eopt -2328.50702

O	1.010038	1.188152	0.669402
O	-0.299234	-0.316462	-0.104608
O	1.727019	-0.932057	0.543171
O	0.518923	-3.572147	-0.499728
H	-0.156803	-3.919152	0.125367
H	0.845215	-2.751744	-0.098869
O	0.241338	5.264015	0.663343
H	0.828681	5.109283	1.430450
H	-0.386832	4.515149	0.676139
O	2.753681	2.209148	-1.443846
H	3.605828	1.732494	-1.325670
H	2.240667	1.988328	-0.649655
O	1.639783	-2.765221	2.827344
H	1.623394	-2.127642	2.094528
H	0.851181	-3.305261	2.695948
O	-1.448045	-4.556394	1.182154
H	-1.138948	-4.519825	2.094734
H	-2.180955	-3.905136	1.129449
O	-2.176318	-0.514842	2.213081
H	-2.707071	0.312174	2.227765
H	-1.550517	-0.391292	1.482843
O	-0.749624	-2.655400	-2.805417
H	-0.294854	-2.966434	-1.992495
H	-0.360324	-1.793707	-2.994719
O	-3.590422	1.908565	2.176501
H	-4.222696	1.625457	1.494531
H	-2.875924	2.353365	1.674921
O	1.917480	4.774005	2.889779
H	1.538767	5.268246	3.625552
H	1.753213	3.833283	3.103726
O	-3.389521	-2.382271	-1.872191
H	-3.806676	-1.583669	-2.247778
H	-2.476192	-2.408094	-2.222762
O	0.980052	0.873689	-3.139799
H	0.375724	0.443976	-2.520492
H	1.656316	1.302569	-2.568151
O	-6.110914	-1.629625	1.099901
H	-6.683998	-2.072593	0.463847
H	-5.253937	-2.102626	1.046727
O	1.457441	2.026533	3.382647
H	2.293654	1.659728	3.695263
H	1.359943	1.694844	2.472303
O	3.773676	-4.446940	1.881377
H	3.053059	-3.888768	2.226689
H	3.618143	-4.474548	0.917546
O	3.187742	-4.487479	-0.913329
H	2.232228	-4.360121	-0.764341
H	3.481550	-3.603046	-1.204803
O	2.369552	-1.387446	-4.056445
H	1.855685	-0.594178	-3.796081
H	1.714882	-2.091928	-4.131570
O	-0.332946	3.424223	-3.408602
H	0.264310	3.960239	-2.845015
H	0.075735	2.538571	-3.409157
O	-0.524300	0.181205	4.477174
H	0.131952	0.809241	4.129649
H	-1.072433	-0.061345	3.708688
O	-4.820447	-0.091533	-2.820079
H	-4.945147	0.257004	-1.915026
H	-4.265581	0.559467	-3.265115
O	3.660617	-1.749212	-1.610059
H	3.212381	-1.649939	-2.478623

H	2.993776	-1.489005	-0.954536
O	-4.906363	0.605856	-0.080462
H	-5.420367	-0.132050	0.315412
H	-3.997449	0.279144	-0.074750
O	-1.480708	3.012326	0.667817
H	-1.861848	2.987924	-0.240372
H	-0.790697	2.331913	0.672963
O	-3.494857	-2.661406	0.888057
H	-3.417562	-2.496048	-0.078769
H	-3.077596	-1.892785	1.327310
O	4.216162	0.156967	1.726520
H	3.980149	0.972174	2.184749
H	3.369345	-0.196999	1.405166
O	1.523043	4.799474	-1.779554
H	1.107824	4.958934	-0.904564
H	2.073606	4.007140	-1.656980
O	-2.582461	3.026034	-1.861458
H	-1.796172	3.140420	-2.444239
H	-2.931813	2.150538	-2.064970
O	5.034891	0.674285	-0.961285
H	4.671278	-0.157773	-1.321149
H	4.868658	0.588696	-0.002256
C	0.858837	-0.042154	0.383231

D3_B3LYP_9_sl

Eopt -952.385472

O	-1.271213	0.273254	-1.249868
O	0.923287	0.597804	-1.515526
O	0.181796	-0.655305	0.185679
O	2.486717	-0.291823	1.499298
H	1.656871	-0.464594	0.980184
H	2.689471	0.626959	1.266328
O	2.044265	2.379375	0.297595
H	1.734651	1.761683	-0.401036
H	1.313575	2.354958	0.937740
O	3.057757	-0.989721	-2.161179
H	3.478122	-1.339802	-1.356289
H	2.301795	-0.445684	-1.843614
O	-3.251932	-0.212838	0.501942
H	-2.514357	-0.031717	-0.138214
H	-2.831997	-0.814428	1.142148
O	-0.391368	1.760177	1.873888
H	-0.238973	0.865438	1.528391
H	-0.882691	2.201595	1.155437
O	-1.447386	-1.892614	1.927579
H	-1.628927	-2.773275	1.582254
H	-0.872831	-1.461037	1.244483
O	-1.581238	2.895192	-0.489700
H	-0.778984	3.340866	-0.785081
H	-1.507785	1.987207	-0.864290
O	4.277067	-1.943500	0.264774
H	3.648794	-1.359904	0.752515
H	3.929150	-2.834562	0.379941
O	-4.962002	-1.851687	-0.925845
H	-4.354328	-1.256160	-0.432348
H	-5.341718	-1.299122	-1.616953
C	-0.054307	0.065844	-0.866780

D3_B3LYP_9_s2

Eopt -952.385449

O	-1.269886	0.274018	-1.251736
O	0.924821	0.599210	-1.514893
O	0.181874	-0.655529	0.184467
O	2.486273	-0.294650	1.499630
H	1.656573	-0.466351	0.979911
H	2.689664	0.624289	1.267817
O	2.046150	2.377988	0.300607
H	1.736348	1.761110	-0.398677
H	1.315049	2.353761	0.940314
O	3.058539	-0.988887	-2.161637
H	3.478506	-1.339915	-1.356952
H	2.302828	-0.444685	-1.843761

O	-3.252061	-0.212415	0.498403
H	-2.514154	-0.031569	-0.141435
H	-2.832275	-0.813048	1.139610
O	-0.390809	1.759806	1.873765
H	-0.238622	0.865075	1.528196
H	-0.881583	2.201562	1.155131
O	-1.448179	-1.889598	1.927925
H	-1.629463	-2.770980	1.584312
H	-0.873298	-1.459367	1.244272
O	-1.579878	2.895565	-0.489604
H	-0.777730	3.341419	-0.785002
H	-1.506557	1.987819	-0.864778
O	4.276502	-1.945586	0.263867
H	3.648227	-1.362342	0.752027
H	3.928281	-2.836671	0.377928
O	-4.967028	-1.851828	-0.922515
H	-4.357425	-1.255993	-0.431751
H	-5.354948	-1.297898	-1.607940
C	-0.053327	0.066505	-0.867576

D3_B3LYP_9_s3 Eopt -952.386534

O	-0.471665	0.700808	-1.014904
O	1.689461	0.269477	-1.381102
O	0.537597	-0.964851	0.098357
O	2.524063	-2.532929	1.082629
H	1.830477	-1.922998	0.726170
H	2.864114	-2.095010	1.870257
O	2.637053	2.779093	-0.819747
H	2.319032	1.872234	-1.045717
H	3.383511	2.642973	-0.226169
O	3.850781	-1.381037	-1.203970
H	3.630896	-1.906596	-0.416423
H	3.068341	-0.782833	-1.281890
O	-2.832175	-0.222372	-0.148581
H	-1.955393	0.145308	-0.451540
H	-2.632311	-1.168908	-0.024849
O	0.333911	0.697060	2.436747
H	0.403702	0.030451	1.724669
H	0.339659	1.542177	1.948233
O	-1.532447	-2.728433	0.219210
H	-1.527179	-3.242624	-0.595300
H	-0.772961	-2.100402	0.136582
O	0.152686	2.936966	0.609102
H	1.053442	3.050735	0.252360
H	-0.213622	2.238691	0.029095
O	-4.712209	0.014666	-2.179118
H	-4.016278	-0.078164	-1.492729
H	-4.246033	-0.064974	-3.017897
C	0.585009	-0.000896	-0.773011
O	-2.524790	0.549707	2.580600
H	-1.550859	0.607870	2.613319
H	-2.706726	0.292206	1.656105

D3_B3LYP_12_s1 Eopt -1181.781462

O	0.332772	-0.491408	1.369166
O	0.390483	0.456905	-0.655163
O	-1.248860	-0.975868	-0.144039
O	1.231025	-1.118255	-2.795434
H	0.903587	-0.488340	-2.117183
H	0.696940	-1.914849	-2.620686
O	-0.824256	-2.145422	3.237675
H	-0.394920	-1.559249	2.572854
H	-1.665808	-2.368188	2.805103
O	1.419175	3.776223	0.772868
H	2.039024	3.083914	0.478048
H	0.642066	3.642466	0.193678
O	2.637730	-2.134429	1.071528
H	3.031768	-1.827733	0.234333
H	1.854516	-1.563574	1.193597
O	-3.419824	2.737649	-0.761192

H	-3.654074	2.643587	0.168727
H	-3.332024	1.817928	-1.098978
O	0.545451	1.907801	2.803930
H	0.825613	2.585248	2.162232
H	0.497667	1.080517	2.281855
O	-3.007968	-2.413161	1.377623
H	-2.370924	-1.863713	0.860753
H	-3.706790	-1.805683	1.642733
O	-0.611575	3.028353	-1.039749
H	-1.574439	3.015256	-0.876287
H	-0.328544	2.095680	-0.934461
O	3.701733	-1.047845	-1.390400
H	2.897723	-1.179887	-1.931923
H	3.565750	-0.167247	-0.994901
O	2.849901	1.393983	-0.065637
H	1.935753	1.030244	-0.220164
H	3.082617	1.096204	0.821849
O	-0.667765	-3.079033	-1.897445
H	-0.237908	-3.773192	-1.385831
H	-0.890787	-2.381679	-1.243600
O	-3.049448	0.190104	-1.792139
H	-2.328477	-0.212287	-1.245029
H	-2.657481	0.340939	-2.659366
C	-0.176573	-0.335191	0.196651

D3_B3LYP_12_s2 Eopt -1181.77761

O	-0.757504	0.178827	0.131728
O	1.249739	0.991054	-0.430862
O	-0.549897	2.310036	-0.539842
O	1.825892	0.387743	-3.069841
H	1.596170	0.665088	-2.153864
H	1.003820	0.462935	-3.567162
O	0.690076	-2.878404	1.745574
H	0.232878	-2.162581	2.226017
H	0.272930	-2.860395	0.862435
O	-3.437972	0.221481	-0.130581
H	-2.449240	0.224345	-0.030269
H	-3.613801	1.119311	-0.467613
O	4.248761	0.796316	1.874364
H	3.746836	0.049210	1.498741
H	3.859511	1.576942	1.436492
O	-0.439634	-2.359312	-0.846726
H	0.383726	-2.394016	-1.371845
H	-0.487194	-1.427877	-0.522022
O	-0.737368	-0.606251	2.747263
H	-0.212266	-0.014180	3.297542
H	-0.670590	-0.245562	1.830538
O	-3.143143	2.919907	-0.979109
H	-3.234857	2.976474	-1.936275
H	-2.196462	2.667495	-0.822888
O	-3.574766	-0.011196	2.720272
H	-3.644182	0.109391	1.754235
H	-2.631570	-0.210406	2.856734
O	2.961290	2.909880	0.426995
H	2.502435	3.489248	1.044810
H	2.271206	2.282541	0.095414
O	2.148398	-2.263101	-2.085689
H	2.034377	-1.409552	-2.548550
H	2.447677	-1.994348	-1.195525
O	2.643004	-1.150484	0.519234
H	2.062447	-0.410117	0.209191
H	2.052152	-1.738349	1.027672
O	-3.085118	-1.993763	-1.930957
H	-3.310024	-1.216708	-1.386464
H	-2.172510	-2.205565	-1.663021
C	-0.029588	1.174137	-0.281484

D3_B3LYP_12_s3 Eopt -1181.781264

O	0.271374	-0.996173	0.830129
O	0.386532	0.618543	-0.724102

O	-0.988072	-1.112508	-1.023206
O	2.636721	0.192396	-2.362471
H	1.816026	0.329250	-1.844261
H	2.846783	-0.753014	-2.237981
O	-1.020476	-3.188788	1.837446
H	-0.530120	-2.415332	1.469416
H	-1.826775	-3.201532	1.298077
O	-0.210003	4.251750	0.317410
H	0.474999	3.636559	0.639933
H	-0.752618	3.694482	-0.275313
O	2.999360	-1.507223	0.878959
H	3.427718	-0.656671	0.661535
H	2.037373	-1.302787	0.875202
O	-3.987120	1.824742	0.023101
H	-3.739185	1.822927	0.954247
H	-4.333927	0.922869	-0.152052
O	0.807530	0.472435	3.088882
H	1.566556	0.036939	3.492041
H	0.618583	-0.051574	2.274420
O	-3.045099	-2.549045	-0.161604
H	-2.240511	-2.042860	-0.467570
H	-3.156491	-3.264791	-0.797429
O	-1.602705	2.441195	-1.375670
H	-2.407310	2.174706	-0.889241
H	-0.937797	1.741054	-1.189776
O	4.062697	1.020656	-0.008295
H	3.691276	0.789214	-0.882402
H	3.335798	1.514433	0.421287
O	1.695055	2.223923	0.999946
H	1.220711	1.614362	0.371809
H	1.512786	1.819400	1.867266
O	3.309010	-2.509631	-1.697822
H	3.172673	-2.251582	-0.758506
H	2.559844	-3.074552	-1.917171
O	-5.065667	-0.687032	-0.519970
H	-4.355644	-1.362443	-0.435879
H	-5.277676	-0.658025	-1.459682
C	-0.119363	-0.503826	-0.306638

D3_B3LYP_18_s1 Eopt -1640.56286

O	-0.948536	0.156731	0.354576
O	1.256812	0.111621	0.005334
O	0.024166	-1.729363	-0.343427
O	2.604424	-1.146838	2.075931
H	2.190793	-0.675430	1.317751
H	1.925517	-1.807924	2.311322
O	-0.812549	3.714599	1.567382
H	-1.196055	3.400411	0.723763
H	-0.893682	2.945508	2.160018
O	-3.298544	-1.008219	0.952855
H	-2.407033	-0.678946	0.670006
H	-3.536925	-1.711124	0.317229
O	-0.073496	3.222691	-2.936123
H	0.841649	3.084473	-2.604039
H	-0.187464	2.576256	-3.641601
O	-4.592731	-0.734978	-2.788919
H	-5.520363	-0.737279	-3.050088
H	-4.513346	-0.021164	-2.117005
O	2.497327	2.950434	-1.887606
H	2.263327	2.982325	-0.938758
H	2.796740	2.030448	-2.018275
O	-0.808058	1.128235	2.958079
H	0.137923	1.164719	3.203260
H	-0.809828	0.804388	2.028910
O	2.623882	-1.855730	-3.725124
H	1.793980	-1.630319	-4.159776
H	2.366292	-2.381331	-2.932984
O	-1.764133	2.479891	-0.805784
H	-1.199094	2.722965	-1.567994
H	-1.374860	1.649555	-0.442900

O	-4.161959	-2.862923	-1.023744
H	-3.392943	-3.354694	-1.332730
H	-4.307708	-2.164028	-1.697171
O	4.389247	-1.928367	-0.091395
H	4.168332	-1.180274	-0.675777
H	3.885864	-1.749515	0.723787
O	-4.288193	1.116254	-0.740556
H	-4.029128	0.430209	-0.094543
H	-3.474283	1.638038	-0.875355
O	3.271424	0.174171	-1.826867
H	3.067230	-0.428952	-2.567669
H	2.509575	0.073754	-1.208799
O	2.015119	1.332999	3.423080
H	2.261023	0.443633	3.104939
H	2.041545	1.880947	2.615631
O	1.758373	2.641153	0.853472
H	1.481804	1.735998	0.560583
H	0.922476	3.100808	1.063747
O	0.304376	-2.898357	2.251578
H	-0.427289	-2.444546	2.715845
H	0.196545	-2.617933	1.321827
O	-1.894656	-1.499966	3.442195
H	-2.468942	-1.485875	2.653816
H	-1.494626	-0.609550	3.440627
O	2.080087	-3.180183	-1.352147
H	1.363127	-2.614168	-0.968046
H	2.892331	-2.876260	-0.907464
C	0.111408	-0.494328	-0.005735

D3_B3LYP_18_s2 Eopt -1640.565767

O	1.092520	0.133692	0.282492
O	-1.103155	0.375873	-0.052413
O	-0.132243	-1.605358	-0.415037
O	-1.298998	2.039550	-2.231047
H	-1.157382	1.439768	-1.464037
H	-0.490648	1.948980	-2.777757
O	1.074108	2.573832	3.122865
H	1.218411	1.612350	3.217641
H	1.396420	2.767206	2.222300
O	3.565312	-0.485501	-0.665976
H	2.631350	-0.355116	-0.371797
H	3.554421	-1.307093	-1.193799
O	-0.974458	-1.621065	3.445246
H	-1.711411	-0.996748	3.262572
H	-0.931874	-2.185359	2.664309
O	1.760531	-3.440718	0.253191
H	1.098481	-2.739328	0.032805
H	2.368498	-3.014705	0.885349
O	-3.066396	0.174440	2.951339
H	-2.547480	0.968596	2.714785
H	-3.396274	-0.141446	2.087940
O	1.685771	2.796110	0.299227
H	0.896580	3.313429	0.046231
H	1.382733	1.854102	0.288339
O	-3.794974	-3.226637	-0.596157
H	-4.634905	-3.355204	-1.050789
H	-3.159863	-2.959867	-1.298170
O	1.470191	-0.264918	2.973644
H	0.649441	-0.730667	3.235033
H	1.344224	-0.109467	2.009738
O	3.431010	-3.044476	-1.927565
H	2.899351	-2.994354	-2.729562
H	2.796747	-3.269795	-1.209481
O	-3.496574	0.206880	-2.679230
H	-3.718266	0.065365	-1.742034
H	-2.775536	0.863586	-2.655801
O	3.608615	-1.920709	1.911023
H	3.752181	-1.406906	1.095706
H	2.925374	-1.417577	2.391375
O	-3.670607	-0.471890	0.212144

H	-3.763916	-1.423757	0.017791
H	-2.709239	-0.273178	0.091832
O	-0.804394	4.103972	-0.306192
H	-1.000111	3.496847	-1.046637
H	-1.142943	3.630863	0.476684
O	-1.497153	2.293345	1.859819
H	-1.272236	1.615231	1.176935
H	-0.674493	2.408500	2.374155
O	1.044267	1.818189	-3.779042
H	1.810446	1.844723	-3.162857
H	1.044230	0.925782	-4.142747
O	3.180632	2.031859	-2.000492
H	3.403369	1.138026	-1.676184
H	2.699151	2.430336	-1.248090
O	-1.922911	-2.220368	-2.392130
H	-1.290770	-1.966165	-1.676849
H	-2.416126	-1.401897	-2.588083
C	-0.047783	-0.373983	-0.063752

D3_B3LYP_18_s3 Eopt -1640.55785

O	-0.984386	0.292968	-0.114673
O	1.194634	0.061310	0.351038
O	0.185565	-1.368767	-1.039971
O	1.179569	-0.246294	3.049052
H	1.152176	-0.101377	2.073340
H	0.370692	-0.766000	3.217761
O	-0.654331	4.032865	-0.506982
H	-0.876283	3.404227	-1.223128
H	-1.085547	3.637238	0.270696
O	-4.506496	-0.484461	0.256859
H	-5.467162	-0.544606	0.311769
H	-4.187670	-1.413600	0.189508
O	1.077783	1.477162	-3.695814
H	1.831633	1.627621	-3.083549
H	1.187890	2.131286	-4.394767
O	-2.081263	-2.186079	-2.244071
H	-1.260573	-1.838268	-1.806063
H	-2.632574	-1.396739	-2.402736
O	3.211161	1.922396	-1.936442
H	2.733694	2.345332	-1.194888
H	3.493627	1.068187	-1.558194
O	-1.845032	2.272959	1.504795
H	-2.703145	2.470307	1.110385
H	-1.456639	1.563074	0.929028
O	4.022237	-3.007019	-1.582931
H	4.700756	-3.452178	-1.063310
H	3.166663	-3.295556	-1.190531
O	-1.342603	1.911517	-2.290826
H	-0.537079	1.775297	-2.830997
H	-1.210527	1.320664	-1.512948
O	-3.420223	-3.019312	0.013472
H	-2.778429	-3.046567	0.733031
H	-2.899195	-2.780115	-0.790043
O	3.895787	-1.189397	2.467112
H	3.918282	-0.955231	1.521769
H	2.995805	-0.954449	2.751269
O	-3.729719	0.176663	-2.470841
H	-3.983661	0.069282	-1.535415
H	-2.985566	0.803287	-2.470522
O	3.745196	-0.448558	-0.372023
H	3.859667	-1.309422	-0.820046
H	2.778041	-0.371462	-0.175553
O	1.636477	2.601747	3.245015
H	1.419944	1.655193	3.317024
H	1.679678	2.755679	2.283250
O	1.734952	2.744300	0.354292
H	1.456150	1.796642	0.369223
H	0.949016	3.233326	0.038661
O	-1.249508	-1.791328	3.028761
H	-1.971426	-1.134058	2.916252

H	-1.063340	-2.104189	2.135445
O	-3.282648	0.104368	2.771382
H	-3.761741	-0.123336	1.950233
H	-2.751680	0.880348	2.515031
O	1.580614	-3.592383	-0.458109
H	1.090514	-2.752038	-0.653900
H	1.124803	-4.275184	-0.962511
C	0.126844	-0.339976	-0.266224

D3_B3LYP_24_sl Eopt -2099.348589

O	1.221770	0.195054	-0.865412
O	-0.783143	-0.350722	-0.027208
O	1.074868	-1.229323	0.849619
O	2.479181	-0.139495	2.940615
H	2.230314	0.806839	2.974556
H	1.995930	-0.483571	2.155933
O	0.033521	-0.954023	4.274892
H	0.924857	-0.694992	3.973168
H	-0.170029	-1.739421	3.734186
O	-2.136518	1.041669	-1.888653
H	-1.623349	1.122759	-2.716301
H	-1.566638	0.516949	-1.268961
O	4.700682	-1.335545	1.468983
H	4.177074	-2.013125	1.003876
H	4.064453	-0.904229	2.067096
O	-2.538725	3.053753	-0.022641
H	-2.186505	2.648388	0.780038
H	-2.364846	2.393178	-0.730777
O	-2.794478	-1.857423	1.277192
H	-3.284754	-1.185239	1.793497
H	-2.085362	-1.347792	0.829124
O	-0.386245	-3.026843	2.264664
H	0.118531	-2.350772	1.744606
H	-1.316070	-2.793651	2.092539
O	-0.453163	1.197952	-4.194607
H	-0.056627	0.321825	-4.035366
H	0.104897	1.798048	-3.660961
O	1.104591	2.592159	-2.286254
H	0.572545	3.267629	-1.814580
H	1.035136	1.778078	-1.741604
O	1.924636	4.269875	1.029002
H	2.321404	5.078836	1.371425
H	2.575577	3.899529	0.388094
O	-0.232413	4.580184	-0.808161
H	-1.015900	4.108247	-0.468227
H	0.438192	4.530673	-0.100253
O	1.313812	2.431413	3.063273
H	1.536481	3.057696	2.346285
H	0.452040	2.045827	2.819514
O	2.867807	-3.072714	-0.070760
H	2.250341	-2.355739	0.204410
H	3.073184	-2.881468	-1.008072
O	-1.149341	0.987836	2.548019
H	-1.047752	0.574388	1.669126
H	-0.812487	0.311531	3.173547
O	-3.942303	0.331763	2.648731
H	-3.026817	0.670888	2.673256
H	-4.353559	0.765653	1.872498
O	3.956036	0.435615	-0.686918
H	2.984777	0.268001	-0.703296
H	4.290105	-0.095376	0.058955
O	0.319998	-4.504493	-0.175635
H	1.224679	-4.142734	-0.226592
H	-0.014183	-4.155724	0.671000
O	-1.114994	-2.723643	-1.861564
H	-0.623489	-3.377371	-1.319403
H	-1.143748	-1.930384	-1.298995
O	0.896399	-1.206658	-3.254312
H	1.042148	-0.651137	-2.457014
H	0.216318	-1.839479	-2.952923

O	-4.636012	-0.188899	-1.825322
H	-3.751974	0.217739	-1.941997
H	-4.444792	-1.117350	-1.585162
O	3.368372	-2.509260	-2.814255
H	2.514783	-2.075637	-3.024516
H	3.996498	-1.782133	-2.730974
O	3.535885	3.199681	-0.937154
H	2.757242	3.074643	-1.515622
H	3.804107	2.282332	-0.725580
O	-5.062998	1.570732	0.369574
H	-4.312986	2.174810	0.229801
H	-4.977760	0.911731	-0.349653
O	-3.923229	-2.848423	-1.072755
H	-3.064961	-2.946167	-1.521647
H	-3.658533	-2.539080	-0.181313
C	0.508257	-0.457572	-0.015064

D3_B3LYP_24_s2 Eopt -2099.343787

O	1.167617	0.640746	-0.513867
O	-0.707048	-0.454367	0.032945
O	1.264491	-1.143088	0.828310
O	2.364451	-0.154174	3.132205
H	1.941805	0.723310	3.230313
H	1.998018	-0.487738	2.282029
O	0.023048	-1.591719	4.156754
H	0.856467	-1.124809	3.959732
H	-0.011047	-2.296548	3.483394
O	-2.190705	0.842161	-1.794942
H	-1.616711	1.213956	-2.493182
H	-1.577637	0.394046	-1.156095
O	4.841701	-0.607723	1.634970
H	4.490682	-1.311549	1.058429
H	4.102781	-0.395747	2.233270
O	-3.464595	2.570482	-0.094076
H	-3.135218	2.335832	0.782527
H	-2.986772	1.968320	-0.714089
O	-2.452088	-2.552251	0.871054
H	-2.717120	-2.983013	0.039833
H	-1.874050	-1.815151	0.589323
O	0.089532	-3.371692	1.840639
H	0.494332	-2.547183	1.468672
H	-0.846611	-3.298784	1.574194
O	-0.301220	1.861574	-3.688680
H	0.242054	1.053297	-3.650060
H	0.080068	2.432656	-2.997502
O	0.660789	3.235226	-1.279202
H	-0.217837	3.634082	-1.104917
H	0.650913	2.312991	-0.940179
O	1.148115	4.242535	1.461593
H	1.077718	3.915643	0.546706
H	0.380150	4.815335	1.573946
O	-1.702267	4.649753	-0.777861
H	-2.357773	3.984274	-0.482235
H	-1.460794	5.137832	0.017854
O	0.734362	2.148849	3.315032
H	0.856799	2.838923	2.633471
H	-0.039355	1.626122	3.030825
O	3.453518	-2.452629	-0.169618
H	2.690548	-1.903074	0.122586
H	3.647278	-2.159942	-1.083002
O	-1.444578	0.368458	2.669149
H	-1.250548	0.097618	1.749751
H	-1.027368	-0.327201	3.218193
O	-4.298233	0.095618	2.778420
H	-3.327668	0.162863	2.707274
H	-4.630728	0.120538	1.862587
O	3.872327	1.159077	-0.437105
H	2.920363	0.909223	-0.408901
H	4.285830	0.664390	0.292965
O	1.275053	-4.327941	-0.654100

H	2.091917	-3.799862	-0.574166
H	0.828177	-4.180317	0.200346
O	-0.398533	-2.547185	-2.090869
H	0.196661	-3.182074	-1.635760
H	-0.605956	-1.883849	-1.408568
O	1.365809	-0.456418	-3.096139
H	1.384317	-0.016626	-2.219384
H	0.781456	-1.222559	-2.943255
O	-4.317789	-0.958090	-2.109666
H	-3.548113	-0.353807	-2.093894
H	-3.936992	-1.849620	-2.015270
O	3.901458	-1.655613	-2.859490
H	3.019456	-1.254301	-3.010639
H	3.902298	-2.463841	-3.384610
O	3.507524	3.828289	-1.269412
H	2.537744	3.787449	-1.301893
H	3.756752	2.946933	-0.932241
O	-5.415228	0.397973	0.137254
H	-4.902504	1.218826	0.036391
H	-5.078041	-0.176741	-0.579017
O	-3.010106	-3.484330	-1.787934
H	-2.076564	-3.293508	-2.019459
H	-3.206427	-4.359091	-2.140769
C	0.579669	-0.312616	0.118591

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O	0.542731	-1.151822	-0.778454
O	-1.134992	0.274360	-0.420774
O	-0.925293	-1.551015	0.859462
O	0.524271	-1.684725	3.239413
H	0.768214	-0.759439	3.446916
H	0.023779	-1.620218	2.400017
O	-3.040113	0.783549	3.470914
H	-3.266809	0.050012	2.858669
H	-3.792854	1.384287	3.433619
O	0.264517	1.865634	-2.092531
H	0.992280	1.368353	-2.519400
H	-0.228656	1.211994	-1.531742
O	1.914060	-3.896630	2.143157
H	1.171234	-4.158972	1.568966
H	1.562715	-3.121549	2.623541
O	1.148041	3.348381	0.058216
H	0.602619	3.016166	0.785409
H	0.875592	2.807399	-0.720458
O	-3.825045	0.333612	-0.754352
H	-4.053713	-0.315640	-1.429993
H	-2.841584	0.271558	-0.652491
O	-3.472990	-1.294561	1.638427
H	-2.512109	-1.336439	1.380411
H	-3.869189	-0.788289	0.908168
O	2.412261	0.441980	-3.280940
H	1.981367	-0.421637	-3.395614
H	2.999278	0.320547	-2.506191
O	4.112423	0.083798	-1.033408
H	3.950639	0.857983	-0.447697
H	3.752822	-0.694333	-0.566450
O	3.723919	1.658149	3.246765
H	4.293321	0.912918	3.473798
H	4.015677	2.381234	3.815070
O	3.751799	2.355638	0.499916
H	2.844515	2.694770	0.358586
H	3.784402	2.109472	1.442969
O	0.985757	1.038842	3.742558
H	1.900575	1.284023	3.514498
H	0.415903	1.379038	3.026316
O	-0.515590	-4.225681	0.543651
H	-0.588972	-3.244751	0.644582
H	-0.457227	-4.362812	-0.422336
O	-1.008230	1.888482	1.865651
H	-1.066126	1.323057	1.063703

H	-1.712403	1.545445	2.457237
O	-2.297966	4.393062	1.302439
H	-1.852252	3.542238	1.473665
H	-1.802255	4.780243	0.555741
O	2.880453	-2.267573	-0.016295
H	1.984321	-1.918295	-0.232477
H	2.730799	-2.823423	0.770568
O	-3.420303	-4.013507	0.602916
H	-2.462490	-4.191464	0.666204
H	-3.531930	-3.134525	1.011574
O	-3.144778	-3.156716	-2.058457
H	-3.301017	-3.444907	-1.133008
H	-2.819357	-2.251976	-1.979072
O	1.053590	-2.216339	-3.206226
H	0.820264	-1.828621	-2.329867
H	1.892337	-2.669681	-3.058885
O	-1.668313	3.745788	-2.937853
H	-1.009465	3.052202	-2.740211
H	-2.523193	3.386063	-2.625673
O	-0.630536	-4.454448	-2.326126
H	-0.041789	-3.759173	-2.670026
H	-1.512196	-4.031172	-2.296781
O	6.869366	-0.208794	-1.366587
H	5.899221	-0.114437	-1.262899
H	7.018108	-0.207083	-2.318003
O	-0.700872	5.379978	-0.851929
H	0.016506	4.804500	-0.528119
H	-1.085809	4.872588	-1.597232
O	-4.173161	2.804428	-2.035972
H	-4.696121	2.631586	-2.826809
H	-4.062026	1.929310	-1.606769
C	-0.501167	-0.818183	-0.118446

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Eopt -2328.73511

O	-1.060668	-0.952904	-0.131299
O	-0.496128	1.114207	-0.777213
O	1.064592	-0.482790	-0.615848
O	3.327982	0.942670	-0.209255
H	3.352847	1.544546	-0.979116
H	2.487016	0.440472	-0.345722
O	-4.121209	-3.206298	1.019727
H	-3.574339	-3.803339	0.471019
H	-4.040305	-2.328806	0.590706
O	-0.095323	-1.937360	2.255079
H	0.735563	-2.445723	2.131794
H	-0.400429	-1.687009	1.353105
O	1.894619	-0.254788	-3.283876
H	1.071963	-0.531419	-3.737558
H	1.640148	-0.283801	-2.336798
O	3.004412	2.377734	-2.685681
H	2.628508	1.554324	-3.044468
H	2.234570	2.842250	-2.295057
O	-1.951313	1.209326	-3.174220
H	-2.865712	0.895160	-3.010178
H	-1.496505	1.138746	-2.308082
O	2.363155	2.088838	2.172051
H	2.703304	1.706038	1.335657
H	1.543353	1.596254	2.378130
O	-4.522517	0.227273	-2.655000
H	-5.111639	0.979508	-2.529893
H	-4.303216	-0.084935	-1.746685
O	-2.545051	-4.908206	-0.624866
H	-1.976888	-5.412576	-0.031895
H	-1.943335	-4.283531	-1.084454
O	1.370495	4.527008	1.080051
H	0.457611	4.608381	1.425823
H	1.718527	3.708794	1.486385
O	0.094093	0.669531	3.165643
H	0.444888	0.649815	4.064365
H	0.122175	-0.267349	2.862639

O	-1.929419	4.022830	-2.394226
H	-2.054126	3.141322	-2.790889
H	-1.001810	3.999867	-2.089802
O	-0.930404	-3.026305	-1.938197
H	-0.005075	-3.294948	-1.793422
H	-1.040944	-2.296720	-1.284105
O	3.778193	-2.342526	-2.817111
H	3.140210	-1.658418	-3.101484
H	4.384119	-1.861815	-2.218671
O	5.382902	-0.755289	-1.102549
H	4.683438	-0.194441	-0.703520
H	5.792884	-1.225527	-0.368321
O	3.784161	0.585459	4.079642
H	3.106184	0.302229	4.703994
H	3.310818	1.155577	3.436990
O	-2.748261	0.231364	3.734616
H	-2.787250	-0.737367	3.591457
H	-1.819770	0.462741	3.551545
O	-0.652495	-1.137836	-4.165848
H	-0.761085	-1.792635	-3.451028
H	-1.137908	-0.346329	-3.857699
O	-1.291893	4.705260	1.958607
H	-1.680099	4.015005	1.376234
H	-1.336208	4.339456	2.849103
O	4.393056	-1.588747	2.431090
H	4.157328	-0.838970	3.019059
H	4.548508	-1.184477	1.569466
O	-2.383526	2.845410	0.215496
H	-2.457675	3.358845	-0.610494
H	-1.745668	2.134376	-0.024406
O	-3.763501	-0.693633	-0.175414
H	-4.005763	-0.005724	0.481384
H	-2.774070	-0.696860	-0.187566
O	0.741147	3.474190	-1.452453
H	0.982507	3.886759	-0.595318
H	0.394590	2.585624	-1.207753
O	1.774447	-3.098364	-0.926494
H	2.515885	-2.988861	-1.554190
H	1.467763	-2.171500	-0.769863
O	-2.629120	-2.570200	3.314389
H	-3.153365	-2.815206	2.522419
H	-1.714830	-2.474468	2.983987
O	-4.283653	1.346665	1.671464
H	-3.739092	0.983434	2.402303
H	-3.685501	1.943086	1.181549
O	2.276768	-3.362080	1.833784
H	2.996124	-2.737635	2.057624
H	2.209369	-3.334016	0.857723
C	-0.163653	-0.098621	-0.507121

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Eopt -2328.73619

O	-1.104434	-0.746459	-0.655976
O	-0.597339	1.361608	-0.096176
O	0.942533	0.047180	-1.044839
O	3.223851	0.974337	0.059076
H	3.282764	1.898081	-0.251653
H	2.345676	0.674215	-0.282752
O	-4.107183	-3.318031	-0.502339
H	-3.690383	-3.502872	-1.367326
H	-4.058652	-2.342823	-0.415664
O	0.010004	-2.630858	1.069281
H	0.808420	-3.061071	0.692491
H	-0.332370	-2.023484	0.377740
O	1.556222	1.849785	-3.054151
H	0.709539	1.842043	-3.542907
H	1.382835	1.234520	-2.307975
O	2.837466	3.589298	-1.094449
H	2.405041	3.143458	-1.843982
H	2.119707	3.695452	-0.435366
O	-2.206522	2.865254	-1.830887

H	-3.107774	2.481526	-1.784606	O	-1.144969	-0.949222	-0.567799
H	-1.669752	2.310432	-1.226606	O	-3.833536	-0.190209	-0.494683
O	2.867176	0.512585	2.772417	H	-4.082664	-0.259223	0.449161
H	2.971016	0.693749	1.812244	H	-2.871450	-0.395227	-0.503550
H	2.034749	0.008033	2.861535	O	5.232719	-1.597007	-0.198294
O	-4.726318	1.637303	-1.689499	H	4.850855	-2.483847	-0.354331
H	-5.274842	2.157509	-1.091818	H	4.576680	-1.147278	0.375296
H	-4.432161	0.861495	-1.159430	O	1.886474	-0.033953	-2.539093
O	-2.906854	-3.717543	-3.048297	H	1.320033	-0.428913	-3.235060
H	-3.641511	-3.680603	-3.671202	H	1.578257	-0.434021	-1.693738
H	-2.417743	-2.878815	-3.180852	O	-2.435060	-2.641420	1.425488
O	1.499468	2.970230	3.363839	H	-1.671175	-2.954542	1.958238
H	0.662092	2.543376	3.643767	H	-2.034331	-2.105404	0.715922
H	2.083028	2.209389	3.181021	O	-4.128032	-0.528428	2.314886
O	0.427009	-0.963559	3.214603	H	-3.517662	-1.276566	2.164632
H	0.696848	-1.529355	3.947771	H	-3.548203	0.248366	2.443659
H	0.324813	-1.567243	2.440405	O	0.167827	-0.703279	3.614869
O	-1.933613	4.702874	0.462785	H	1.126990	-0.654199	3.801953
H	-2.147291	4.222005	-0.356631	H	0.053113	-0.293756	2.733865
H	-0.997455	4.471882	0.621282	O	-4.188436	2.388623	-1.435037
O	-1.413672	-1.329955	-3.309404	H	-4.058663	1.469571	-1.110525
H	-0.576943	-1.683653	-3.634189	H	-3.552950	2.484007	-2.154359
H	-1.262387	-1.167325	-2.346617	O	2.950140	-0.693321	4.055934
O	4.052252	0.804714	-3.946135	H	3.181731	0.133319	4.493665
H	3.176369	1.164041	-3.708503	H	3.117791	-0.533787	3.098768
H	4.283154	0.224573	-3.201027	O	4.020592	-4.126789	-0.582134
O	4.476850	-0.942669	-1.591876	H	4.457622	-4.735603	0.023841
H	4.135954	-0.224993	-1.018370	H	3.141391	-3.955650	-0.183164
H	3.668544	-1.401928	-1.895781	O	-3.155668	3.788010	0.763546
O	4.776920	-1.493732	3.070103	H	-2.276552	4.122724	0.494003
H	5.633482	-1.060831	3.157727	H	-3.509739	3.329326	-0.026396
H	4.126611	-0.761954	2.988276	O	1.455515	2.638183	-1.948170
O	-2.539394	-1.822485	3.571948	H	1.255061	2.669213	-1.003451
H	-2.553191	-2.552349	2.916986	H	1.545465	1.680541	-2.163524
H	-1.639847	-1.463599	3.519976	O	-0.364932	3.122019	3.813812
O	-1.091328	1.513362	-4.088784	H	-0.660708	4.033506	3.916511
H	-1.201882	0.572483	-3.861750	H	-1.119623	2.651876	3.397654
H	-1.517808	1.997010	-3.352985	O	1.486464	-3.565052	0.491847
O	-0.823516	1.528334	4.033544	H	0.897560	-4.136240	-0.015158
H	-1.397779	1.788984	3.283670	H	1.278535	-2.643874	0.200264
H	-0.460144	0.663827	3.774060	O	-4.194706	-4.319047	-0.041990
O	4.764983	-2.833388	0.596717	H	-3.556946	-3.811696	0.494487
H	4.767801	-2.330702	1.437063	H	-4.554796	-3.660953	-0.666425
H	4.746597	-2.162289	-0.111029	O	-5.189494	-2.273603	-1.770064
O	-2.391898	2.167723	1.807121	H	-4.691995	-1.534150	-1.358078
H	-2.414992	3.103940	1.538836	H	-4.773276	-2.409987	-2.628411
H	-1.820710	1.748295	1.122680	O	-0.969702	3.183493	-3.237797
O	-3.798287	-0.546016	-0.269311	H	-0.132653	3.074800	-2.737873
H	-3.971422	-0.345081	0.675720	H	-1.549018	3.699814	-2.665733
H	-2.814303	-0.533974	-0.365745	O	4.333255	2.686203	-1.574808
O	0.714143	3.635596	0.737383	H	4.539187	1.767314	-1.846145
H	1.008138	3.448392	1.654548	H	3.386336	2.785657	-1.782973
H	0.341701	2.782827	0.415829	O	-0.156886	-3.365256	2.858696
O	1.972818	-2.111312	-2.260078	H	0.443782	-3.475391	2.097980
H	1.678271	-2.195550	-3.173442	H	-0.007838	-2.442242	3.161034
H	1.469924	-1.352425	-1.865022	O	-0.573871	4.728891	0.097542
O	-2.413432	-3.910881	1.668717	H	-0.010379	4.024267	0.484116
H	-2.990731	-3.729535	0.897403	H	-0.438062	4.662184	-0.854641
H	-1.531266	-3.582214	1.404095	O	-1.777336	0.496152	-3.124401
O	-4.210182	0.118269	2.420728	H	-1.506631	1.436760	-3.113861
H	-3.626657	-0.542865	2.849300	H	-1.518266	0.133122	-2.260550
H	-3.647045	0.905078	2.293297	O	0.975989	2.770141	1.351692
O	2.226201	-3.864219	-0.091755	H	0.639274	2.993688	2.244362
H	3.086130	-3.538073	0.245879	H	0.593359	1.877684	1.179650
H	2.106596	-3.376053	-0.929138	O	3.299632	-0.309161	1.354295
C	-0.255024	0.227714	-0.594282	H	3.479652	0.653412	1.273174
				H	2.447880	-0.467733	0.881905
				O	-2.348911	1.687748	2.421571
				H	-2.680550	2.408769	1.841496
				H	-1.707110	1.193363	1.864429

D3_B3LYP_27_s3 Eopt -2328.734483

O	1.041672	-0.937553	-0.094224
O	-0.349758	0.389808	1.043726

O	-0.695265	-2.990545	-2.350245
H	0.089864	-3.484807	-2.090911
H	-0.786582	-2.273250	-1.675702
O	4.696594	0.011691	-2.439543
H	4.914266	-0.568207	-1.679429
H	3.729063	-0.079873	-2.546856
O	3.754724	2.429901	1.184170
H	3.986130	2.542035	0.239313
H	2.796325	2.623616	1.242056
O	0.082028	-1.179906	-4.371631
H	-0.579832	-0.509146	-4.105028
H	-0.123523	-1.923093	-3.768434
C	-0.153589	-0.492860	0.129262

D3_B3LYP_Radical_9_s1			
O	-0.612327	-2.088457	-0.310232
O	-0.448182	-0.104806	-1.174206
O	-0.299662	-0.396198	1.040598
O	0.492068	2.338769	1.469196
H	0.161199	1.426097	1.410216
H	0.337378	2.689764	0.574651
O	-3.134494	1.067849	-1.207142
H	-2.228873	0.774817	-1.392510
H	-3.141890	1.174618	-0.241159
O	0.370684	2.688313	-1.384532
H	1.317088	2.501709	-1.348997
H	-0.038605	1.809370	-1.343449
O	2.579053	-2.493878	-0.561895
H	1.662920	-2.757515	-0.719513
H	2.554972	-2.074997	0.325375
O	-3.021455	0.557103	1.696713
H	-2.063541	0.429135	1.663779
H	-3.370923	-0.260548	1.304349
O	2.417609	-1.100148	1.870540
H	2.736538	-0.253997	1.491514
H	1.454660	-1.011266	1.808513
O	-3.750382	-1.625644	-0.110198
H	-3.637982	-0.868496	-0.707547
H	-2.887821	-2.063915	-0.117391
O	3.051186	1.329379	0.604354
H	2.225675	1.756271	0.901619
H	2.835687	0.952325	-0.274277
O	2.444162	0.014690	-1.836843
H	2.567964	-0.882331	-1.459401
H	1.479715	0.119287	-1.841410
C	-0.445042	-0.826017	-0.134197

D3_B3LYP_Radical_9_s2			
O	0.196132	-0.034955	-1.127014
O	-0.085048	-2.119965	-0.794511
O	-0.103760	-0.756792	0.968693
O	-2.751487	-1.810419	1.629290
H	-1.834703	-1.496237	1.572083
H	-3.041560	-1.799967	0.700704
O	3.106924	-2.401392	-0.198267
H	2.213952	-2.590001	-0.514234
H	2.973846	-1.789383	0.547013
O	-3.170853	-1.472102	-1.271666
H	-3.025667	-0.536298	-1.025103
H	-2.285396	-1.827299	-1.423821
O	1.194181	2.937067	0.168657
H	1.796708	2.243997	-0.125568
H	0.709938	2.539951	0.923523
O	2.713766	-0.107065	1.579034
H	1.752155	-0.229740	1.563001
H	2.904732	0.325372	0.731510
O	-0.362067	1.771815	2.163695
H	-1.226607	2.136668	1.941182
H	-0.342590	0.892692	1.738530
O	3.071777	0.347957	-1.360399

H	3.300665	-0.579259	-1.188671
H	2.103678	0.323886	-1.417125
O	-2.849207	1.087426	-0.128848
H	-2.394582	0.652318	0.602392
H	-2.167676	1.642200	-0.561791
O	-1.013207	2.691022	-1.547460
H	-0.227285	2.791513	-0.968959
H	-0.770020	1.973005	-2.143487
C	-0.002798	-0.955698	-0.266800

D3_B3LYP_Radical_9_s3			
O	0.735010	-0.365102	-1.851927
O	1.732489	1.194064	-0.776981
O	1.668764	-0.857159	0.106050
O	4.469260	-1.157420	0.713916
H	3.506468	-1.084854	0.586859
H	4.617614	-0.911185	1.634022
O	-0.449685	3.015413	-0.193302
H	0.322267	2.460582	-0.398955
H	-0.143828	3.620988	0.491955
O	4.744482	1.213505	-0.867491
H	4.770269	0.413436	-0.309680
H	3.796764	1.383154	-0.966206
O	-1.942624	-1.164250	-0.699235
H	-1.306791	-0.816700	-1.341136
H	-1.450424	-1.878806	-0.242207
O	0.341419	0.094148	2.603411
H	0.881687	-0.239406	1.871333
H	-0.467190	0.419454	2.162286
O	-0.229719	-2.972662	0.578369
H	-0.053707	-3.708457	-0.019200
H	0.487318	-2.334418	0.409088
O	-1.928064	1.003664	1.126940
H	-1.452243	1.726945	0.669235
H	-1.912008	0.253002	0.497937
O	-4.704669	-1.014381	-1.195350
H	-3.749372	-1.159149	-1.047261
H	-5.141984	-1.748927	-0.750670
C	1.389421	-0.036634	-0.802810
O	-4.740409	1.266684	0.555528
H	-3.799342	1.274706	0.809620
H	-4.812052	0.497403	-0.039576

D3_B3LYP_Radical_12_s1			
O	-0.174764	0.301114	0.999499
O	0.018616	-0.676089	-0.950101
O	-0.174997	1.525438	-0.815857
O	-2.632416	-0.967134	-2.379705
H	-1.702802	-1.020467	-2.113168
H	-2.861153	-0.031291	-2.210421
O	-0.890380	2.601325	2.963268
H	-0.729814	1.729282	2.580724
H	-0.799126	3.202733	2.199991
O	2.440258	-3.326590	0.576969
H	1.481626	-3.472186	0.504574
H	2.645661	-2.723017	-0.167411
O	-2.967996	-0.612007	1.810816
H	-3.124554	-1.303463	1.137196
H	-2.084319	-0.275087	1.607914
O	4.352387	0.699838	-0.762170
H	4.555727	0.611309	0.175732
H	3.704124	1.434080	-0.817268
O	2.021799	-1.199328	2.435888
H	2.197076	-1.944995	1.828963
H	1.337336	-0.681978	1.988595
O	-0.615788	4.098297	0.550259
H	-0.454633	3.271416	0.066905
H	0.241197	4.540131	0.568470
O	2.801456	-1.494921	-1.533521
H	3.360365	-0.743133	-1.242854

Eopt -952.18389

Eopt -952.183365

Eopt -952.180242

Eopt -1181.782999

H	1.891612	-1.174332	-1.434394
O	-3.311994	-2.617809	-0.173869
H	-3.178260	-2.042963	-0.954310
H	-2.425811	-2.978918	0.004373
O	-0.507498	-3.223429	0.408625
H	-0.336269	-2.355335	0.003285
H	-0.595056	-3.031532	1.350877
O	-2.971014	1.800701	-1.861674
H	-3.601232	1.937604	-1.144887
H	-2.098313	1.859327	-1.442090
O	2.491244	2.768790	-1.013851
H	1.604792	2.372893	-0.986973
H	2.589233	3.098481	-1.914754
C	-0.108120	0.382648	-0.270944

D3_B3LYP_Radical_12_s2

O	0.582072	-0.451002	0.199529
O	-1.220890	-1.041763	-0.968875
O	0.522938	-2.347350	-0.886263
O	-1.436982	0.658924	-3.347387
H	-1.303161	0.029103	-2.619493
H	-0.570280	0.750273	-3.759672
O	-0.869330	2.199362	2.331599
H	-0.399099	1.425198	2.691763
H	-0.338686	2.454129	1.553647
O	3.474407	-0.216349	-0.056972
H	2.506813	-0.233027	0.041962
H	3.646231	-0.983292	-0.637593
O	-4.644207	-0.901077	1.399838
H	-4.054879	-0.152068	1.196754
H	-4.238285	-1.647873	0.920974
O	0.564894	2.482916	-0.168793
H	-0.222678	2.681971	-0.717882
H	0.584030	1.512667	-0.124198
O	0.679552	-0.140501	3.042198
H	0.228476	-0.803339	3.578102
H	0.565427	-0.431785	2.120720
O	3.432188	-2.534761	-1.699431
H	3.565084	-2.283044	-2.620767
H	2.470668	-2.531160	-1.577978
O	3.562374	-0.546954	2.826611
H	3.645431	-0.483503	1.858609
H	2.610720	-0.429189	2.990278
O	-3.300252	-2.931830	-0.117140
H	-2.916937	-3.577902	0.486888
H	-2.553512	-2.375060	-0.393851
O	-1.855571	2.836705	-1.571105
H	-1.712615	2.155924	-2.258491
H	-2.292529	2.347252	-0.848891
O	-2.753776	1.083622	0.544122
H	-2.244166	0.387941	0.098206
H	-2.145742	1.432819	1.230866
O	3.226122	2.381106	-1.282615
H	3.429530	1.492305	-0.938449
H	2.317817	2.543052	-0.971910
C	-0.047664	-1.254965	-0.543686

D3_B3LYP_Radical_12_s3

O	-0.441726	0.581440	1.462006
O	0.695875	-0.007421	-0.358169
O	1.664501	0.991716	1.374214
O	-1.577717	-0.029318	-2.240788
H	-0.851590	0.043317	-1.599808
H	-2.356838	0.357356	-1.785904
O	-2.533812	2.550428	0.968795
H	-1.757417	1.989894	1.125536
H	-2.203562	3.319377	0.463064
O	2.914810	-3.436651	0.135764
H	1.947934	-3.385062	0.231335
H	3.136088	-2.629372	-0.367716

Eopt -1181.782868

Eopt -1181.783787

O	-4.225500	-1.693921	0.200597
H	-3.523436	-2.098655	-0.355744
H	-3.867546	-1.695029	1.095677
O	5.319982	0.736899	-0.650152
H	5.747098	0.359687	0.127090
H	4.771150	1.474343	-0.307955
O	-1.080323	-2.056467	2.604237
H	-2.033381	-2.190389	2.541288
H	-0.940316	-1.134005	2.333449
O	-1.645420	4.818391	-0.461617
H	-1.235772	4.495727	-1.273151
H	-2.439223	5.280052	-0.757185
O	3.257634	-1.042201	-1.365246
H	3.982093	-0.440063	-1.097857
H	2.447574	-0.630850	-1.021280
O	-2.253840	-2.685390	-1.512520
H	-2.028455	-1.797851	-1.860791
H	-1.498642	-2.899349	-0.931913
O	0.061992	-2.896116	0.158551
H	0.306224	-2.005567	-0.142815
H	-0.331636	-2.734604	1.040504
O	-3.850769	0.909179	-0.889431
H	-4.018405	0.057415	-0.439891
H	-3.427058	1.483340	-0.217913
O	3.618628	2.787072	0.194398
H	4.021557	3.254443	0.935380
H	2.905571	2.259156	0.590663
C	0.642242	0.507596	0.785138

D3_B3LYP_Radical_18_s1

O	0.931688	0.142806	-0.122639
O	-1.281680	0.026375	0.094111
O	-0.096779	-1.766668	-0.312001
O	-2.119516	1.351150	-2.341296
H	-1.900622	0.954996	-1.480872
H	-1.333065	1.142615	-2.891129
O	0.746956	3.254776	2.412431
H	1.091334	2.366712	2.630168
H	0.966707	3.360871	1.469086
O	3.650926	0.108874	-1.068406
H	2.728353	-0.044058	-0.806811
H	3.984727	-0.768098	-1.354192
O	-0.402846	-1.022708	3.644944
H	-1.269772	-0.583765	3.500952
H	-0.375425	-1.736664	2.997219
O	4.378413	-3.069857	1.045910
H	5.175074	-3.479604	1.400252
H	4.383911	-2.146632	1.381023
O	-2.878026	0.261679	3.287839
H	-2.569578	1.078530	2.852969
H	-3.298419	-0.242425	2.568265
O	1.114545	3.080012	-0.486241
H	0.209598	3.390563	-0.702411
H	1.005034	2.129467	-0.317090
O	-3.761634	-3.803761	0.297073
H	-3.169280	-4.262765	0.903240
H	-3.221307	-3.618262	-0.500054
O	1.699525	0.560349	2.664709
H	0.991182	0.022478	3.080062
H	1.510659	0.482838	1.714716
O	4.667089	-2.440717	-1.654784
H	3.976824	-2.903545	-2.143319
H	4.575896	-2.747627	-0.726293
O	-4.119683	-0.784589	-2.156544
H	-4.201690	-0.781046	-1.187170
H	-3.511441	-0.049121	-2.351400
O	4.313556	-0.361018	1.725724
H	4.155504	-0.104249	0.797393
H	3.483559	-0.137365	2.182469
O	-3.842114	-1.020578	0.821894

Eopt -1640.566472

H	-3.851404	-1.997037	0.754409
H	-2.940712	-0.769842	0.555860
O	-1.582184	3.807064	-0.927246
H	-1.804091	3.063276	-1.519201
H	-1.798621	3.471878	-0.038459
O	-1.845250	2.411404	1.644608
H	-1.596191	1.647719	1.095837
H	-0.991216	2.735967	2.000607
O	0.189416	0.627417	-3.761406
H	0.975641	1.115241	-3.430807
H	0.301405	-0.272472	-3.434088
O	2.421092	2.060865	-2.842647
H	2.950884	1.384666	-2.382745
H	1.990389	2.548349	-2.115334
O	-2.334906	-2.976936	-1.987039
H	-1.552572	-2.601381	-1.558257
H	-2.931266	-2.211107	-2.123327
C	-0.154789	-0.501103	-0.108920

D3_B3LYP_Radical_18_s2

Eopt -1640.56789

O	0.879883	0.115987	-0.167837
O	-1.326694	-0.022585	0.101865
O	-0.197336	-1.679468	-0.768205
O	-2.160211	1.902731	-1.889275
H	-1.915059	1.289355	-1.175820
H	-1.393053	1.857917	-2.500313
O	0.831106	2.450773	3.097953
H	1.153068	1.528703	3.061873
H	1.022195	2.795102	2.206327
O	3.574459	0.302463	-1.135786
H	2.657531	0.063301	-0.924514
H	3.953561	-0.482182	-1.586889
O	-0.390479	-1.980701	3.232142
H	-1.245992	-1.498048	3.240510
H	-0.411618	-2.509493	2.426106
O	5.211014	-2.976319	0.389387
H	4.576663	-3.675345	0.583421
H	4.874210	-2.182502	0.860168
O	-2.828573	-0.587810	3.316184
H	-2.514539	0.308702	3.094418
H	-3.291267	-0.878597	2.510084
O	1.111495	3.031999	0.258891
H	0.212117	3.409267	0.155807
H	0.978683	2.073471	0.167486
O	-3.884331	-3.726590	-0.515144
H	-4.768675	-3.961571	-0.817643
H	-3.437151	-3.344648	-1.300571
O	1.709709	-0.228841	2.619045
H	1.002447	-0.848281	2.902272
H	1.507970	-0.071387	1.681885
O	4.792090	-1.982002	-2.190225
H	4.140100	-2.525013	-2.647169
H	4.922507	-2.413394	-1.317903
O	-4.197573	-0.152987	-2.200326
H	-4.277818	-0.377114	-1.257630
H	-3.571667	0.594087	-2.219704
O	4.391119	-0.556296	1.492284
H	4.146978	-0.182409	0.623087
H	3.555080	-0.582140	1.988419
O	-3.913145	-1.136155	0.635160
H	-3.970855	-2.063218	0.326485
H	-3.007272	-0.863489	0.409882
O	-1.576259	3.900938	0.093627
H	-1.822992	3.329478	-0.658903
H	-1.781206	3.358603	0.876359
O	-1.806980	1.896051	2.232741
H	-1.596246	1.298970	1.494518
H	-0.933071	2.100168	2.627941
O	0.099900	1.621203	-3.525962
H	0.906774	1.972001	-3.088763

H	0.199861	0.662616	-3.498749
O	2.387338	2.683174	-2.290768
H	2.902847	1.896212	-2.036191
H	1.971799	2.965574	-1.454032
O	-2.535223	-2.407958	-2.599213
H	-1.725102	-2.194248	-2.114305
H	-3.081115	-1.596330	-2.534605
C	-0.218359	-0.499162	-0.265941

D3_B3LYP_Radical_18_s3

Eopt -1640.56085

O	-1.066535	-0.089525	0.193777
O	1.061124	-0.270425	-0.385307
O	-0.201091	1.388798	-1.125625
O	1.131804	-2.056772	-2.651263
H	1.200686	-1.512525	-1.848924
H	0.249920	-1.814243	-3.000589
O	-0.496117	-2.652189	3.166591
H	-0.607170	-1.686188	3.269945
H	-1.099916	-2.870709	2.434313
O	-4.395863	0.302385	-0.149042
H	-5.357187	0.274976	-0.078867
H	-4.197771	1.053768	-0.753037
O	1.687203	1.219172	3.641542
H	2.344706	0.638268	3.197626
H	1.870152	1.134277	4.583906
O	-2.054352	3.430213	0.307760
H	-1.276828	2.941019	0.004878
H	-2.454516	2.854020	0.993917
O	3.513492	-0.443900	2.337054
H	2.939076	-1.202406	2.116871
H	3.716266	-0.045984	1.469819
O	-2.131929	-2.791462	0.765732
H	-2.983959	-2.612631	1.182094
H	-1.751565	-1.913340	0.596853
O	4.103355	3.262634	-0.618885
H	4.540202	3.440402	-1.459308
H	3.162347	3.501213	-0.763575
O	-0.856465	0.185379	3.072103
H	0.017682	0.566846	3.304804
H	-0.834001	0.100148	2.104766
O	-3.656220	2.425902	-1.770379
H	-3.040244	2.020372	-2.392153
H	-3.086355	2.844746	-1.089771
O	3.743278	-0.629290	-3.104895
H	3.819045	-0.242033	-2.214588
H	2.892396	-1.094849	-3.096298
O	-3.309065	1.701774	2.148160
H	-3.665316	1.123392	1.447170
H	-2.564120	1.216405	2.537142
O	3.801116	0.497382	-0.397890
H	3.935365	1.466303	-0.479352
H	2.836609	0.375333	-0.422945
O	1.321010	-4.301938	-0.816383
H	1.205846	-3.634945	-1.516095
H	1.446844	-3.773499	-0.008053
O	1.692392	-2.462066	1.409920
H	1.380514	-1.760079	0.812708
H	0.966034	-2.567624	2.061446
O	-1.425703	-1.061996	-3.417231
H	-2.140636	-1.343041	-2.805169
H	-1.248517	-0.143760	-3.180295
O	-3.502893	-1.905630	-1.730812
H	-3.840203	-1.133845	-1.233175
H	-3.042525	-2.427104	-1.054490
O	1.409552	3.860383	-0.987706
H	0.912634	3.027082	-0.976197
H	1.078353	4.355636	-0.228898
C	-0.044768	0.328997	-0.435710

D3_B3LYP_Radical_24_s1

Eopt -2099.351409

O	-0.808920	0.221358	-1.373162
O	0.942513	0.025645	-0.035828
O	-0.934342	0.987086	0.643360
O	-3.127612	0.341895	2.436057
H	-3.252055	-0.633328	2.419477
H	-2.390398	0.492814	1.823141
O	-1.035014	0.051921	4.410260
H	-1.840661	0.187216	3.876214
H	-0.459917	0.792276	4.146859
O	2.631086	-1.030800	-2.095099
H	2.528104	-0.569237	-2.954635
H	2.031170	-0.564214	-1.487421
O	-4.396981	2.312050	0.691180
H	-3.630654	2.896692	0.557399
H	-4.097623	1.656594	1.346420
O	1.742197	-3.422328	-0.858943
H	1.116807	-3.031385	-0.235431
H	2.038947	-2.668885	-1.407917
O	2.588484	0.567429	2.318797
H	2.680911	-0.318020	2.737546
H	2.055608	0.395864	1.523364
O	0.466496	2.204466	3.111459
H	-0.117064	1.927960	2.389303
H	1.271099	1.662692	2.969610
O	2.292298	0.513554	-4.407104
H	1.697825	1.173857	-3.997305
H	1.745726	0.050603	-5.052262
O	-1.537161	-2.149426	-3.092521
H	-1.056716	-2.982232	-2.901112
H	-1.164437	-1.488399	-2.492005
O	-4.055150	-3.626112	0.182932
H	-4.965561	-3.880163	0.370432
H	-4.109190	-3.013456	-0.586632
O	-0.136673	-4.533832	-2.641424
H	0.530731	-4.222090	-1.996258
H	-0.704351	-5.135762	-2.147035
O	-3.108684	-2.434373	2.516776
H	-3.394981	-2.842158	1.672537
H	-2.136214	-2.466992	2.521659
O	-1.825759	3.732473	0.147914
H	-1.528227	2.812604	0.232093
H	-1.733533	3.937161	-0.807578
O	-0.190516	-2.075482	2.764841
H	-0.046650	-1.667354	1.901567
H	-0.428236	-1.327261	3.356373
O	2.683652	-2.040314	3.270323
H	1.727690	-2.167549	3.129151
H	3.118767	-2.398625	2.467130
O	-3.821250	0.795861	-1.622681
H	-2.859005	0.714031	-1.557863
H	-4.077365	1.294384	-0.819156
O	0.873818	4.302035	1.081667
H	-0.039502	4.241466	0.743560
H	0.867995	3.718739	1.861052
O	2.292558	2.692950	-0.743467
H	1.819571	3.283844	-0.116460
H	2.032427	1.800627	-0.470320
O	0.598795	2.330737	-2.997067
H	0.044410	1.621673	-2.635022
H	1.208621	2.549560	-2.260659
O	5.007002	-0.811482	-0.574683
H	4.238982	-0.845576	-1.178367
H	4.925695	0.052116	-0.122707
O	-1.379651	4.326018	-2.552286
H	-0.696434	3.660073	-2.770377
H	-2.141631	4.089817	-3.093339
O	-4.128869	-1.991328	-2.028275
H	-3.241622	-2.127721	-2.421419
H	-4.140914	-1.041027	-1.801413
O	3.987086	-2.970377	0.960916

H	3.254112	-3.234286	0.376955
H	4.384443	-2.198689	0.506398
O	4.661832	1.677491	0.769079
H	4.067983	2.166951	0.176242
H	4.046799	1.281784	1.418451
C	-0.238563	0.397686	-0.245735

D3_B3LYP_Radical_24_s2

O	1.189416	0.971199	-0.292059
O	-0.438913	-0.505568	0.098367
O	1.466126	-0.492853	1.242685
O	1.124899	0.581322	4.024102
H	0.348702	1.179567	3.968056
H	1.315240	0.343265	3.104730
O	-0.617428	-1.668993	4.306630
H	0.037125	-0.943173	4.298379
H	-0.182524	-2.404030	3.830027
O	-1.915340	0.494024	-2.173117
H	-1.294044	0.914056	-2.808141
H	-1.357937	0.153148	-1.451540
O	5.577023	0.208539	1.241199
H	5.054855	-0.576987	0.988637
H	5.399113	0.336140	2.179984
O	-3.584180	2.106055	-0.688939
H	-3.332383	1.938190	0.227464
H	-2.959648	1.567049	-1.226744
O	-1.173910	-3.267854	0.754607
H	-0.899892	-3.724472	-0.050151
H	-0.944955	-2.336663	0.592663
O	0.589556	-3.783430	2.833672
H	1.446106	-3.435286	2.559363
H	0.004166	-3.652371	2.056538
O	-0.048932	1.692102	-3.865069
H	0.644401	1.024603	-3.715355
H	0.144817	2.392243	-3.210798
O	0.403397	3.473739	-1.687047
H	-0.483510	3.842474	-1.481238
H	0.501648	2.702024	-1.109207
O	-0.871613	4.331653	2.209148
H	-1.737605	4.609535	1.887934
H	-0.593243	5.039742	2.802235
O	-2.148652	4.500855	-1.204710
H	-2.690923	3.715128	-0.986583
H	-2.116612	5.019008	-0.392361
O	-1.243865	2.055422	3.852252
H	-1.142397	2.823628	3.258047
H	-1.656531	1.351098	3.316257
O	3.878981	-1.911306	0.258876
H	3.111503	-1.369467	0.502734
H	4.086518	-1.671582	-0.672400
O	-2.215971	-0.253297	2.482486
H	-1.696284	-0.283409	1.663557
H	-1.719167	-0.828127	3.106041
O	-4.761834	-1.332632	1.746207
H	-3.885685	-0.984183	1.994401
H	-4.928007	-0.989617	0.846462
O	3.976308	2.004377	-0.261936
H	3.109593	1.573734	-0.226355
H	4.552518	1.451535	0.302433
O	2.037234	-3.970646	-0.525940
H	2.694975	-3.320263	-0.208693
H	1.495786	-4.172985	0.247169
O	0.328796	-2.496140	-2.179912
H	0.929419	-3.035434	-1.618116
H	-0.085920	-1.880838	-1.557612
O	1.932047	-0.270980	-2.975791
H	1.861281	0.213700	-2.138845
H	1.403717	-1.079786	-2.818508
O	-3.712109	-1.542122	-2.848720
H	-3.041177	-0.846544	-2.699458

Eopt -2099.348874

H	-3.218309	-2.380436	-2.757625
O	4.492852	-1.266965	-2.379697
H	3.618540	-0.945631	-2.683452
H	4.639308	-2.092052	-2.856289
O	2.817466	4.629028	-0.591024
H	1.968953	4.332080	-0.965293
H	3.298570	3.803621	-0.410017
O	-5.303086	-0.296022	-0.840017
H	-4.825266	0.550060	-0.789748
H	-4.800283	-0.818927	-1.495195
O	-2.107801	-3.890068	-2.670419
H	-1.243948	-3.468100	-2.489031
H	-2.352350	-4.320777	-1.843260
C	0.693005	-0.018334	0.333709

D3_B3LYP_Radical_24_s3

Eopt -2099.34529

O	-1.158115	-1.704460	-0.230498
O	-0.392576	0.366624	0.115854
O	-1.908204	-0.561453	1.429605
O	-0.685486	-1.965948	3.825378
H	0.283848	-1.932167	3.684982
H	-1.065939	-1.519635	3.056651
O	2.606535	2.634398	2.440242
H	1.665416	2.820203	2.225546
H	2.681785	2.709237	3.398369
O	1.140434	0.384952	-2.381989
H	0.833716	-0.367469	-2.934335
H	0.597590	0.345207	-1.576044
O	-5.831173	-2.406323	0.437207
H	-5.475099	-1.493538	0.482523
H	-6.123321	-2.607492	1.333292
O	3.630785	0.090915	-1.095646
H	3.296034	0.078634	-0.175942
H	2.812016	0.114242	-1.633534
O	-0.012012	2.905287	1.605815
H	-0.004035	3.500683	0.828497
H	-0.167131	2.022291	1.228524
O	-2.399118	3.518844	2.934962
H	-2.511826	2.880656	3.648267
H	-1.545075	3.286634	2.513128
O	0.244388	-1.844954	-3.808517
H	-0.712159	-1.738716	-3.653081
H	0.508619	-2.495007	-3.130769
O	0.757224	-3.551160	-1.554401
H	0.192513	-3.000118	-0.989243
H	0.257923	-4.366373	-1.685833
O	3.099239	-4.291474	2.455685
H	3.997172	-4.412565	2.788216
H	2.602540	-5.043485	2.801001
O	4.966409	-2.403000	-1.335520
H	4.483523	-1.557644	-1.263217
H	4.349959	-3.079156	-0.991851
O	2.091706	-1.834717	3.499810
H	2.429936	-2.678793	3.148355
H	2.199561	-1.189360	2.772377
O	-4.654700	0.135423	0.452614
H	-3.791772	-0.122752	0.812686
H	-4.493829	0.261479	-0.510631
O	2.345729	0.044547	1.420004
H	1.459248	0.104951	1.030326
H	2.494245	0.921282	1.833655
O	4.269331	4.210376	0.717396
H	3.713255	3.702300	1.333815
H	4.209331	3.726135	-0.131279
O	-3.380808	-3.757524	-0.022232
H	-2.710815	-3.059641	-0.022772
H	-4.224200	-3.296225	0.155096
O	-4.092655	2.962876	0.774548
H	-4.366403	2.027953	0.799016
H	-3.548443	3.103928	1.577124

O	-2.208244	2.515674	-1.214378
H	-2.846051	2.725669	-0.492666
H	-1.643464	1.818735	-0.846043
O	-2.455124	-1.576245	-2.859203
H	-2.104020	-1.698253	-1.960444
H	-2.980127	-2.367018	-3.033014
O	1.564700	3.161162	-2.858875
H	1.353764	2.212094	-2.772906
H	1.007486	3.603334	-2.191022
O	-4.125156	0.626348	-2.239510
H	-3.594790	-0.147886	-2.511025
H	-3.464752	1.311519	-2.024903
O	3.206876	-4.405398	-0.397799
H	2.340379	-4.100511	-0.726575
H	3.147476	-4.368914	0.574345
O	4.133979	2.824722	-1.727682
H	4.055112	1.886473	-1.465372
H	3.260597	3.028595	-2.120884
O	-0.111080	4.303669	-0.846127
H	-0.334728	5.239693	-0.902940
H	-0.936346	3.813854	-1.052881
C	-1.121966	-0.611392	0.413242

D3_B3LYP_Radical_27_s1

Eopt -2328.742729

O	0.549476	1.039967	-0.522950
O	0.632859	-1.062689	-0.016761
O	-1.334694	-0.110821	-0.335679
O	-2.938580	-2.314466	0.700705
H	-2.679775	-3.084949	0.154106
H	-2.426129	-1.581288	0.320850
O	2.970184	4.275861	-0.741314
H	2.369546	4.309604	-1.512086
H	3.185138	3.329820	-0.624702
O	-0.829725	3.102955	1.075333
H	-1.714019	3.302119	0.698604
H	-0.392229	2.543233	0.415201
O	-1.901948	-1.888887	-2.750539
H	-1.145421	-1.598894	-3.307584
H	-1.795551	-1.369078	-1.939599
O	-2.023513	-4.287686	-1.118051
H	-1.899424	-3.573526	-1.770094
H	-1.173761	-4.342986	-0.642559
O	2.284587	-1.901304	-2.369111
H	3.112564	-1.377509	-2.281954
H	1.753797	-1.644163	-1.598831
O	-1.627016	-1.552524	3.145554
H	-2.050508	-1.867848	2.324016
H	-1.197096	-0.706732	2.918641
O	4.614091	-0.426588	-1.996654
H	5.169586	-0.997050	-1.452720
H	4.262642	0.252348	-1.379649
O	1.257758	4.428152	-3.015392
H	0.581901	5.082059	-2.804240
H	0.771940	3.586902	-3.130189
O	0.597769	-3.383553	3.035873
H	1.352401	-2.798045	2.834363
H	-0.162682	-2.776776	3.123801
O	-0.489551	1.129030	3.080536
H	-1.031767	1.354872	3.846171
H	-0.740536	1.782295	2.394841
O	2.965522	-4.333054	-1.022383
H	2.803732	-3.553354	-1.588788
H	2.145434	-4.400294	-0.497540
O	0.023799	1.877799	-3.273419
H	-0.938607	1.939811	-3.119710
H	0.363597	1.603973	-2.405469
O	-4.336608	-0.300461	-2.941484
H	-3.565486	-0.889247	-3.030776
H	-4.682315	-0.492687	-2.044754
O	-5.231974	-0.882402	-0.309290

H	-4.584693	-1.565633	-0.056154
H	-4.946986	-0.123881	0.235340
O	-3.921456	-0.020059	3.929429
H	-3.623887	0.657913	4.547137
H	-3.139172	-0.587227	3.779883
O	1.986769	2.648288	3.467948
H	1.861135	3.374631	2.822331
H	1.172555	2.117318	3.401966
O	0.303441	-0.892074	-4.156654
H	0.210757	0.051629	-3.930753
H	1.041735	-1.210713	-3.601335
O	2.648097	-1.566636	2.140762
H	3.334113	-2.113266	1.694621
H	2.034714	-1.311475	1.434814
O	-3.914805	1.036871	1.338266
H	-3.952063	0.727601	2.269386
H	-3.054457	0.736245	1.014083
O	4.577731	-3.118637	0.886670
H	4.051495	-3.563004	0.183925
H	5.161031	-2.510206	0.418401
O	3.451890	1.497613	-0.354293
H	3.654511	1.335856	0.598047
H	2.516139	1.255752	-0.444292
O	0.446981	-4.060430	0.307836
H	0.449163	-3.952061	1.284111
H	0.466719	-3.146831	-0.012503
O	-2.630757	1.809657	-2.185835
H	-3.296412	1.180689	-2.538774
H	-2.163606	1.278269	-1.519783
O	1.453831	4.699153	1.588013
H	1.984601	4.568726	0.773596
H	0.593953	4.285004	1.387176
O	3.904137	0.976951	2.314875
H	3.241717	1.564771	2.738660
H	3.496929	0.088204	2.327092
O	-3.404543	3.488030	0.009404
H	-3.740121	2.777861	0.586863
H	-3.236085	3.027231	-0.834687
C	-0.080127	-0.040077	-0.291612

D3_B3LYP_Radical_27_s2

Eopt -2328.741903

O	-0.873809	-0.818106	-0.296611
O	-0.249811	1.290618	-0.164405
O	1.267355	-0.231513	-0.355507
O	3.585367	1.442848	0.296959
H	3.486507	2.186509	-0.334404
H	2.867260	0.839311	0.052177
O	-4.040063	-3.179248	-0.374876
H	-3.388534	-3.584321	-0.982268
H	-3.937012	-2.214493	-0.496293
O	-0.241293	-2.734217	1.657899
H	0.480281	-3.370304	1.467967
H	-0.408632	-2.263234	0.824042
O	2.149469	0.966174	-2.914097
H	1.358757	0.762354	-3.462862
H	1.900320	0.635622	-2.037898
O	3.023374	3.382172	-1.651238
H	2.654242	2.672080	-2.207913
H	2.273524	3.688912	-1.105264
O	-1.488338	2.233617	-2.681456
H	-2.444299	2.016316	-2.604717
H	-1.096692	1.914131	-1.853845
O	2.345858	1.431387	2.813553
H	2.784053	1.524836	1.944014
H	1.545855	0.896351	2.651619
O	-4.175960	1.626565	-2.389734
H	-4.450790	2.361704	-1.829070
H	-4.030667	0.883057	-1.762009
O	-2.166779	-4.380321	-2.104765
H	-2.662841	-4.655866	-2.883718

H	-1.608748	-3.633485	-2.408582
O	0.870200	3.857721	2.775856
H	0.002712	3.399415	2.793099
H	1.499775	3.115630	2.855091
O	0.029261	-0.257406	2.938452
H	0.236613	-0.416080	3.867370
H	0.066020	-1.140414	2.512759
O	-1.612014	4.697086	-1.163055
H	-1.594812	4.005465	-1.849007
H	-0.750830	4.587175	-0.712847
O	-0.584600	-2.174748	-2.780758
H	0.327442	-2.480646	-2.573355
H	-0.844526	-1.701963	-1.971664
O	3.873686	-1.294358	-2.897837
H	3.324079	-0.497397	-3.022888
H	4.362992	-1.124839	-2.064937
O	5.148070	-0.825269	-0.440653
H	4.849225	0.089668	-0.292857
H	4.524352	-1.333837	0.115839
O	3.656820	-0.883462	3.673894
H	4.608044	-0.733341	3.717722
H	3.269948	-0.009509	3.455292
O	-2.878160	-0.867434	3.334581
H	-2.943671	-1.753920	2.917933
H	-1.953173	-0.602961	3.206070
O	-0.191111	0.269441	-4.217002
H	-0.339986	-0.578831	-3.756416
H	-0.727868	0.924522	-3.726932
O	-1.428872	2.279521	2.757729
H	-1.898708	2.424443	1.911931
H	-0.974895	1.427020	2.664315
O	3.135413	-1.942871	1.166816
H	3.326824	-1.610331	2.071966
H	2.409826	-1.387788	0.841529
O	-2.916918	2.785700	0.430275
H	-2.504631	3.536044	-0.047804
H	-2.744909	2.024888	-0.138421
O	-3.643819	-0.405592	-0.613234
H	-3.978865	-0.040896	0.237742
H	-2.674975	-0.432618	-0.512780
O	0.825346	3.937419	0.010274
H	0.905306	4.026442	0.986764
H	0.533969	3.018971	-0.104185
O	1.919466	-2.999529	-1.931363
H	1.805500	-2.737141	-1.010132
H	2.615894	-2.394314	-2.275106
O	-2.900693	-3.402134	2.161490
H	-3.315195	-3.339986	1.274224
H	-1.943101	-3.309804	1.988355
O	-4.524441	0.686115	1.767527
H	-3.912399	0.190750	2.357534
H	-4.109448	1.548912	1.633059
O	1.922862	-4.410677	1.176463
H	2.459894	-3.588691	1.147885
H	1.878551	-4.713111	0.262030
C	0.032587	0.052267	-0.268595

D3_B3LYP_Radical_27_s3

Eopt -2328.739391

O	-0.968194	1.004418	-0.728892
O	0.495590	0.036707	0.539449
O	-1.255484	-1.110408	-0.266566
O	0.016648	-3.621016	0.353635
H	0.777383	-3.715644	-0.265226
H	-0.411285	-2.788854	0.088996
O	-1.798335	4.404588	-1.570240
H	-2.295149	3.624071	-1.884523
H	-0.867230	4.114884	-1.564182
O	-2.964094	1.829926	1.356780
H	-3.732533	1.217185	1.392615
H	-2.533237	1.650504	0.508873

O	-1.856499	-2.167010	-2.833470
H	-1.499382	-1.914307	-1.963986
H	-1.257336	-2.843432	-3.171289
O	2.145935	-3.737492	-1.374938
H	1.837624	-3.089374	-2.040064
H	2.841219	-3.249107	-0.890582
O	2.706644	0.142643	-1.422756
H	2.848614	0.972874	-1.932205
H	2.027693	0.336604	-0.758729
O	0.858617	-2.046532	2.495366
H	0.652820	-2.762568	1.858658
H	0.681514	-1.247961	1.969004
O	3.249088	2.498923	-2.730669
H	3.975058	2.794640	-2.168305
H	2.448986	2.932583	-2.367718
O	-3.220020	2.125287	-2.517707
H	-3.849384	2.404159	-3.192952
H	-2.550945	1.583710	-2.992947
O	3.595436	-1.391877	2.432846
H	3.592210	-0.413269	2.377083
H	2.657141	-1.651957	2.512621
O	-0.958456	1.211432	3.137447
H	-0.251473	0.877260	2.569359
H	-1.706652	1.370017	2.517694
O	6.706514	-1.131414	-0.122145
H	7.026282	-1.253877	0.778730
H	5.820666	-1.553410	-0.136478
O	-1.288651	0.505181	-3.704647
H	-1.564629	-0.411057	-3.512122
H	-0.606810	0.682733	-3.044431
O	-3.851214	-3.856186	-1.534999
H	-3.219536	-3.270809	-1.984764
H	-3.407596	-4.110080	-0.702297
O	-2.600660	-4.564917	0.914794
H	-1.665031	-4.465543	0.665053
H	-2.803580	-3.715578	1.355314
O	-1.391463	-1.419463	4.087766
H	-1.327895	-0.465056	3.887299
H	-0.601110	-1.783907	3.643658
O	-0.203897	3.946591	2.714788
H	-0.942765	4.237590	2.139785
H	-0.482165	3.065511	3.026322
O	1.464303	-1.654343	-3.138837
H	0.531044	-1.418911	-3.187849
H	1.866614	-0.980096	-2.551566
O	3.809604	1.400056	2.191210
H	4.396855	1.382897	1.408460
H	3.013165	1.864768	1.872901
O	-3.001531	-1.957382	1.899137
H	-2.488689	-1.796722	2.722557
H	-2.433030	-1.610974	1.191080
O	5.255494	1.294695	-0.216750
H	5.852424	0.522464	-0.155700
H	4.458295	0.937467	-0.636829
O	0.826849	3.295079	-1.609482
H	1.093304	3.183554	-0.669053
H	0.406011	2.450598	-1.820569
O	4.070061	-2.038238	-0.195204
H	3.882829	-1.841639	0.752853
H	3.695127	-1.276697	-0.673623
O	-4.113796	-0.276432	-1.303212
H	-3.885550	0.597817	-1.674335
H	-3.263777	-0.637993	-1.015401
O	-2.444132	4.582633	1.134271
H	-2.196058	4.564209	0.184976
H	-2.795927	3.687619	1.292677
O	1.552209	2.681429	0.992235
H	0.960111	3.183986	1.596474
H	1.117227	1.819024	0.881001
O	-4.985014	-0.054532	1.338265

H	-4.384255	-0.750808	1.672369
H	-4.855386	-0.108250	0.369043
C	-0.565705	-0.064937	-0.136257

D3BJ_B3LYP_9_s1			Eopt -952.388665
O	-1.286971	0.192234	-1.271065
O	0.923579	0.349252	-1.546300
O	0.098283	-0.556339	0.328027
O	2.457106	-0.126788	1.524522
H	1.605898	-0.350116	1.062536
H	2.658012	0.752020	1.163279
O	2.118388	2.336057	-0.013547
H	1.776650	1.643325	-0.621418
H	1.377999	2.453509	0.607420
O	2.824822	-1.559114	-1.993526
H	3.340587	-1.688128	-1.176791
H	2.150166	-0.880162	-1.763857
O	-3.338162	-0.082220	0.428747
H	-2.570802	0.026622	-0.194672
H	-2.926446	-0.519059	1.196471
O	-0.313874	2.119736	1.601411
H	-0.206085	1.175057	1.400450
H	-0.811402	2.460025	0.832175
O	-1.590531	-1.377162	2.248513
H	-1.764443	-2.312410	2.097116
H	-0.989764	-1.103589	1.509139
O	-1.559404	2.885114	-0.851139
H	-0.786700	3.296800	-1.254297
H	-1.490617	1.934027	-1.100429
O	4.281443	-1.831039	0.446449
H	3.628093	-1.226624	0.875222
H	4.069632	-2.708880	0.782172
O	-4.656262	-2.204420	-0.740090
H	-4.165714	-1.452120	-0.336937
H	-4.038258	-2.594103	-1.367369
C	-0.087358	-0.011447	-0.834372

D3BJ_B3LYP_9_s2			Eopt -952.388705
O	-1.286470	0.192007	-1.273060
O	0.924513	0.347152	-1.545856
O	0.096394	-0.555991	0.328403
O	2.455051	-0.127744	1.525974
H	1.604019	-0.350937	1.063620
H	2.656178	0.751072	1.164830
O	2.119435	2.334187	-0.013514
H	1.777644	1.641272	-0.621153
H	1.378447	2.453063	0.606472
O	2.822520	-1.565156	-1.990227
H	3.339882	-1.691375	-1.174071
H	2.149054	-0.884609	-1.761814
O	-3.339852	-0.079185	0.424725
H	-2.571820	0.028400	-0.198052
H	-2.928788	-0.513418	1.194274
O	-0.314550	2.121856	1.598872
H	-0.207163	1.176908	1.399004
H	-0.811042	2.461656	0.828747
O	-1.594946	-1.370178	2.249474
H	-1.770557	-2.305379	2.099934
H	-0.993287	-1.099251	1.509854
O	-1.556790	2.885554	-0.855732
H	-0.783359	3.296138	-1.258615
H	-1.488693	1.934171	-1.104071
O	4.283903	-1.827024	0.447645
H	3.628640	-1.224932	0.876724
H	4.077940	-2.705066	0.786306
O	-4.651610	-2.209812	-0.735816
H	-4.163400	-1.454313	-0.335971
H	-4.029349	-2.606091	-1.354682
C	-0.087519	-0.012104	-0.834741

D3BJ_B3LYP_9_s3 Eopt -952.390317

O	-0.471665	0.700808	-1.014904
O	1.689461	0.269477	-1.381102
O	0.537597	-0.964851	0.098357
O	2.524063	-2.532929	1.082629
H	1.830477	-1.922998	0.726170
H	2.864114	-2.095010	1.870257
O	2.637053	2.779093	-0.819747
H	2.319032	1.872234	-1.045717
H	3.383511	2.642973	-0.226169
O	3.850781	-1.381037	-1.203970
H	3.630896	-1.906596	-0.416423
H	3.068341	-0.782833	-1.281890
O	-2.832175	-0.222372	-0.148581
H	-1.955393	0.145308	-0.451540
H	-2.632311	-1.168908	-0.024849
O	0.333911	0.697060	2.436747
H	0.403702	0.030451	1.724669
O	0.339659	1.542177	1.948233
O	-1.532447	-2.728433	0.219210
H	-1.527179	-3.242624	-0.595300
H	-0.772961	-2.100402	0.136582
O	0.152686	2.936966	0.609102
H	1.053442	3.050735	0.252360
H	-0.213622	2.238691	-0.029095
O	-4.712209	0.014666	-2.179118
H	-4.016278	-0.078164	-1.492729
H	-4.246033	-0.064974	-3.017897
C	0.585009	-0.000896	-0.773011
O	-2.524790	0.549707	2.580600
H	-1.550859	0.607870	2.613319
H	-2.706726	0.292206	1.656105

D3BJ_B3LYP_12_s1 Eopt -1181.782999

O	0.332772	-0.491408	1.369166
O	0.390483	0.456905	-0.655163
O	-1.248860	-0.975868	-0.144039
O	1.231025	-1.118255	-2.795434
H	0.903587	-0.488340	-2.117183
H	0.696940	-1.914849	-2.620686
O	-0.824256	-2.145422	3.237675
H	-0.394920	-1.559249	2.572854
H	-1.665808	-2.368188	2.805103
O	1.419175	3.776223	0.772868
H	2.039024	3.083914	0.478048
H	0.642066	3.642466	0.193678
O	2.637730	-2.134429	1.071528
H	3.031768	-1.827733	0.234333
H	1.854516	-1.563574	1.193597
O	-3.419824	2.737649	-0.761192
H	-3.654074	2.643587	0.168727
H	-3.332024	1.817928	-1.098978
O	0.545451	1.907801	2.803930
H	0.825613	2.585248	2.162232
H	0.497667	1.080517	2.281855
O	-3.007968	-2.413161	1.377623
H	-2.370924	-1.863713	0.860753
H	-3.706790	-1.805683	1.642733
O	-0.611575	3.028353	-1.039749
H	-1.574439	3.015256	-0.876287
H	-0.328544	2.095680	-0.934461
O	3.701733	-1.047845	-1.390400
H	2.897723	-1.179887	-1.931923
H	3.565750	-0.167247	-0.994901
O	2.849901	1.393983	-0.065637
H	1.935753	1.030244	-0.220164
H	3.082617	1.096204	0.821849
O	-0.667765	-3.079033	-1.897445
H	-0.237908	-3.773192	-1.385831
H	-0.890787	-2.381679	-1.243600

O	-3.049448	0.190104	-1.792139
H	-2.328477	-0.212287	-1.245029
H	-2.657481	0.340939	-2.659366
C	-0.176573	-0.335191	0.196651

D3BJ_B3LYP_12_s2 Eopt -1181.782868

O	-0.757504	0.178827	0.131728
O	1.249739	0.991054	-0.430862
O	-0.549897	2.310036	-0.539842
O	1.825892	0.387743	-3.069841
H	1.596170	0.665088	-2.153864
H	1.003820	0.462935	-3.567162
O	0.690076	-2.878404	1.745574
H	0.232878	-2.162581	2.226017
H	0.272930	-2.860395	0.862435
O	-3.437972	0.221481	-0.130581
H	-2.449240	0.224345	-0.030269
H	-3.613801	1.119311	-0.467613
O	4.248761	0.796316	1.874364
H	3.746836	0.049210	1.498741
H	3.859511	1.576942	1.436492
O	-0.439634	-2.359312	-0.846726
H	0.383726	-2.394016	-1.371845
H	-0.487194	-1.427877	-0.522022
O	-0.737368	-0.606251	2.747263
H	-0.212266	-0.014180	3.297542
H	-0.670590	-0.245562	1.830538
O	-3.143143	2.919907	-0.979109
H	-3.234857	2.976474	-1.936275
H	-2.196462	2.667495	-0.822888
O	-3.574766	-0.011196	2.720272
H	-3.644182	0.109391	1.754235
H	-2.631570	-0.210406	2.856734
O	2.961290	2.909880	0.426995
H	2.502435	3.489248	1.044810
H	2.271206	2.282541	0.095414
O	2.148398	-2.263101	-2.085689
H	2.034377	-1.409552	-2.548550
H	2.447677	-1.994348	-1.195525
O	2.643004	-1.150484	0.519234
H	2.062447	-0.410117	0.209191
H	2.052152	-1.738349	1.027672
O	-3.085118	-1.993763	-1.930957
H	-3.310024	-1.216708	-1.386464
H	-2.172510	-2.205565	-1.663021
C	-0.029588	1.174137	-0.281484

D3BJ_B3LYP_12_s3 Eopt -1181.783787

O	0.271374	-0.996173	0.830129
O	0.386532	0.618543	-0.724102
O	-0.988072	-1.112508	-1.023206
O	2.636721	0.192396	-2.362471
H	1.816026	0.329250	-1.844261
H	2.846783	-0.753014	-2.237981
O	-1.020476	-3.188788	1.837446
H	-0.530120	-2.415332	1.469416
H	-1.826775	-3.201532	1.298077
O	-0.210003	4.251750	0.317410
H	0.474999	3.636559	0.639933
H	-0.752618	3.694482	-0.275313
O	2.999360	-1.507223	0.878959
H	3.427718	-0.656671	0.661535
H	2.037373	-1.302787	0.875202
O	-3.987120	1.824742	0.023101
H	-3.739185	1.822927	0.954247
H	-4.333927	0.922869	-0.152052
O	0.807530	0.472435	3.088882
H	1.566556	0.036939	3.492041
H	0.618583	-0.051574	2.274420
O	-3.045099	-2.549045	-0.161604

H	-2.240511	-2.042860	-0.467570
H	-3.156491	-3.264791	-0.797429
O	-1.602705	2.441195	-1.375670
H	-2.407310	2.174706	-0.889241
H	-0.937797	1.741054	-1.189776
O	4.062697	1.020656	-0.008295
H	3.691276	0.789214	-0.882402
H	3.335798	1.514433	0.421287
O	1.695055	2.223923	0.999946
H	1.220711	1.614362	0.371809
H	1.512786	1.819400	1.867266
O	3.309010	-2.509631	-1.697822
H	3.172673	-2.251582	-0.758506
H	2.559844	-3.074552	-1.917171
O	-5.065667	-0.687032	-0.519970
H	-4.355644	-1.362443	-0.435879
H	-5.277676	-0.658025	-1.459682
C	-0.119363	-0.503826	-0.306638

D3BJ_B3LYP_18_s1 Eopt -1640.566472

O	-0.948536	0.156731	0.354576
O	1.256812	0.111621	0.005334
O	0.024166	-1.729363	-0.343427
O	2.604424	-1.146838	2.075931
H	2.190793	-0.675430	1.317751
H	1.925517	-1.807924	2.311322
O	-0.812549	3.714599	1.567382
H	-1.196055	3.400411	0.723763
H	-0.893682	2.945508	2.160018
O	-3.298544	-1.008219	0.952855
H	-2.407033	-0.678946	0.670006
H	-3.536925	-1.711124	0.317229
O	-0.073496	3.222691	-2.936123
H	0.841649	3.084473	-2.604039
H	-0.187464	2.576256	-3.641601
O	-4.592731	-0.734978	-2.788919
H	-5.520363	-0.737279	-3.050088
H	-4.513346	-0.021164	-2.117005
O	2.497327	2.950434	-1.887606
H	2.263327	2.982325	-0.938758
H	2.796740	2.030448	-2.018275
O	-0.808058	1.128235	2.958079
H	0.137923	1.164719	3.203260
H	-0.809828	0.804388	2.028910
O	2.623882	-1.855730	-3.725124
H	1.793980	-1.630319	-4.159776
H	2.366292	-2.381331	-2.932984
O	-1.764133	2.479891	-0.805784
H	-1.199094	2.722965	-1.567994
H	-1.374860	1.649555	-0.442900
O	-4.161959	-2.862923	-1.023744
H	-3.392943	-3.354694	-1.332730
H	-4.307708	-2.164028	-1.697171
O	4.389247	-1.928367	-0.091395
H	4.168332	-1.180274	-0.675777
H	3.885864	-1.749515	0.723787
O	-4.288193	1.116254	-0.740556
H	-4.029128	0.430209	-0.094543
H	-3.474283	1.638038	-0.875355
O	3.271424	0.174171	-1.826867
H	3.067230	-0.428952	-2.567669
H	2.509575	0.073754	-1.208799
O	2.015119	1.332999	3.423080
H	2.261023	0.443633	3.104939
H	2.041545	1.880947	2.615631
O	1.758373	2.641153	0.853472
H	1.481804	1.735998	0.560583
H	0.922476	3.100808	1.063747
O	0.304376	-2.898357	2.251578
H	-0.427289	-2.444546	2.715845

H	0.196545	-2.617933	1.321827
O	-1.894656	-1.499966	3.442195
H	-2.468942	-1.485875	2.653816
H	-1.494626	-0.609550	3.440627
O	2.080087	-3.180183	-1.352147
H	1.363127	-2.614168	-0.968046
H	2.892331	-2.876260	-0.907464
C	0.111408	-0.494328	-0.005735

D3BJ_B3LYP_18_s2 Eopt -1640.56789

O	1.092520	0.133692	0.282492
O	-1.103155	0.375873	-0.052413
O	-0.132243	-1.605358	-0.415037
O	-1.298998	2.039550	-2.231047
H	-1.157382	1.439768	-1.464037
H	-0.490648	1.948980	-2.777757
O	1.074108	2.573832	3.122865
H	1.218411	1.612350	3.217641
H	1.396420	2.767206	2.222300
O	3.565312	-0.485501	-0.665976
H	2.631350	-0.355116	-0.371797
H	3.554421	-1.307093	-1.193799
O	-0.974458	-1.621065	3.445246
H	-1.711411	-0.996748	3.262572
H	-0.931874	-2.185359	2.664309
O	1.760531	-3.440718	0.253191
H	1.098481	-2.739328	0.032805
H	2.368498	-3.014705	0.885349
O	-3.066396	0.174440	2.951339
H	-2.547480	0.968596	2.714785
H	-3.396274	-0.141446	2.087940
O	1.685771	2.796110	0.299227
H	0.896580	3.313429	0.046231
H	1.382733	1.854102	0.288339
O	-3.794974	-3.226637	-0.596157
H	-4.634905	-3.355204	-1.050789
H	-3.159863	-2.959867	-1.298170
O	1.470191	-0.264918	2.973644
H	0.649441	-0.730667	3.235033
H	1.344224	-0.109467	2.009738
O	3.431010	-3.044476	-1.927565
H	2.899351	-2.994354	-2.729562
H	2.796747	-3.269795	-1.209481
O	-3.496574	0.206880	-2.679230
H	-3.718266	0.065365	-1.742034
H	-2.775536	0.863586	-2.655801
O	3.608615	-1.920709	1.911023
H	3.752181	-1.406906	1.095706
H	2.925374	-1.417577	2.391375
O	-3.670607	-0.471890	0.212144
H	-3.763916	-1.423757	0.017791
H	-2.709239	-0.273178	0.091832
O	-0.804394	4.103972	-0.306192
H	-1.000111	3.496847	-1.046637
H	-1.142943	3.630863	0.476684
O	-1.497153	2.293345	1.859819
H	-1.272236	1.615231	1.176935
H	-0.674493	2.408500	2.374155
O	1.044267	1.818189	-3.779042
H	1.810446	1.844723	-3.162857
H	1.044230	0.925782	-4.142747
O	3.180632	2.031859	-2.000492
H	3.403369	1.138026	-1.676184
H	2.699151	2.430336	-1.248090
O	-1.922911	-2.220368	-2.392130
H	-1.290770	-1.966165	-1.676849
H	-2.416126	-1.401897	-2.588083
C	-0.047783	-0.373983	-0.063752

D3BJ_B3LYP_18_s3 Eopt -1640.56085

O	-0.984386	0.292968	-0.114673
O	1.194634	0.061310	0.351038
O	0.185565	-1.368767	-1.039971
O	1.179569	-0.246294	3.049052
H	1.152176	-0.101377	2.073340
H	0.370692	-0.766000	3.217761
O	-0.654331	4.032865	-0.506982
H	-0.876283	3.404227	-1.223128
H	-1.085547	3.637238	0.270696
O	-4.506496	-0.484461	0.256859
H	-5.467162	-0.544606	0.311769
H	-4.187670	-1.413600	0.189508
O	1.077783	1.477162	-3.695814
H	1.831633	1.627621	-3.083549
H	1.187890	2.131286	-4.394767
O	-2.081263	-2.186079	-2.244071
H	-1.260573	-1.838268	-1.806063
H	-2.632574	-1.396739	-2.402736
O	3.211161	1.922396	-1.936442
H	2.733694	2.345332	-1.194888
H	3.493627	1.068187	-1.558194
O	-1.845032	2.272959	1.504795
H	-2.703145	2.470307	1.110385
H	-1.456639	1.563074	0.929028
O	4.022237	-3.007019	-1.582931
H	4.700756	-3.452178	-1.063310
H	3.166663	-3.295556	-1.190531
O	-1.342603	1.911517	-2.290826
H	-0.537079	1.775297	-2.830997
H	-1.210527	1.320664	-1.512948
O	-3.420223	-3.019312	0.013472
H	-2.778429	-3.046567	0.733031
H	-2.899195	-2.780115	-0.790043
O	3.895787	-1.189397	2.467112
H	3.918282	-0.955231	1.521769
H	2.995805	-0.954449	2.751269
O	-3.729719	0.176663	-2.470841
H	-3.983661	0.069282	-1.535415
H	-2.985566	0.803287	-2.470522
O	3.745196	-0.448558	-0.372023
H	3.859667	-1.309422	-0.820046
H	2.778041	-0.371462	-0.175553
O	1.636477	2.601747	3.245015
H	1.419944	1.655193	3.317024
H	1.679678	2.755679	2.283250
O	1.734952	2.744300	0.354292
H	1.456150	1.796642	0.369223
H	0.949016	3.233326	0.038661
O	-1.249508	-1.791328	3.028761
H	-1.971426	-1.134058	2.916252
H	-1.063340	-2.104189	2.135445
O	-3.282648	0.104368	2.771382
H	-3.761741	-0.123336	1.950233
H	-2.751680	0.880348	2.515031
O	1.580614	-3.592383	-0.458109
H	1.090514	-2.752038	-0.653900
H	1.124803	-4.275184	-0.962511
C	0.126844	-0.339976	-0.266224

D3BJ_B3LYP_24_s1

Eopt -2099.351409

O	1.221770	0.195054	-0.865412
O	-0.783143	-0.350722	-0.027208
O	1.074868	-1.229323	0.849619
O	2.479181	-0.139495	2.940615
H	2.230314	0.806839	2.974556
H	1.995930	-0.483571	2.155933
O	0.033521	-0.954023	4.274892
H	0.924857	-0.694992	3.973168
H	-0.170029	-1.739421	3.734186
O	-2.136518	1.041669	-1.888653

H	-1.623349	1.122759	-2.716301
H	-1.566638	0.516949	-1.268961
O	4.700682	-1.335545	1.468983
H	4.177074	-2.013125	1.003876
H	4.064453	-0.904229	2.067096
O	-2.538725	3.053753	-0.022641
H	-2.186505	2.648388	0.780038
H	-2.364846	2.393178	-0.730777
O	-2.794478	-1.857423	1.277192
H	-3.284754	-1.185239	1.793497
H	-2.085362	-1.347792	0.829124
O	-0.386245	-3.026843	2.264664
H	0.118531	-2.350772	1.744606
H	-1.316070	-2.793651	2.092539
O	-0.453163	1.197952	-4.194607
H	-0.056627	0.321825	-4.035366
H	0.104897	1.798048	-3.660961
O	1.104591	2.592159	-2.286254
H	0.572545	3.267629	-1.814580
H	1.035136	1.778078	-1.741604
O	1.924636	4.269875	1.029002
H	2.321404	5.078836	1.371425
H	2.575577	3.899529	0.388094
O	-0.232413	4.580184	-0.808161
H	-1.015900	4.108247	-0.468227
H	0.438192	4.530673	-0.100253
O	1.313812	2.431413	3.063273
H	1.536481	3.057696	2.346285
H	0.452040	2.045827	2.819514
O	2.867807	-3.072714	-0.070760
H	2.250341	-2.355739	0.204410
H	3.073184	-2.881468	-1.008072
O	-1.149341	0.987836	2.548019
H	-1.047752	0.574388	1.669126
H	-0.812487	0.311531	3.173547
O	-3.942303	0.331763	2.648731
H	-3.026817	0.670888	2.673256
H	-4.353559	0.765653	1.872498
O	3.956036	0.435615	-0.686918
H	2.984777	0.268001	-0.703296
H	4.290105	-0.095376	0.058955
O	0.319998	-4.504493	-0.175635
H	1.224679	-4.142734	-0.226592
H	-0.014183	-4.155724	0.671000
O	-1.114994	-2.723643	-1.861564
H	-0.623489	-3.377371	-1.319403
H	-1.143748	-1.930384	-1.298995
O	0.896399	-1.206658	-3.254312
H	1.042148	-0.651137	-2.457014
H	0.216318	-1.839479	-2.952923
O	-4.636012	-0.188899	-1.825322
H	-3.751974	0.217739	-1.941997
H	-4.444792	-1.117350	-1.585162
O	3.368372	-2.509260	-2.814255
H	2.514783	-2.075637	-3.024516
H	3.996498	-1.782133	-2.730974
O	3.535885	3.199681	-0.937154
H	2.757242	3.074643	-1.515622
H	3.804107	2.282332	-0.725580
O	-5.062998	1.570732	0.369574
H	-4.312986	2.174810	0.229801
H	-4.977760	0.911731	-0.349653
O	-3.923229	-2.848423	-1.072755
H	-3.064961	-2.946167	-1.521647
H	-3.658533	-2.539080	-0.181313
C	0.508257	-0.457572	-0.015064

D3BJ_B3LYP_24_s2

Eopt -2099.348874

O	1.167617	0.640746	-0.513867
O	-0.707048	-0.454367	0.032945

O	1.264491	-1.143088	0.828310
O	2.364451	-0.154174	3.132205
H	1.941805	0.723310	3.230313
H	1.998018	-0.487738	2.282029
O	0.023048	-1.591719	4.156754
H	0.856467	-1.124809	3.959732
H	-0.011047	-2.296548	3.483394
O	-2.190705	0.842161	-1.794942
H	-1.616711	1.213956	-2.493182
H	-1.577637	0.394046	-1.156095
O	4.841701	-0.607723	1.634970
H	4.490682	-1.311549	1.058429
H	4.102781	-0.395747	2.233270
O	-3.464595	2.570482	-0.094076
H	-3.135218	2.335832	0.782527
H	-2.986772	1.968320	-0.714089
O	-2.452088	-2.552251	0.871054
H	-2.717120	-2.983013	0.039833
H	-1.874050	-1.815151	0.589323
O	0.089532	-3.371692	1.840639
H	0.494332	-2.547183	1.468672
H	-0.846611	-3.298784	1.574194
O	-0.301220	1.861574	-3.688680
H	0.242054	1.053297	-3.650060
H	0.080068	2.432656	-2.997502
O	0.660789	3.235226	-1.279202
H	-0.217837	3.634082	-1.104917
H	0.650913	2.312991	-0.940179
O	1.148115	4.242535	1.461593
H	1.077718	3.915643	0.546706
H	0.380150	4.815335	1.573946
O	-1.702267	4.649753	-0.777861
H	-2.357773	3.984274	-0.482235
H	-1.460794	5.137832	0.017854
O	0.734362	2.148849	3.315032
H	0.856799	2.838923	2.633471
H	-0.039355	1.626122	3.030825
O	3.453518	-2.452629	-0.169618
H	2.690548	-1.903074	0.122586
H	3.647278	-2.159942	-1.083002
O	-1.444578	0.368458	2.669149
H	-1.250548	0.097618	1.749751
H	-1.027368	-0.327201	3.218193
O	-4.298233	0.095618	2.778420
H	-3.327668	0.162863	2.707274
H	-4.630728	0.120538	1.862587
O	3.872327	1.159077	-0.437105
H	2.920363	0.909223	-0.408901
H	4.285830	0.664390	0.292965
O	1.275053	-4.327941	-0.654100
H	2.091917	-3.799862	-0.574166
H	0.828177	-4.180317	0.200346
O	-0.398533	-2.547185	-2.090869
H	0.196661	-3.182074	-1.635760
H	-0.605956	-1.883849	-1.408568
O	1.365809	-0.456418	-3.096139
H	1.384317	-0.016626	-2.219384
H	0.781456	-1.222559	-2.943255
O	-4.317789	-0.958090	-2.109666
H	-3.548113	-0.353807	-2.093894
H	-3.936992	-1.849620	-2.015270
O	3.901458	-1.655613	-2.859490
H	3.019456	-1.254301	-3.010639
H	3.902298	-2.463841	-3.384610
O	3.507524	3.828289	-1.269412
H	2.537744	3.787449	-1.301893
H	3.756752	2.946933	-0.932241
O	-5.415228	0.397973	0.137254
H	-4.902504	1.218826	0.036391
H	-5.078041	-0.176741	-0.579017

O	-3.010106	-3.484330	-1.787934
H	-2.076564	-3.293508	-2.019459
H	-3.206427	-4.359091	-2.140769
C	0.579669	-0.312616	0.118591

D3BJ_B3LYP_24_s3

Eopt -2099.34529

O	0.542731	-1.151822	-0.778454
O	-1.134992	0.274360	-0.420774
O	-0.925293	-1.551015	0.859462
O	0.524271	-1.684725	3.239413
H	0.768214	-0.759439	3.446916
H	0.023779	-1.620218	2.400017
O	-3.040113	0.783549	3.470914
H	-3.266809	0.050012	2.858669
H	-3.792854	1.384287	3.433619
O	0.264517	1.865634	-2.092531
H	0.992280	1.368353	-2.519400
H	-0.228656	1.211994	-1.531742
O	1.914060	-3.896630	2.143157
H	1.171234	-4.158972	1.568966
H	1.562715	-3.121549	2.623541
O	1.148041	3.348381	0.058216
H	0.602619	3.016166	0.785409
H	0.875592	2.807399	-0.720458
O	-3.825045	0.333612	-0.754352
H	-4.053713	-0.315640	-1.429993
H	-2.841584	0.271558	-0.652491
O	-3.472990	-1.294561	1.638427
H	-2.512109	-1.336439	1.380411
H	-3.869189	-0.788289	0.908168
O	2.412261	0.441980	-3.280940
H	1.981367	-0.421637	-3.395614
H	2.999278	0.320547	-2.506191
O	4.112423	0.083798	-1.033408
H	3.950639	0.857983	-0.447697
H	3.752822	-0.694333	-0.566450
O	3.723919	1.658149	3.246765
H	4.293321	0.912918	3.473798
H	4.015677	2.381234	3.815070
O	3.751799	2.355638	0.499916
H	2.844515	2.694770	0.358586
H	3.784402	2.109472	1.442969
O	0.985757	1.038842	3.742558
H	1.900575	1.284023	3.514498
H	0.415903	1.379038	3.026316
O	-0.515590	-4.225681	0.543651
H	-0.588972	-3.244751	0.644582
H	-0.457227	-4.362812	-0.422336
O	-1.008230	1.888482	1.865651
H	-1.066126	1.323057	1.063703
H	-1.712403	1.545445	2.457237
O	-2.297966	4.393062	1.302439
H	-1.852252	3.542238	1.473665
H	-1.802255	4.780243	0.555741
O	2.880453	-2.267573	-0.016295
H	1.984321	-1.918295	-0.232477
H	2.730799	-2.823423	0.770568
O	-3.420303	-4.013507	0.602916
H	-2.462490	-4.191464	0.666204
H	-3.531930	-3.134525	1.011574
O	-3.144778	-3.156716	-2.058457
H	-3.301017	-3.444907	-1.133008
H	-2.819357	-2.251976	-1.979072
O	1.053590	-2.216339	-3.206226
H	0.820264	-1.828621	-2.329867
H	1.892337	-2.669681	-3.058885
O	-1.668313	3.745788	-2.937853
H	-1.009465	3.052202	-2.740211
H	-2.523193	3.386063	-2.625673
O	-0.630536	-4.454448	-2.326126

H	-0.041789	-3.759173	-2.670026
H	-1.512196	-4.031172	-2.296781
O	6.869366	-0.208794	-1.366587
H	5.899221	-0.114437	-1.262899
H	7.018108	-0.207083	-2.318003
O	-0.700872	5.379978	-0.851929
H	0.016506	4.804500	-0.528119
H	-1.085809	4.872588	-1.597232
O	-4.173161	2.804428	-2.035972
H	-4.696121	2.631586	-2.826809
H	-4.062026	1.929310	-1.606769
C	-0.501167	-0.818183	-0.118446

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Eopt -2328.742729

O	-1.060668	-0.952904	-0.131299
O	-0.496128	1.114207	-0.777213
O	1.064592	-0.482790	-0.615848
O	3.327982	0.942670	-0.209255
H	3.352847	1.544546	-0.979116
H	2.487016	0.440472	-0.345722
O	-4.121209	-3.206298	1.019727
H	-3.574339	-3.803339	0.471019
H	-4.040305	-2.328806	0.590706
O	-0.095323	-1.937360	2.255079
H	0.735563	-2.445723	2.131794
H	-0.400429	-1.687009	1.353105
O	1.894619	-0.254788	-3.283876
H	1.071963	-0.531419	-3.737558
H	1.640148	-0.283801	-2.336798
O	3.004412	2.377734	-2.685681
H	2.628508	1.554324	-3.044468
H	2.234570	2.842250	-2.295057
O	-1.951313	1.209326	-3.174220
H	-2.865712	0.895160	-3.010178
H	-1.496505	1.138746	-2.308082
O	2.363155	2.088838	2.172051
H	2.703304	1.706038	1.335657
H	1.543353	1.596254	2.378130
O	-4.522517	0.227273	-2.655000
H	-5.111639	0.979508	-2.529893
H	-4.303216	-0.084935	-1.746685
O	-2.545051	-4.908206	-0.624866
H	-1.976888	-5.412576	-0.031895
H	-1.943335	-4.283531	-1.084454
O	1.370495	4.527008	1.080051
H	0.457611	4.608381	1.425823
H	1.718527	3.708794	1.486385
O	0.094093	0.669531	3.165643
H	0.444888	0.649815	4.064365
H	0.122175	-0.267349	2.862639
O	-1.929419	4.022830	-2.394226
H	-2.054126	3.141322	-2.790889
H	-1.001810	3.999867	-2.089802
O	-0.930404	-3.026305	-1.938197
H	-0.005075	-3.294948	-1.793422
H	-1.040944	-2.296720	-1.284105
O	3.778193	-2.342526	-2.817111
H	3.140210	-1.658418	-3.101484
H	4.384119	-1.861815	-2.218671
O	5.382902	-0.755289	-1.102549
H	4.683438	-0.194441	-0.703520
H	5.792884	-1.225527	-0.368321
O	3.784161	0.585459	4.079642
H	3.106184	0.302229	4.703994
H	3.310818	1.155577	3.436990
O	-2.748261	0.231364	3.734616
H	-2.787250	-0.737367	3.591457
H	-1.819770	0.462741	3.551545
O	-0.652495	-1.137836	-4.165848
H	-0.761085	-1.792635	-3.451028

H	-1.137908	-0.346329	-3.857699
O	-1.291893	4.705260	1.958607
H	-1.680099	4.015005	1.376234
H	-1.336208	4.339456	2.849103
O	4.393056	-1.588747	2.431090
H	4.157328	-0.838970	3.019059
H	4.548508	-1.184477	1.569466
O	-2.383526	2.845410	0.215496
H	-2.457675	3.358845	-0.610494
H	-1.745668	2.134376	-0.024406
O	-3.763501	-0.693633	-0.175414
H	-4.005763	-0.005724	0.481384
H	-2.774070	-0.696860	-0.187566
O	0.741147	3.474190	-1.452453
H	0.982507	3.886759	-0.595318
H	0.394590	2.585624	-1.207753
O	1.774447	-3.098364	-0.926494
H	2.515885	-2.988861	-1.554190
H	1.467763	-2.171500	-0.769863
O	-2.629120	-2.570200	3.314389
H	-3.153365	-2.815206	2.522419
H	-1.714830	-2.474468	2.983987
O	-4.283653	1.346665	1.671464
H	-3.739092	0.983434	2.402303
H	-3.685501	1.943086	1.181549
O	2.276768	-3.362080	1.833784
H	2.996124	-2.737635	2.057624
H	2.209369	-3.334016	0.857723
C	-0.163653	-0.098621	-0.507121

D3BJ B3LYP_27_s2

Eopt -2328.741903

O	-1.104434	-0.746459	-0.655976
O	-0.597339	1.361608	-0.096176
O	0.942533	0.047180	-1.044839
O	3.223851	0.974337	0.059076
H	3.282764	1.898081	-0.251653
H	2.345676	0.674215	-0.282752
O	-4.107183	-3.318031	-0.502339
H	-3.690383	-3.502872	-1.367326
H	-4.058652	-2.342823	-0.415664
O	0.010004	-2.630858	1.069281
H	0.808420	-3.061071	0.692491
H	-0.332370	-2.023484	0.377740
O	1.556222	1.849785	-3.054151
H	0.709539	1.842043	-3.542907
H	1.382835	1.234520	-2.307975
O	2.837466	3.589298	-1.094449
H	2.405041	3.143458	-1.843982
H	2.119707	3.695452	-0.435366
O	-2.206522	2.865254	-1.830887
H	-3.107774	2.481526	-1.784606
H	-1.669752	2.310432	-1.226606
O	2.867176	0.512585	2.772417
H	2.971016	0.693749	1.812244
H	2.034749	0.008033	2.861535
O	-4.726318	1.637303	-1.689499
H	-5.274842	2.157509	-1.091818
H	-4.432161	0.861495	-1.159430
O	-2.906854	-3.717543	-3.048297
H	-3.641511	-3.680603	-3.671202
H	-2.417743	-2.878815	-3.180852
O	1.499468	2.970230	3.363839
H	0.662092	2.543376	3.643767
H	2.083028	2.209389	3.181021
O	0.427009	-0.963559	3.214603
H	0.696848	-1.529355	3.947771
H	0.324813	-1.567243	2.440405
O	-1.933613	4.702874	0.462785
H	-2.147291	4.222005	-0.356631
H	-0.997455	4.471882	0.621282

O	-1.413672	-1.329955	-3.309404
H	-0.576943	-1.683653	-3.634189
H	-1.262387	-1.167325	-2.346617
O	4.052252	0.804714	-3.946135
H	3.176369	1.164041	-3.708503
H	4.283154	0.224573	-3.201027
O	4.476850	-0.942669	-1.591876
H	4.135954	-0.224993	-1.018370
H	3.668544	-1.401928	-1.895781
O	4.776920	-1.493732	3.070103
H	5.633482	-1.060831	3.157727
H	4.126611	-0.761954	2.988276
O	-2.539394	-1.822485	3.571948
H	-2.553191	-2.552349	2.916986
H	-1.639847	-1.463599	3.519976
O	-1.091328	1.513362	-4.088784
H	-1.201882	0.572483	-3.861750
H	-1.517808	1.997010	-3.352985
O	-0.823516	1.528334	4.033544
H	-1.397779	1.788984	3.283670
H	-0.460144	0.663827	3.774060
O	4.764983	-2.833388	0.596717
H	4.767801	-2.330702	1.437063
H	4.746597	-2.162289	-0.111029
O	-2.391898	2.167723	1.807121
H	-2.414992	3.103940	1.538836
H	-1.820710	1.748295	1.122680
O	-3.798287	-0.546016	-0.269311
H	-3.971422	-0.345081	0.675720
H	-2.814303	-0.533974	-0.365745
O	0.714143	3.635596	0.737383
H	1.008138	3.448392	1.654548
H	0.341701	2.782827	0.415829
O	1.972818	-2.111312	-2.260078
H	1.678271	-2.195550	-3.173442
H	1.469924	-1.352425	-1.865022
O	-2.413432	-3.910881	1.668717
H	-2.990731	-3.729535	0.897403
H	-1.531266	-3.582214	1.404095
O	-4.210182	0.118269	2.420728
H	-3.626657	-0.542865	2.849300
H	-3.647045	0.905078	2.293297
O	2.226201	-3.864219	-0.091755
H	3.086130	-3.538073	0.245879
H	2.106596	-3.376053	-0.929138
C	-0.255024	0.227714	-0.594282

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Eopt -2328.739391

O	1.041672	-0.937553	-0.094224
O	-0.349758	0.389808	1.043726
O	-1.144969	-0.949222	-0.567799
O	-3.833536	-0.190209	-0.494683
H	-4.082664	-0.259223	0.449161
H	-2.871450	-0.395227	-0.503550
O	5.232719	-1.597007	-0.198294
H	4.850855	-2.483847	-0.354331
H	4.576680	-1.147278	0.375296
O	1.886474	-0.033953	-2.539093
H	1.320033	-0.428913	-3.235060
H	1.578257	-0.434021	-1.693738
O	-2.435060	-2.641420	1.425488
H	-1.671175	-2.954542	1.958238
H	-2.034331	-2.105404	0.715922
O	-4.128032	-0.528428	2.314886
H	-3.517662	-1.276566	2.164632
H	-3.548203	0.248366	2.443659
O	0.167827	-0.703279	3.614869
H	1.126990	-0.654199	3.801953
H	0.053113	-0.293756	2.733865
O	-4.188436	2.388623	-1.435037

H	-4.058663	1.469571	-1.110525
H	-3.552950	2.484007	-2.154359
O	2.950140	-0.693321	4.055934
H	3.181731	0.133319	4.493665
H	3.117791	-0.533787	3.098768
O	4.020592	-4.126789	-0.582134
H	4.457622	-4.735603	0.023841
H	3.141391	-3.955650	-0.183164
O	-3.155668	3.788010	0.763546
H	-2.276552	4.122724	0.494003
H	-3.509739	3.329326	-0.026396
O	1.455515	2.638183	-1.948170
H	1.255061	2.669213	-1.003451
H	1.545465	1.680541	-2.163524
O	-0.364932	3.122019	3.813812
H	-0.660708	4.033506	3.916511
H	-1.119623	2.651876	3.397654
O	1.486464	-3.565052	0.491847
H	0.897560	-4.136240	-0.015158
H	1.278535	-2.643874	0.200264
O	-4.194706	-4.319047	-0.041990
H	-3.556946	-3.811696	0.494487
H	-4.554796	-3.660953	-0.666425
O	-5.189494	-2.273603	-1.770064
H	-4.691995	-1.534150	-1.358078
H	-4.773276	-2.409987	-2.628411
O	-0.969702	3.183493	-3.237797
H	-0.132653	3.074800	-2.737873
H	-1.549018	3.699814	-2.665733
O	4.333255	2.686203	-1.574808
H	4.539187	1.767314	-1.846145
H	3.386336	2.785657	-1.782973
O	-0.156886	-3.365256	2.858696
H	0.443782	-3.475391	2.097980
H	-0.007838	-2.442242	3.161034
O	-0.573871	4.728891	0.097542
H	-0.010379	4.024267	0.484116
H	-0.438062	4.662184	-0.854641
O	-1.777336	0.496152	-3.124401
H	-1.506631	1.436760	-3.113861
H	-1.518266	0.133122	-2.260550
O	0.975989	2.770141	1.351692
H	0.639274	2.993688	2.244362
H	0.593359	1.877684	1.179650
O	3.299632	-0.309161	1.354295
H	3.479652	0.653412	1.273174
H	2.447880	-0.467733	0.881905
O	-2.348911	1.687748	2.421571
H	-2.680550	2.408769	1.841496
H	-1.707110	1.193363	1.864429
O	-0.695265	-2.990545	-2.350245
H	0.089864	-3.484807	-2.090911
H	-0.786582	-2.273250	-1.675702
O	4.696594	0.011691	-2.439543
H	4.914266	-0.568207	-1.679429
H	3.729063	-0.079873	-2.546856
O	3.754724	2.429901	1.184170
H	3.986130	2.542035	0.239313
H	2.796325	2.623616	1.242056
O	0.082028	-1.179906	-4.371631
H	-0.579832	-0.509146	-4.105028
H	-0.123523	-1.923093	-3.768434
C	-0.153589	-0.492860	0.129262

D3BJ_B3LYP_Radical_9_s1

Eopt -952.184987

O	-0.724432	-0.307322	-1.284027
O	-0.885394	1.564460	-0.254734
O	-0.668343	-0.292741	0.945185
O	1.579320	0.468992	2.531111
H	0.781925	0.274834	2.007443

H	1.369933	1.278421	3.011183
O	-3.851455	1.629788	0.219020
H	-2.922354	1.845782	0.051983
H	-3.806496	0.829305	0.769483
O	1.708641	2.781477	-0.972091
H	2.330229	2.267518	-0.413725
H	0.837686	2.413254	-0.765234
O	1.655735	-2.029086	-1.456739
H	0.968050	-1.362379	-1.604025
H	1.473917	-2.339695	-0.545607
O	-3.490663	-1.136555	1.203843
H	-2.539662	-0.970959	1.294726
H	-3.617675	-1.210033	0.242097
O	0.888466	-2.664071	1.160941
H	1.606071	-2.389065	1.743375
H	0.296152	-1.890852	1.122735
O	-3.684625	-0.613806	-1.683151
H	-3.853541	0.247271	-1.263486
H	-2.719257	-0.645424	-1.754582
O	3.457431	1.317890	0.623279
H	2.816345	0.976387	1.278297
H	3.658059	0.566035	0.027656
O	4.061831	-0.744824	-1.153247
H	3.191668	-1.182525	-1.298225
H	4.248993	-0.278019	-1.975302
C	-0.748688	0.296089	-0.160651

D3BJ_B3LYP_Radical_9_s2

Eopt -952.183825

O	-0.202751	0.211255	-1.001506
O	-0.773045	2.047668	-0.048571
O	-0.473129	0.257827	1.218005
O	2.091908	0.401500	2.429746
H	1.175609	0.399574	2.093751
H	2.197396	1.259767	2.866202
O	-3.777679	1.533748	-0.140785
H	-2.895511	1.931063	-0.162744
H	-3.679793	0.785511	0.475402
O	1.969609	3.059670	-0.850611
H	2.433220	2.226819	-0.612598
H	1.044302	2.881972	-0.637410
O	0.546300	-2.575358	-1.143488
H	0.143445	-1.707051	-1.284992
H	0.498539	-2.679574	-0.169851
O	-3.131286	-1.012340	1.146120
H	-2.247732	-0.681323	1.371588
H	-3.064207	-1.210301	0.195132
O	0.227773	-2.493321	1.646391
H	1.107706	-2.428672	2.042923
H	-0.050920	-1.567710	1.525236
O	-2.925942	-0.756187	-1.781936
H	-3.311809	0.081020	-1.469961
H	-1.972712	-0.602719	-1.709217
O	3.339702	0.773951	-0.062630
H	2.928163	0.607251	0.806470
H	3.192667	-0.034633	-0.592689
O	3.110867	-1.558754	-1.576536
H	2.210156	-1.929359	-1.424384
H	3.117643	-1.285142	-2.502000
C	-0.474130	0.806039	0.085923

D3BJ_B3LYP_Radical_9_s3

Eopt -952.184882

O	0.735010	-0.365102	-1.851927
O	1.732489	1.194064	-0.776981
O	1.668764	-0.857159	0.106050
O	4.469260	-1.157420	0.713916
H	3.506468	-1.084854	0.586859
H	4.617614	-0.911185	1.634022
O	-0.449685	3.015413	-0.193302
H	0.322267	2.460582	-0.398955
H	-0.143828	3.620988	0.491955

O	4.744482	1.213505	-0.867491
H	4.770269	0.413436	-0.309680
H	3.796764	1.383154	-0.966206
O	-1.942624	-1.164250	-0.699235
H	-1.306791	-0.816700	-1.341136
H	-1.450424	-1.878806	-0.242207
O	0.341419	0.094148	2.603411
H	0.881687	-0.239406	1.871333
H	-0.467190	0.419454	2.162286
O	-0.229719	-2.972662	0.578369
H	-0.053707	-3.708457	-0.019200
H	0.487318	-2.334418	0.409088
O	-1.928064	1.003664	1.126940
H	-1.452243	1.726945	0.669235
H	-1.912008	0.253002	0.497937
O	-4.704669	-1.014381	-1.195350
H	-3.749372	-1.159149	-1.047261
H	-5.141984	-1.748927	-0.750670
C	1.389421	-0.036634	-0.802810
O	-4.740409	1.266684	0.555528
H	-3.799342	1.274706	0.809620
H	-4.812052	0.497403	-0.039576

D3BJ_B3LYP_Radical_12_s1

Eopt -1181.577228

O	-0.174764	0.301114	0.999499
O	0.018616	-0.676089	-0.950101
O	-0.174997	1.525438	-0.815857
O	-2.632416	-0.967134	-2.379705
H	-1.702802	-1.020467	-2.113168
H	-2.861153	-0.031291	-2.210421
O	-0.890380	2.601325	2.963268
H	-0.729814	1.729282	2.580724
H	-0.799126	3.202733	2.199991
O	2.440258	-3.326590	0.576969
H	1.481626	-3.472186	0.504574
H	2.645661	-2.723017	-0.167411
O	-2.967996	-0.612007	1.810816
H	-3.124554	-1.303463	1.137196
H	-2.084319	-0.275087	1.607914
O	4.352387	0.699838	-0.762170
H	4.555727	0.611309	0.175732
H	3.704124	1.434080	-0.817268
O	2.021799	-1.199328	2.435888
H	2.197076	-1.944995	1.828963
H	1.337336	-0.681978	1.988595
O	-0.615788	4.098297	0.550259
H	-0.454633	3.271416	0.066905
H	0.241197	4.540131	0.568470
O	2.801456	-1.494921	-1.533521
H	3.360365	-0.743133	-1.242854
H	1.891612	-1.174332	-1.434394
O	-3.311994	-2.617809	-0.173869
H	-3.178260	-2.042963	-0.954310
H	-2.425811	-2.978918	0.004373
O	-0.507498	-3.223429	0.408625
H	-0.336269	-2.355335	0.003285
H	-0.595056	-3.031532	1.350877
O	-2.971014	1.800701	-1.861674
H	-3.601232	1.937604	-1.144887
H	-2.098313	1.859327	-1.442090
O	2.491244	2.768790	-1.013851
H	1.604792	2.372893	-0.986973
H	2.589233	3.098481	-1.914754
C	-0.108120	0.382648	-0.270944

D3BJ_B3LYP_Radical_12_s2

Eopt -1181.57315

O	0.582072	-0.451002	0.199529
O	-1.220890	-1.041763	-0.968875
O	0.522938	-2.347350	-0.886263
O	-1.436982	0.658924	-3.347387

H	-1.303161	0.029103	-2.619493
H	-0.570280	0.750273	-3.759672
O	-0.869330	2.199362	2.331599
H	-0.399099	1.425198	2.691763
H	-0.338686	2.454129	1.553647
O	3.474407	-0.216349	-0.056972
H	2.506813	-0.233027	0.041962
H	3.646231	-0.983292	-0.637593
O	-4.644207	-0.901077	1.399838
H	-4.054879	-0.152068	1.196754
H	-4.238285	-1.647873	0.920974
O	0.564894	2.482916	-0.168793
H	-0.222678	2.681971	-0.717882
H	0.584030	1.512667	-0.124198
O	0.679552	-0.140501	3.042198
H	0.228476	-0.803339	3.578102
H	0.565427	-0.431785	2.120720
O	3.432188	-2.534761	-1.699431
H	3.565084	-2.283044	-2.620767
H	2.470668	-2.531160	-1.577978
O	3.562374	-0.546954	2.826611
H	3.645431	-0.483503	1.858609
H	2.610720	-0.429189	2.990278
O	-3.300252	-2.931830	-0.117140
H	-2.916937	-3.577902	0.486888
H	-2.553512	-2.375060	-0.393851
O	-1.855571	2.836705	-1.571105
H	-1.712615	2.155924	-2.258491
H	-2.292529	2.347252	-0.848891
O	-2.753776	1.083622	0.544122
H	-2.244166	0.387941	0.098206
H	-2.145742	1.432819	1.230866
O	3.226122	2.381106	-1.282615
H	3.429530	1.492305	-0.938449
H	2.317817	2.543052	-0.971910
C	-0.047664	-1.254965	-0.543686

D3BJ_B3LYP_Radical_12_s3

Eopt -1181.573298

O	-0.441726	0.581440	1.462006
O	0.695875	-0.007421	-0.358169
O	1.664501	0.991716	1.374214
O	-1.577717	-0.029318	-2.240788
H	-0.851590	0.043317	-1.599808
H	-2.356838	0.357356	-1.785904
O	-2.533812	2.550428	0.968795
H	-1.757417	1.989894	1.125536
H	-2.203562	3.319377	0.463064
O	2.914810	-3.436651	0.135764
H	1.947934	-3.385062	0.231335
H	3.136088	-2.629372	-0.367716
O	-4.225500	-1.693921	0.200597
H	-3.523436	-2.098655	-0.355744
H	-3.867546	-1.695029	1.095677
O	5.319982	0.736899	-0.650152
H	5.747098	0.359687	0.127090
H	4.771150	1.474343	-0.307955
O	-1.080323	-2.056467	2.604237
H	-2.033381	-2.190389	2.541288
H	-0.940316	-1.134005	2.333449
O	-1.645420	4.818391	-0.461617
H	-1.235772	4.495727	-1.273151
H	-2.439223	5.280052	-0.757185
O	3.257634	-1.042201	-1.365246
H	3.982093	-0.440063	-1.097857
H	2.447574	-0.630850	-1.021280
O	-2.253840	-2.685390	-1.512520
H	-2.028455	-1.797851	-1.860791
H	-1.498642	-2.899349	-0.931913
O	0.061992	-2.896116	0.158551
H	0.306224	-2.005567	-0.142815

H	-0.331636	-2.734604	1.040504
O	-3.850769	0.909179	-0.889431
H	-4.018405	0.057415	-0.439891
H	-3.427058	1.483340	-0.217913
O	3.618628	2.787072	0.194398
H	4.021557	3.254443	0.935380
H	2.905571	2.259156	0.590663
C	0.642242	0.507596	0.785138

D3BJ_B3LYP_Radical_18_sl

Eopt -1640.352858

O	0.931688	0.142806	-0.122639
O	-1.281680	0.026375	0.094111
O	-0.096779	-1.766668	-0.312001
O	-2.119516	1.351150	-2.341296
H	-1.900622	0.954996	-1.480872
H	-1.333065	1.142615	-2.891129
O	0.746956	3.254776	2.412431
H	1.091334	2.366712	2.630168
H	0.966707	3.360871	1.469086
O	3.650926	0.108874	-1.068406
H	2.728353	-0.044058	-0.806811
H	3.984727	-0.768098	-1.354192
O	-0.402846	-1.022708	3.644944
H	-1.269772	-0.583765	3.500952
H	-0.375425	-1.736664	2.997219
O	4.378413	-3.069857	1.045910
H	5.175074	-3.479604	1.400252
H	4.383911	-2.146632	1.381023
O	-2.878026	0.261679	3.287839
H	-2.569578	1.078530	2.852969
H	-3.298419	-0.242425	2.568265
O	1.114545	3.080012	-0.486241
H	0.209598	3.390563	-0.702411
H	1.005034	2.129467	-0.317090
O	-3.761634	-3.803761	0.297073
H	-3.169280	-4.262765	0.903240
H	-3.221307	-3.618262	-0.500054
O	1.699525	0.560349	2.664709
H	0.991182	0.022478	3.080062
H	1.510659	0.482838	1.714716
O	4.667089	-2.440717	-1.654784
H	3.976824	-2.903545	-2.143319
H	4.575896	-2.747627	-0.726293
O	-4.119683	-0.784589	-2.156544
H	-4.201690	-0.781046	-1.187170
H	-3.511441	-0.049121	-2.351400
O	4.313556	-0.361018	1.725724
H	4.155504	-0.104249	0.797393
H	3.483559	-0.137365	2.182469
O	-3.842114	-1.020578	0.821894
H	-3.851404	-1.997037	0.754409
H	-2.940712	-0.769842	0.555860
O	-1.582184	3.807064	-0.927246
H	-1.804091	3.063276	-1.519201
H	-1.798621	3.471878	-0.038459
O	-1.845250	2.411404	1.644608
H	-1.596191	1.647719	1.095837
H	-0.991216	2.735967	2.000607
O	0.189416	0.627417	-3.761406
H	0.975641	1.115241	-3.430807
H	0.301405	-0.272472	-3.434088
O	2.421092	2.060865	-2.842647
H	2.950884	1.384666	-2.382745
H	1.990389	2.548349	-2.115334
O	-2.334906	-2.976936	-1.987039
H	-1.552572	-2.601381	-1.558257
H	-2.931266	-2.211107	-2.123327
C	-0.154789	-0.501103	-0.108920

D3BJ_B3LYP_Radical_18_s2

Eopt -1640.351673

O	-1.147086	0.104383	0.121468
O	1.020952	0.548016	-0.124383
O	0.307459	-1.497709	-0.187365
O	1.698875	1.376674	2.499583
H	1.542369	1.209008	1.554968
H	1.074274	0.752945	2.930648
O	-1.898713	3.456622	-1.564156
H	-2.052046	2.594438	-1.995021
H	-2.064706	3.276670	-0.620845
O	-3.345488	-1.338568	1.061593
H	-2.583818	-0.831263	0.728411
H	-2.955540	-2.223761	1.212170
O	0.080837	-0.271652	-3.521136
H	0.815605	0.360961	-3.361149
H	0.224973	-0.989816	-2.893334
O	-1.509707	-3.299712	-1.628513
H	-0.795064	-2.668702	-1.465487
H	-2.307251	-2.738878	-1.743011
O	2.159161	1.556360	-3.153426
H	1.737883	2.204651	-2.559784
H	2.754444	1.048918	-2.573779
O	-2.019130	2.546979	1.209880
H	-1.213039	3.042900	1.469433
H	-1.669511	1.739354	0.792288
O	3.690769	-2.741402	-1.111546
H	4.603568	-3.033821	-1.011032
H	3.314835	-2.762364	-0.205617
O	-2.258209	0.738987	-2.416443
H	-1.458651	0.429100	-2.896838
H	-2.011978	0.589592	-1.488100
O	-1.847050	-3.729483	1.145331
H	-1.055399	-3.339839	1.535458
H	-1.710724	-3.643870	0.178009
O	4.013539	-0.205069	1.830992
H	4.031757	-0.031137	0.873066
H	3.294852	0.362150	2.167863
O	-3.773964	-1.660326	-1.790709
H	-3.786673	-1.553198	-0.821138
H	-3.341546	-0.850043	-2.117078
O	3.606985	0.065265	-1.073507
H	3.707581	-0.901835	-1.192592
H	2.699182	0.161532	-0.734180
O	0.416536	3.837828	1.701675
H	0.860799	3.073178	2.112199
H	0.642134	3.762993	0.756175
O	0.851025	3.174313	-1.110783
H	0.852364	2.279433	-0.727813
H	-0.088327	3.322798	-1.352999
O	-0.099186	-0.536792	3.442602
H	-1.001884	-0.160964	3.337403
H	-0.018854	-1.197261	2.744571
O	-2.658431	0.543653	3.201632
H	-3.023195	-0.129066	2.600245
H	-2.490061	1.312736	2.625985
O	2.522982	-2.547043	1.437376
H	1.678250	-2.229537	1.086417
H	3.025660	-1.730809	1.646823
C	0.045078	-0.246303	-0.058945

D3BJ_B3LYP_Radical_18_s3

O	-1.066535	-0.089525	0.193777
O	1.061124	-0.270425	-0.385307
O	-0.201091	1.388798	-1.125625
O	1.131804	-2.056772	-2.651263
H	1.200686	-1.512525	-1.848924
H	0.249920	-1.814243	-3.000589
O	-0.496117	-2.652189	3.166591
H	-0.607170	-1.686188	3.269945
H	-1.099916	-2.870709	2.434313
O	-4.395863	0.302385	-0.149042

Eopt -1640.353578

H	-5.357187	0.274976	-0.078867
H	-4.197771	1.053768	-0.753037
O	1.687203	1.219172	3.641542
H	2.344706	0.638268	3.197626
H	1.870152	1.134277	4.583906
O	-2.054352	3.430213	0.307760
H	-1.276828	2.941019	0.004878
H	-2.454516	2.854020	0.993917
O	3.513492	-0.443900	2.337054
H	2.939076	-1.202406	2.116871
H	3.716266	-0.045984	1.469819
O	-2.131929	-2.791462	0.765732
H	-2.983959	-2.612631	1.182094
H	-1.751565	-1.913340	0.596853
O	4.103355	3.262634	-0.618885
H	4.540202	3.440402	-1.459308
H	3.162347	3.501213	-0.763575
O	-0.856465	0.185379	3.072103
H	0.017682	0.566846	3.304804
H	-0.834001	0.100148	2.104766
O	-3.656220	2.425902	-1.770379
H	-3.040244	2.020372	-2.392153
H	-3.086355	2.844746	-1.089771
O	3.743278	-0.629290	-3.104895
H	3.819045	-0.242033	-2.214588
H	2.892396	-1.094849	-3.096298
O	-3.309065	1.701774	2.148160
H	-3.665316	1.123392	1.447170
H	-2.564120	1.216405	2.537142
O	3.801116	0.497382	-0.397890
H	3.935365	1.466303	-0.479352
H	2.836609	0.375333	-0.422945
O	1.321010	-4.301938	-0.816383
H	1.205846	-3.634945	-1.516095
H	1.446844	-3.773499	-0.008053
O	1.692392	-2.462066	1.409920
H	1.380514	-1.760079	0.812708
H	0.966034	-2.567624	2.061446
O	-1.425703	-1.061996	-3.417231
H	-2.140636	-1.343041	-2.805169
H	-1.248517	-0.143760	-3.180295
O	-3.502893	-1.905630	-1.730812
H	-3.840203	-1.133845	-1.233175
H	-3.042525	-2.427104	-1.054490
O	1.409552	3.860383	-0.987706
H	0.912634	3.027082	-0.976197
H	1.078353	4.355636	-0.228898
C	-0.044768	0.328997	-0.435710

D3BJ_B3LYP_Radical_24_s1

O	-0.808920	0.221358	-1.373162
O	0.942513	0.025645	-0.035828
O	-0.934342	0.987086	0.643360
O	-3.127612	0.341895	2.436057
H	-3.252055	-0.633328	2.419477
H	-2.390398	0.492814	1.823141
O	-1.035014	0.051921	4.410260
H	-1.840661	0.187216	3.876214
H	-0.459917	0.792276	4.146859
O	2.631086	-1.030800	-2.095099
H	2.528104	-0.569237	-2.954635
H	2.031170	-0.564214	-1.487421
O	-4.396981	2.312050	0.691180
H	-3.630654	2.896692	0.557399
H	-4.097623	1.656594	1.346420
O	1.742197	-3.422328	-0.858943
H	1.116807	-3.031385	-0.235431
H	2.038947	-2.668885	-1.407917
O	2.588484	0.567429	2.318797
H	2.680911	-0.318020	2.737546

Eopt -2099.128424

H	2.055608	0.395864	1.523364
O	0.466496	2.204466	3.111459
H	-0.117064	1.927960	2.389303
H	1.271099	1.662692	2.969610
O	2.292298	0.513554	-4.407104
H	1.697825	1.173857	-3.997305
H	1.745726	0.050603	-5.052262
O	-1.537161	-2.149426	-3.092521
H	-1.056716	-2.982232	-2.901112
H	-1.164437	-1.488399	-2.492005
O	-4.055150	-3.626112	0.182932
H	-4.965561	-3.880163	0.370432
H	-4.109190	-3.013456	-0.586632
O	-0.136673	-4.533832	-2.641424
H	0.530731	-4.222090	-1.996258
H	-0.704351	-5.135762	-2.147035
O	-3.108684	-2.434373	2.516776
H	-3.394981	-2.842158	1.672537
H	-2.136214	-2.466992	2.521659
O	-1.825759	3.732473	0.147914
H	-1.528227	2.812604	0.232093
H	-1.733533	3.937161	-0.807578
O	-0.190516	-2.075482	2.764841
H	-0.046650	-1.667354	1.901567
H	-0.428236	-1.327261	3.356373
O	2.683652	-2.040314	3.270323
H	1.727690	-2.167549	3.129151
H	3.118767	-2.398625	2.467130
O	-3.821250	0.795861	-1.622681
H	-2.859005	0.714031	-1.557863
H	-4.077365	1.294384	-0.819156
O	0.873818	4.302035	1.081667
H	-0.039502	4.241466	0.743560
H	0.867995	3.718739	1.861052
O	2.292558	2.692950	-0.743467
H	1.819571	3.283844	-0.116460
H	2.032427	1.800627	-0.470320
O	0.598795	2.330737	-2.997067
H	0.044410	1.621673	-2.635022
H	1.208621	2.549560	-2.260659
O	5.007002	-0.811482	-0.574683
H	4.238982	-0.845576	-1.178367
H	4.925695	0.052116	-0.122707
O	-1.379651	4.326018	-2.552286
H	-0.696434	3.660073	-2.770377
H	-2.141631	4.089817	-3.093339
O	-4.128869	-1.991328	-2.028275
H	-3.241622	-2.127721	-2.421419
H	-4.140914	-1.041027	-1.801413
O	3.987086	-2.970377	0.960916
H	3.254112	-3.234286	0.376955
H	4.384443	-2.198689	0.506398
O	4.661832	1.677491	0.769079
H	4.067983	2.166951	0.176242
H	4.046799	1.281784	1.418451
C	-0.238563	0.397686	-0.245735

D3BJ_B3LYP_Radical_24_s2

O	1.189416	0.971199	-0.292059
O	-0.438913	-0.505568	0.098367
O	1.466126	-0.492853	1.242685
O	1.124899	0.581322	4.024102
H	0.348702	1.179567	3.968056
H	1.315240	0.343265	3.104730
O	-0.617428	-1.668993	4.306630
H	0.037125	-0.943173	4.298379
H	-0.182524	-2.404030	3.830027
O	-1.915340	0.494024	-2.173117
H	-1.294044	0.914056	-2.808141
H	-1.357937	0.153148	-1.451540

Eopt -2099.122618

O	5.577023	0.208539	1.241199
H	5.054855	-0.576987	0.988637
H	5.399113	0.336140	2.179984
O	-3.584180	2.106055	-0.688939
H	-3.332383	1.938190	0.227464
H	-2.959648	1.567049	-1.226744
O	-1.173910	-3.267854	0.754607
H	-0.899892	-3.724472	-0.050151
H	-0.944955	-2.336663	0.592663
O	0.589556	-3.783430	2.833672
H	1.446106	-3.435286	2.559363
H	0.004166	-3.652371	2.056538
O	-0.048932	1.692102	-3.865069
H	0.644401	1.024603	-3.715355
H	0.144817	2.392243	-3.210798
O	0.403397	3.473739	-1.687047
H	-0.483510	3.842474	-1.481238
H	0.501648	2.702024	-1.109207
O	-0.871613	4.331653	2.209148
H	-1.737605	4.609535	1.887934
H	-0.593243	5.039742	2.802235
O	-2.148652	4.500855	-1.204710
H	-2.690923	3.715128	-0.986583
H	-2.116612	5.019008	-0.392361
O	-1.243865	2.055422	3.852252
H	-1.142397	2.823628	3.258047
H	-1.656531	1.351098	3.316257
O	3.878981	-1.911306	0.258876
H	3.111503	-1.369467	0.502734
H	4.086518	-1.671582	-0.672400
O	-2.215971	-0.253297	2.482486
H	-1.696284	-0.283409	1.663557
H	-1.719167	-0.828127	3.106041
O	-4.761834	-1.332632	1.746207
H	-3.885685	-0.984183	1.994401
H	-4.928007	-0.989617	0.846462
O	3.976308	2.004377	-0.261936
H	3.109593	1.573734	-0.226355
H	4.552518	1.451535	0.302433
O	2.037234	-3.970646	-0.525940
H	2.694975	-3.320263	-0.208693
H	1.495786	-4.172985	0.247169
O	0.328796	-2.496140	-2.179912
H	0.929419	-3.035434	-1.618116
H	-0.085920	-1.880838	-1.557612
O	1.932047	-0.270980	-2.975791
H	1.861281	0.213700	-2.138845
H	1.403717	-1.079786	-2.818508
O	-3.712109	-1.542122	-2.848720
H	-3.041177	-0.846544	-2.699458
H	-3.218309	-2.380436	-2.757625
O	4.492852	-1.266965	-2.379697
H	3.618540	-0.945631	-2.683452
H	4.639308	-2.092052	-2.856289
O	2.817466	4.629028	-0.591024
H	1.968953	4.332080	-0.965293
H	3.298570	3.803621	-0.410017
O	-5.303086	-0.296022	-0.840017
H	-4.825266	0.550060	-0.789748
H	-4.800283	-0.818927	-1.495195
O	-2.107801	-3.890068	-2.670419
H	-1.243948	-3.468100	-2.489031
H	-2.352350	-4.320777	-1.843260
C	0.693005	-0.018334	0.333709

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O	-1.158115	-1.704460	-0.230498
O	-0.392576	0.366624	0.115854
O	-1.908204	-0.561453	1.429605
O	-0.685486	-1.965948	3.825378

Eopt -2099.130624

H	0.283848	-1.932167	3.684982
H	-1.065939	-1.519635	3.056651
O	2.606535	2.634398	2.440242
H	1.665416	2.820203	2.225546
H	2.681785	2.709237	3.398369
O	1.140434	0.384952	-2.381989
H	0.833716	-0.367469	-2.934335
H	0.597590	0.345207	-1.576044
O	-5.831173	-2.406323	0.437207
H	-5.475099	-1.493538	0.482523
H	-6.123321	-2.607492	1.333292
O	3.630785	0.090915	-1.095646
H	3.296034	0.078634	-0.175942
H	2.812016	0.114242	-1.633534
O	-0.012012	2.905287	1.605815
H	-0.004035	3.500683	0.828497
H	-0.167131	2.022291	1.228524
O	-2.399118	3.518844	2.934962
H	-2.511826	2.880656	3.648267
H	-1.545075	3.286634	2.513128
O	0.244388	-1.844954	-3.808517
H	-0.712159	-1.738716	-3.653081
H	0.508619	-2.495007	-3.130769
O	0.757224	-3.551160	-1.554401
H	0.192513	-3.000118	-0.989243
H	0.257923	-4.366373	-1.685833
O	3.099239	-4.291474	2.455685
H	3.997172	-4.412565	2.788216
H	2.602540	-5.043485	2.801001
O	4.966409	-2.403000	-1.335520
H	4.483523	-1.557644	-1.263217
H	4.349959	-3.079156	-0.991851
O	2.091706	-1.834717	3.499810
H	2.429936	-2.678793	3.148355
H	2.199561	-1.189360	2.772377
O	-4.654700	0.135423	0.452614
H	-3.791772	-0.122752	0.812686
H	-4.493829	0.261479	-0.510631
O	2.345729	0.044547	1.420004
H	1.459248	0.104951	1.030326
H	2.494245	0.921282	1.833655
O	4.269331	4.210376	0.717396
H	3.713255	3.702300	1.333815
H	4.209331	3.726135	-0.131279
O	-3.380808	-3.757524	-0.022232
H	-2.710815	-3.059641	-0.022772
H	-4.224200	-3.296225	0.155096
O	-4.092655	2.962876	0.774548
H	-4.366403	2.027953	0.799016
H	-3.548443	3.103928	1.577124
O	-2.208244	2.515674	-1.214378
H	-2.846051	2.725669	-0.492666
H	-1.643464	1.818735	-0.846043
O	-2.455124	-1.576245	-2.859203
H	-2.104020	-1.698253	-1.960444
H	-2.980127	-2.367018	-3.033014
O	1.564700	3.161162	-2.858875
H	1.353764	2.212094	-2.772906
H	1.007486	3.603334	-2.191022
O	-4.125156	0.626348	-2.239510
H	-3.594790	-0.147886	-2.511025
H	-3.464752	1.311519	-2.024903
O	3.206876	-4.405398	-0.397799
H	2.340379	-4.100511	-0.726575
H	3.147476	-4.368914	0.574345
O	4.133979	2.824722	-1.727682
H	4.055112	1.886473	-1.465372
H	3.260597	3.028595	-2.120884
O	-0.111080	4.303669	-0.846127
H	-0.334728	5.239693	-0.902940

H	-0.936346	3.813854	-1.052881
C	-1.121966	-0.611392	0.413242

D3BJ_B3LYP_Radical_27_sl			Eopt -2328.52048
O	0.549476	1.039967	-0.522950
O	0.632859	-1.062689	-0.016761
O	-1.334694	-0.110821	-0.335679
O	-2.938580	-2.314466	0.700705
H	-2.679775	-3.084949	0.154106
H	-2.426129	-1.581288	0.320850
O	2.970184	4.275861	-0.741314
H	2.369546	4.309604	-1.512086
H	3.185138	3.329820	-0.624702
O	-0.829725	3.102955	1.075333
H	-1.714019	3.302119	0.698604
H	-0.392229	2.543233	0.415201
O	-1.901948	-1.888887	-2.750539
H	-1.145421	-1.598894	-3.307584
H	-1.795551	-1.369078	-1.939599
O	-2.023513	-4.287686	-1.118051
H	-1.899424	-3.573526	-1.770094
H	-1.173761	-4.342986	-0.642559
O	2.284587	-1.901304	-2.369111
H	3.112564	-1.377509	-2.281954
H	1.753797	-1.644163	-1.598831
O	-1.627016	-1.552524	3.145554
H	-2.050508	-1.867848	2.324016
H	-1.197096	-0.706732	2.918641
O	4.614091	-0.426588	-1.996654
H	5.169586	-0.997050	-1.452720
H	4.262642	0.252348	-1.379649
O	1.257758	4.428152	-3.015392
H	0.581901	5.082059	-2.804240
H	0.771940	3.586902	-3.130189
O	0.597769	-3.383553	3.035873
H	1.352401	-2.798045	2.834363
H	-0.162682	-2.776776	3.123801
O	-0.489551	1.129030	3.080536
H	-1.031767	1.354872	3.846171
H	-0.740536	1.782295	2.394841
O	2.965522	-4.333054	-1.022383
H	2.803732	-3.553354	-1.588788
H	2.145434	-4.400294	-0.497540
O	0.023799	1.877799	-3.273419
H	-0.938607	1.939811	-3.119710
H	0.363597	1.603973	-2.405469
O	-4.336608	-0.300461	-2.941484
H	-3.565486	-0.889247	-3.030776
H	-4.682315	-0.492687	-2.044754
O	-5.231974	-0.882402	-0.309290
H	-4.584693	-1.565633	-0.056154
H	-4.946986	-0.123881	0.235340
O	-3.921456	-0.020059	3.929429
H	-3.623887	0.657913	4.547137
H	-3.139172	-0.587227	3.779883
O	1.986769	2.648288	3.467948
H	1.861135	3.374631	2.822331
H	1.172555	2.117318	3.401966
O	0.303441	-0.892074	-4.156654
H	0.210757	0.051629	-3.930753
H	1.041735	-1.210713	-3.601335
O	2.648097	-1.566636	2.140762
H	3.334113	-2.113266	1.694621
H	2.034714	-1.311475	1.434814
O	-3.914805	1.036871	1.338266
H	-3.952063	0.727601	2.269386
H	-3.054457	0.736245	1.014083
O	4.577731	-3.118637	0.886670
H	4.051495	-3.563004	0.183925
H	5.161031	-2.510206	0.418401

O	3.451890	1.497613	-0.354293
H	3.654511	1.335856	0.598047
H	2.516139	1.255752	-0.444292
O	0.446981	-4.060430	0.307836
H	0.449163	-3.952061	1.284111
H	0.466719	-3.146831	-0.012503
O	-2.630757	1.809657	-2.185835
H	-3.296412	1.180689	-2.538774
H	-2.163606	1.278269	-1.519783
O	1.453831	4.699153	1.588013
H	1.984601	4.568726	0.773596
H	0.593953	4.285004	1.387176
O	3.904137	0.976951	2.314875
H	3.241717	1.564771	2.738660
H	3.496929	0.088204	2.327092
O	-3.404543	3.488030	0.009404
H	-3.740121	2.777861	0.586863
H	-3.236085	3.027231	-0.834687
C	-0.080127	-0.040077	-0.291612

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Eopt -2328.522753

O	-0.699592	-0.669925	-0.343855
O	0.152542	1.330006	-0.088892
O	1.482498	-0.398470	-0.044639
O	4.014161	0.792320	1.068356
H	4.147464	1.522884	0.427332
H	3.260025	0.307687	0.699811
O	-4.468598	-1.947260	-1.619752
H	-3.832930	-2.353603	-2.243128
H	-4.088129	-1.078035	-1.385990
O	-1.354036	-2.827542	1.480645
H	-0.652939	-3.513992	1.438888
H	-1.064717	-2.117414	0.883633
O	3.046652	0.476425	-2.411880
H	2.342764	0.456420	-3.098539
H	2.574554	0.239100	-1.597768
O	4.108394	2.750616	-0.957595
H	3.749834	2.099113	-1.587670
H	3.325672	3.225393	-0.618427
O	-0.505372	2.412143	-2.869068
H	-1.478981	2.326630	-2.978502
H	-0.324574	2.045134	-1.989907
O	2.130596	1.273292	3.134300
H	2.851715	1.235368	2.472371
H	1.348995	0.989316	2.642336
O	-3.266093	2.160418	-3.070465
H	-3.611819	3.037341	-2.868481
H	-3.359954	1.648541	-2.238247
O	-2.677758	-3.221419	-3.395566
H	-2.923751	-2.970817	-4.293021
H	-1.788102	-2.833030	-3.256753
O	1.219852	4.017712	2.796056
H	0.245747	3.913148	2.780630
H	1.564262	3.128398	2.995545
O	-1.892824	-1.625289	3.935902
H	-1.924211	-2.304502	4.618972
H	-1.630895	-2.096834	3.116140
O	-0.479589	4.928323	-1.478313
H	-0.488514	4.178248	-2.102336
H	0.283135	4.728061	-0.901886
O	-0.201122	-2.022440	-2.895372
H	0.551956	-2.612511	-2.665753
H	-0.430075	-1.585646	-2.058461
O	4.239375	-2.111313	-2.201872
H	3.876191	-1.220978	-2.373929
H	4.556401	-2.068788	-1.275982
O	5.069618	-1.923938	0.505884
H	5.009283	-0.963590	0.637477
H	4.249005	-2.255198	0.922509
O	2.590862	-1.379859	4.123083

H	3.490767	-1.438456	4.463993
H	2.478229	-0.444481	3.862223
O	-4.503062	-1.244334	2.884528
H	-4.455130	-1.894806	2.152197
H	-3.643479	-1.344889	3.340017
O	0.886159	0.302146	-4.165172
H	0.508506	-0.510203	-3.774258
H	0.354265	1.030981	-3.788898
O	-1.590179	3.767369	2.718342
H	-1.910569	3.748450	1.789613
H	-1.841839	2.913852	3.089002
O	2.545390	-2.600662	1.611628
H	2.564894	-2.208460	2.513040
H	2.088462	-1.939777	1.066272
O	-2.525075	3.828697	0.101278
H	-1.811469	4.215232	-0.451709
H	-2.639565	2.927091	-0.225424
O	-3.332725	0.534782	-0.831180
H	-3.698699	0.790606	0.046916
H	-2.424120	0.237130	-0.659087
O	1.675926	3.870338	0.053944
H	1.570651	4.002786	1.023414
H	1.253831	3.011669	-0.101273
O	1.931986	-3.656488	-2.172376
H	1.759818	-3.882541	-1.250781
H	2.752122	-3.111666	-2.154288
O	-4.102851	-3.177372	0.868228
H	-4.231505	-2.773262	-0.016226
H	-3.138856	-3.150298	1.019976
O	-4.378781	1.205657	1.630569
H	-4.395757	0.344868	2.110978
H	-3.720170	1.743378	2.085655
O	0.715973	-4.680032	1.458500
H	1.420545	-3.997410	1.507270
H	0.808187	-5.079553	0.585898
C	0.310812	0.065450	-0.156228

D3BJ_B3LYP_Radical_27_s3

Eopt -2328.514196

O	-0.838950	-1.020071	0.807344
O	0.581284	0.086048	-0.331928
O	-1.295753	1.104340	0.307045
O	-0.017220	3.576423	-0.446526
H	0.732580	3.797922	0.151374
H	-0.413359	2.765146	-0.086151
O	-1.501805	-4.481763	1.519331
H	-2.111428	-3.784062	1.826097
H	-0.618737	-4.064431	1.509473
O	-2.821001	-1.829762	-1.236296
H	-3.603459	-1.233071	-1.202746
H	-2.365209	-1.697435	-0.391509
O	-1.186391	2.659508	2.731536
H	-1.199788	2.018689	2.001912
H	-0.407018	3.200482	2.555364
O	2.112216	4.175797	1.168093
H	1.843496	3.949451	2.066144
H	2.756380	3.479858	0.909234
O	2.446239	0.367998	1.974324
H	2.868345	-0.502457	2.150044
H	1.814602	0.193617	1.260082
O	0.671057	2.376300	-2.821071
H	0.450618	2.842648	-1.983910
H	0.119824	1.585347	-2.808069
O	3.513287	-2.178772	2.347100
H	3.986743	-2.090356	1.501275
H	2.659089	-2.590230	2.102882
O	-3.303582	-2.431027	2.420698
H	-3.992359	-2.816231	2.974733
H	-2.683850	-1.995517	3.037455
O	3.277283	1.639459	-2.217580
H	3.439040	0.722188	-2.511777

H	2.344004	1.838234	-2.442048
O	-0.761745	-1.059718	-2.890489
H	-0.088836	-0.689841	-2.302410
H	-1.528571	-1.252935	-2.302197
O	6.224376	0.690835	0.285800
H	6.677944	0.899621	-0.538806
H	5.472662	1.321263	0.330802
O	-1.341786	-0.809556	3.628640
H	-1.888766	-0.014408	3.671897
H	-1.026487	-0.829008	2.708456
O	-3.389724	4.063970	1.529277
H	-2.625565	3.616109	1.934469
H	-3.122828	4.229524	0.604109
O	-2.562668	4.531745	-1.147037
H	-1.627024	4.413993	-0.899100
H	-2.800486	3.657143	-1.514903
O	-2.012352	0.942431	-4.340696
H	-1.492792	0.233953	-3.902746
H	-1.360191	1.590616	-4.630413
O	-0.124776	-3.835743	-2.788119
H	-0.843024	-4.156836	-2.201442
H	-0.338362	-2.894761	-2.934812
O	1.120643	0.442675	4.470369
H	0.268302	0.013689	4.282952
H	1.568274	0.460451	3.603562
O	3.965486	-1.000349	-2.978794
H	4.161148	-1.234635	-2.047680
H	3.219692	-1.558933	-3.225406
O	-3.002437	1.875068	-1.926878
H	-2.651847	1.593236	-2.800348
H	-2.358220	1.552802	-1.274898
O	4.382562	-1.314128	-0.245047
H	5.093726	-0.656054	-0.074572
H	3.567707	-0.815002	-0.101722
O	1.015261	-3.143819	1.457730
H	1.327731	-3.247380	0.527311
H	0.527111	-2.306427	1.438137
O	3.866417	2.159279	0.402041
H	3.605314	1.942781	-0.524278
H	3.427178	1.483547	0.960880
O	-3.892896	0.287133	1.581662
H	-3.740026	-0.643378	1.828205
H	-3.039154	0.591976	1.235041
O	-2.270477	-4.580520	-1.152283
H	-1.965512	-4.599446	-0.219173
H	-2.640684	-3.683764	-1.250582
O	1.959791	-3.293121	-1.100894
H	1.208536	-3.503701	-1.703717
H	2.178377	-2.371810	-1.284156
O	-4.874140	0.004019	-1.027081
H	-4.327005	0.700191	-1.444914
H	-4.670883	0.105151	-0.074027
C	-0.553804	0.097372	0.265025

M06_3_s1			Eopt -493.346246
O	2.715138	0.227492	-0.118502
O	0.669317	0.909359	0.455949
O	0.975519	-1.138924	-0.395427
O	-1.605006	-1.347592	-0.866511
H	-1.862969	-0.431580	-1.040688
H	-0.629842	-1.263890	-0.667171
O	-1.329278	-0.285570	1.842016
H	-0.575120	0.151679	1.381847
H	-1.712160	-0.823455	1.136407
O	-1.559430	1.558797	-0.918536
H	-0.732908	1.308304	-0.439176
H	-2.208423	1.695034	-0.221423
C	1.465224	-0.004097	-0.023618

M06_3_s2			Eopt -493.349487
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C	-0.006555	-0.002948	0.042191
O	-0.337780	-1.247429	0.070471
O	-0.918092	0.907008	0.025240
O	1.236767	0.332919	0.031336
O	2.804026	-1.770266	-0.055906
H	2.178283	-0.991867	-0.019167
H	2.234257	-2.541346	0.005761
O	-2.941858	-1.516208	-0.053203
H	-3.300569	-0.624576	-0.052532
H	-1.951810	-1.383660	-0.008034
O	0.155805	3.296402	-0.033169
H	1.108407	3.169926	-0.046729
H	-0.220190	2.369801	-0.010601

M06_3_s3			Eopt -493.343175
C	-1.595662	-0.146190	-0.099980
O	-1.310788	0.852333	0.669080
O	-2.751127	-0.257363	-0.630619
O	-0.684589	-1.043920	-0.331665
O	1.237436	-0.980312	1.348555
H	0.444475	-0.969305	0.707426
H	1.261101	-0.091211	1.716420
O	2.688672	-0.396741	-0.949306
H	2.279537	-0.712395	-0.119800
H	2.086290	-0.691786	-1.639695
O	1.033881	1.910429	-0.086513
H	0.199730	1.466520	0.204457
H	1.594958	1.199902	-0.425174

M06_6_s1			Eopt -722.614631
O	1.134990	0.180870	-1.831276
O	-0.585124	1.063232	-0.720676
O	-0.631114	-1.084646	-1.333926
O	1.322989	-2.582188	0.000729
O	2.565001	0.183345	0.487853
O	1.120182	2.637792	0.646850
H	2.154388	0.136076	-0.402843
H	1.868159	-1.877257	0.368655
H	1.536801	3.248895	0.032370
H	0.514735	2.087204	0.093014
H	2.338206	1.087085	0.759937
H	0.640133	-2.109570	-0.513890
O	0.254882	-0.292230	2.254496
O	-1.986701	-1.417878	0.929278
O	-3.119736	1.080774	0.071248
H	-1.510103	-1.323845	0.064286
H	-2.190976	1.034087	-0.275438
H	-0.505619	-0.678013	1.784962
H	-3.674042	0.755717	-0.643984
H	-2.575639	-0.649295	0.923564
H	0.948945	-0.196892	1.585841
C	-0.024657	0.055541	-1.302179

M06_6_s2			Eopt -722.619815
O	0.655348	1.286551	-0.127168
O	-1.485918	0.698812	-0.232664
O	0.075659	-0.859113	0.093906
O	2.147892	-0.967590	1.911414
O	3.258539	0.898927	0.034863
O	-1.755462	3.365353	-0.272712
H	2.275095	1.048339	-0.025549
H	2.787353	-0.360144	1.517389
H	-0.862288	3.719906	-0.258381
H	-1.629803	2.384745	-0.264010
H	3.666738	1.758965	-0.098335
H	1.398771	-0.941816	1.280951
O	-1.826403	-2.606727	-0.763438
O	-3.486359	-0.786251	0.731479
H	-1.118189	-1.986871	-0.480722
H	-2.709624	-0.261054	0.415538

H	-3.260146	-1.057011	1.625850
H	-2.610185	-2.226964	-0.342699
C	-0.246046	0.381794	-0.088881
O	2.308281	-1.344208	-1.469682
H	1.501960	-1.202172	-0.933831
H	2.903977	-0.652701	-1.150903

M06_6_s3 Eopt -722.61653

O	0.918627	0.298938	-1.783761
O	-1.165300	0.591145	-1.051868
O	-0.251017	-1.442099	-1.010580
O	2.107977	-2.168554	0.171505
O	2.727686	0.661748	0.262399
O	-0.117973	2.797561	-0.015893
H	2.149796	0.582801	-0.524305
H	2.512267	-1.299091	0.306681
H	-0.845376	3.366001	0.253755
H	-0.542456	2.029679	-0.479536
H	2.087908	0.752029	0.988908
H	1.279138	-1.955660	-0.308569
O	0.517434	0.943085	2.036914
O	-1.035032	-1.379559	1.589373
O	-3.300107	-0.514770	0.084475
H	-0.738739	-1.481965	0.655963
H	-2.508051	-0.112277	-0.360074
H	-0.040948	0.162375	1.865105
H	-3.926918	0.206786	0.187614
H	-1.943128	-1.062866	1.479912
H	0.226057	1.617219	1.398044
C	-0.154654	-0.184165	-1.287336

M06_9_s1 Eopt -951.884233

O	0.951454	1.720216	-0.977927
O	0.993547	-0.406130	-1.658281
O	0.042636	0.125889	0.283142
O	-0.461805	-2.340524	1.036949
H	-0.168264	-1.455226	0.694880
H	0.142563	-2.981704	0.650161
O	2.702863	-1.837813	0.010719
H	2.052027	-1.458806	-0.611951
H	2.522891	-1.377999	0.843521
O	-1.240825	-1.911633	-1.821053
H	-1.342887	-2.270429	-0.930131
H	-0.383998	-1.425659	-1.774680
O	-1.529891	2.788290	-0.404015
H	-0.611026	2.487502	-0.566603
H	-1.716498	2.496553	0.500646
O	2.173150	0.221877	2.100005
H	1.338252	0.236592	1.597322
H	2.795655	0.662945	1.502925
O	-1.625752	1.283630	2.091256
H	-2.298224	0.594120	1.984153
H	-0.911252	0.962813	1.503711
O	3.669165	1.066327	-0.289215
H	3.593547	0.110655	-0.416889
H	2.821753	1.418300	-0.612580
O	-3.085489	-1.048090	1.135180
H	-2.288738	-1.597785	1.123885
H	-3.047169	-0.547738	0.300210
O	-2.833090	0.384201	-1.306563
H	-2.307397	1.163212	-1.056208
H	-2.197128	-0.306070	-1.565698
C	0.659699	0.486466	-0.794708

M06_9_s2 Eopt -951.884607

O	-1.391877	-0.111577	-1.390557
O	0.732154	0.544646	-1.513739
O	0.057743	-0.711212	0.199136
O	2.217512	0.285077	1.457827
H	1.462790	-0.111315	0.957624

H	2.244475	1.199425	1.146329
O	1.237606	2.738555	0.105103
H	1.129335	1.997260	-0.524130
H	0.571402	2.545874	0.783346
O	2.920712	-1.114400	-1.749309
H	3.447650	-1.135356	-0.936279
H	2.173916	-0.510291	-1.566486
O	-3.420106	-0.105444	0.551033
H	-2.731902	-0.037381	-0.137585
H	-3.015126	-0.710864	1.190802
O	-0.928761	1.622100	1.698350
H	-0.625411	0.751253	1.396662
H	-1.462637	1.947786	0.956026
O	-1.636627	-1.845581	1.977561
H	-1.831994	-2.752227	1.722418
H	-1.054100	-1.498942	1.263795
O	-1.818111	2.625574	-0.897142
H	-0.917320	2.970678	-0.918880
H	-1.731590	1.709273	-1.219519
O	4.446948	-1.101638	0.702617
H	3.672903	-0.604356	1.041075
H	4.349087	-1.989432	1.059065
O	-2.361893	-2.679271	-1.054371
H	-2.944497	-2.596180	-0.293047
H	-2.001621	-1.776828	-1.171436
C	-0.196293	-0.095502	-0.906974

M06_9_s3 Eopt -951.885474

O	-1.392021	-0.155520	-1.372989
O	0.730272	0.506388	-1.502558
O	0.042728	-0.672558	0.258819
O	2.217046	0.363113	1.462960
H	1.457136	-0.049221	0.984609
H	2.230286	1.270854	1.132221
O	1.191806	2.765001	0.048830
H	1.102226	2.004434	-0.559326
H	0.529562	2.576743	0.732300
O	2.895330	-1.187903	-1.706793
H	3.449666	-1.146300	-0.913035
H	2.157136	-0.567878	-1.544830
O	-3.446039	-0.047761	0.490658
H	-2.716684	-0.066476	-0.160599
H	-3.132582	-0.647159	1.181002
O	-0.962567	1.673539	1.677226
H	-0.656505	0.796291	1.395551
H	-1.499677	1.977894	0.928297
O	-1.759044	-1.965465	1.781616
H	-1.302452	-2.217471	2.589543
H	-1.092842	-1.483974	1.233920
O	-1.849301	2.600138	-0.948705
H	-0.949659	2.947908	-0.974270
H	-1.757734	1.676745	-1.247156
O	4.466988	-0.991668	0.700621
H	3.686011	-0.504984	1.038056
H	4.417914	-1.859594	1.112146
O	-2.210245	-2.801595	-0.955206
H	-2.171849	-2.850500	0.008819
H	-1.934550	-1.883932	-1.142370
C	-0.202504	-0.109841	-0.878453

M06_12_s1 Eopt -1181.153173

O	-0.924289	-0.935502	1.377328
O	0.702478	-0.193168	0.061230
O	-0.937125	1.182518	0.665895
O	0.222148	0.296090	-2.614856
H	0.489595	0.167623	-1.681716
H	-0.743644	0.378850	-2.543683
O	-3.690272	-0.716302	1.363733
H	-2.716187	-0.795912	1.389676
H	-3.833822	0.241330	1.364998

O	3.646172	-1.175748	1.292778
H	3.147186	-1.779142	0.719512
H	3.541707	-0.306275	0.873838
O	-1.898004	-2.305589	-0.921756
H	-1.156764	-2.451569	-1.534739
H	-1.488484	-1.990409	-0.097331
O	2.399485	3.956523	-0.038025
H	2.206066	4.170721	0.879503
H	1.555020	3.625365	-0.407480
O	1.300551	-1.636405	2.959902
H	2.074475	-1.397872	2.427200
H	0.534938	-1.458385	2.384853
O	-3.384557	2.145822	1.358361
H	-2.481946	1.797219	1.198626
H	-3.394677	2.407640	2.283687
O	3.032688	1.183194	-0.225079
H	2.954279	2.139166	-0.076553
H	2.120432	0.840699	-0.149130
O	0.349130	-2.571593	-2.658507
H	0.350656	-1.607831	-2.786607
H	0.877859	-2.706653	-1.852643
O	1.613074	-2.647356	-0.131935
H	1.198341	-1.751837	0.010137
H	1.195306	-3.225075	0.515094
O	-2.501819	0.389745	-1.671884
H	-2.412002	-0.554712	-1.449812
H	-2.128501	0.841816	-0.899166
O	0.113656	2.870905	-1.129728
H	-0.240462	2.241204	-0.454344
H	0.354584	2.299252	-1.869915
C	-0.391748	0.021617	0.709389

M06_12_s2			Eopt -1181.152226
O	-0.260647	-0.363209	0.250598
O	0.453110	0.617185	-1.615656
O	-1.676845	0.830940	-0.987869
O	1.485367	-1.931403	-2.025635
H	1.123206	-1.031911	-1.896657
H	0.979608	-2.495468	-1.417584
O	1.901139	0.744351	2.746157
H	0.982207	1.054744	2.696659
H	1.858741	-0.189148	2.480126
O	-2.231595	-2.114550	0.685058
H	-1.526932	-1.433996	0.553386
H	-2.830637	-1.962975	-0.064132
O	0.415594	3.378625	0.390446
H	1.217107	2.834719	0.346687
H	0.096006	3.385621	-0.528057
O	1.757361	-1.745047	1.354093
H	2.577056	-1.675182	0.839034
H	1.109636	-1.198705	0.851171
O	-0.825689	1.509829	2.155320
H	-0.555273	2.271627	1.612820
H	-0.688317	0.755398	1.542868
O	-3.697936	-0.938974	-1.441351
H	-3.533640	-1.320357	-2.308894
H	-2.968872	-0.296146	-1.302213
O	-3.463808	0.256948	1.954418
H	-3.117818	-0.564884	1.575488
H	-2.684718	0.826232	2.035498
O	-0.160352	3.135034	-2.417755
H	-1.119542	3.167041	-2.485420
H	0.040185	2.189333	-2.231660
O	3.798360	-1.161306	-0.596881
H	3.080266	-1.490289	-1.168134
H	3.538265	-0.244834	-0.406389
O	2.533354	1.356898	0.018424
H	1.800928	1.012295	-0.538527
H	2.316207	1.106976	0.933863
O	0.144126	-3.633219	-0.092869

H	-0.729112	-3.252619	0.092424
H	0.734764	-3.178923	0.529574
C	-0.511939	0.365771	-0.792318

M06_12_s3			Eopt -1181.150349
O	-0.450651	-0.271469	0.576061
O	0.476341	0.400841	-1.338564
O	-0.692301	-1.492813	-1.272779
O	2.502122	-1.513791	-2.005182
H	1.832790	-0.810259	-1.936394
H	2.129781	-2.238217	-1.474618
O	-1.530468	-2.480630	1.811407
H	-1.097846	-1.715528	1.379537
H	-2.320260	-2.605509	1.271372
O	0.986151	4.357829	-0.487574
H	1.597208	3.618143	-0.344546
H	0.124282	3.914082	-0.515483
O	1.864825	-1.393476	1.779372
H	2.622425	-1.053140	1.271170
H	1.094718	-0.912785	1.429737
O	-2.774127	1.028330	1.484779
H	-2.051982	0.457138	1.168158
H	-3.379639	1.071138	0.733664
O	0.390245	1.813780	2.146399
H	0.674331	1.358837	2.945758
H	0.068734	1.099680	1.555055
O	-3.218573	-1.794102	-0.471662
H	-2.271730	-1.771496	-0.758053
H	-3.670031	-2.339354	-1.123556
O	-1.219385	2.539503	-0.631296
H	-1.518799	2.306810	0.259074
H	-0.545763	1.867257	-0.851828
O	3.963288	-0.380105	0.141353
H	3.585333	-0.819524	-0.641125
H	3.508137	0.481659	0.155888
O	2.292795	1.861890	0.070603
H	1.635819	1.341427	-0.448892
H	1.870668	1.927039	0.943970
O	1.150669	-3.335882	-0.213543
H	1.436851	-2.811028	0.553483
H	0.372765	-2.850445	-0.542375
O	-3.526705	0.897108	-1.402005
H	-3.372681	-0.025523	-1.136726
H	-2.682333	1.356162	-1.277020
C	-0.226096	-0.457111	-0.685866

M06_15_s1			Eopt -1410.422097
O	0.005440	-0.963851	1.101398
O	1.120357	0.549336	-0.083709
O	-0.568113	-0.552998	-1.018858
O	2.800192	-0.325100	-2.112910
H	2.178790	0.137541	-1.519796
H	2.404751	-1.210455	-2.177451
O	-0.904605	-3.591570	0.524125
H	-0.519616	-2.723095	0.736620
H	-1.691679	-3.350497	0.013452
O	1.261298	3.256963	2.164447
H	1.855830	2.490592	2.222468
H	1.112947	3.375078	1.209016
O	2.300208	-2.629459	0.852877
H	3.062582	-2.052429	0.673061
H	1.589118	-2.021206	1.116757
O	-1.676087	3.262935	-2.010213
H	-2.056275	2.766780	-1.266301
H	-1.177262	2.581367	-2.496646
O	-0.910340	1.453015	2.384547
H	-0.198451	2.115610	2.327032
H	-0.487040	0.610984	2.149768
O	-2.806937	-2.145968	-1.082891
H	-2.028468	-1.555941	-1.010881

H	-3.518703	-1.676387	-0.627955
O	0.840150	3.231825	-0.618230
H	-0.017935	3.426729	-1.027111
H	0.863035	2.257488	-0.551404
O	4.347049	-0.731342	0.265880
H	3.906738	-0.553776	-0.583682
H	3.900771	-0.149588	0.903514
O	2.648176	0.750637	2.044317
H	2.014312	0.623836	1.286642
H	2.351734	0.139309	2.726585
O	1.246501	-2.722150	-1.811462
H	1.597108	-2.814188	-0.907209
H	0.477871	-2.141086	-1.702865
O	-0.040486	1.197192	-3.028460
H	-0.190928	0.559890	-2.292495
H	0.818013	1.589321	-2.836282
C	0.184289	-0.326123	0.000917
O	-4.611738	-0.285655	0.235537
H	-3.970688	0.448978	0.192363
H	-5.281546	-0.020556	0.873175
O	-2.430649	1.409335	0.001093
H	-1.959582	1.506653	0.851810
H	-1.917192	0.738615	-0.481531
O	-2.612076	-1.284239	2.137889
H	-3.298842	-1.015812	1.511579
H	-1.771864	-1.177163	1.659526

M06_15_s2			Eopt -1410.422285
O	0.453597	0.055422	0.690313
O	0.032256	-0.049024	-1.491086
O	-1.622444	-0.319188	-0.021870
O	2.067685	-1.901174	-1.313365
H	1.411172	-1.177610	-1.386121
H	2.163621	-2.066677	-0.358813
O	2.107644	3.029159	1.202092
H	1.195662	2.892043	1.504063
H	2.551325	2.180121	1.362105
O	-0.026750	-1.618431	2.752099
H	0.125278	-0.952849	2.042512
H	-0.598210	-2.271488	2.313892
O	-0.991554	3.182184	-0.888651
H	-0.059758	3.034572	-1.109786
H	-1.466737	2.576240	-1.484441
O	3.107409	0.353864	1.066597
H	3.596593	0.368247	0.228426
H	2.168140	0.248203	0.794408
O	-0.662984	2.304498	1.804098
H	-0.923181	2.661270	0.936034
H	-0.262103	1.444075	1.567116
O	-1.792449	-2.946856	0.985837
H	-1.237346	-3.300792	0.270488
H	-1.882571	-2.009187	0.738384
O	-2.301768	0.246207	3.168674
H	-1.593419	-0.410932	3.095554
H	-1.973390	1.002768	2.661977
O	-2.080185	1.248443	-2.690608
H	-2.849266	0.956725	-2.188079
H	-1.346198	0.694226	-2.349879
O	3.926535	0.269111	-1.697849
H	3.409564	-0.552925	-1.663896
H	3.252941	0.966753	-1.764275
O	1.728397	2.127901	-1.500752
H	1.169260	1.323160	-1.460360
H	1.890968	2.385241	-0.576476
O	2.510507	-2.407770	1.493845
H	1.671979	-2.295875	1.969189
H	2.903316	-1.519417	1.503613
C	-0.383472	-0.106568	-0.273839
O	-3.529929	1.688738	0.213721
H	-2.796268	1.049075	0.152315

H	-3.105801	2.549994	0.150270
O	-2.549433	-1.833060	-2.082347
H	-2.264336	-1.213246	-1.373185
H	-2.431936	-1.338609	-2.899817
O	-0.359355	-3.512907	-1.419155
H	0.472577	-3.013984	-1.421571
H	-1.028448	-2.906637	-1.783355

M06_15_s3			Eopt -1410.422093
O	0.584543	0.352233	1.254301
O	-0.675168	0.053778	-0.557643
O	1.519991	-0.268231	-0.673461
O	-0.090214	1.954355	-2.573758
H	-0.350615	1.187331	-2.033418
H	0.760184	2.223018	-2.187772
O	3.157927	1.060378	1.967358
H	2.258690	0.785934	1.698987
H	3.725180	0.723040	1.259823
O	-4.369925	-0.833724	0.102866
H	-3.923442	0.021044	0.245065
H	-3.837159	-1.448019	0.625079
O	0.494787	3.194565	1.073632
H	-0.231626	3.391425	0.455065
H	0.431276	2.239274	1.240856
O	0.519100	-2.155173	2.542447
H	0.622592	-1.235092	2.242036
H	1.060880	-2.651989	1.912711
O	-1.538913	0.826654	2.947029
H	-1.246525	1.609400	3.424749
H	-0.805870	0.625811	2.328494
O	2.071812	-2.868890	0.223348
H	1.978494	-1.961210	-0.121873
H	2.865208	-3.227519	-0.186544
O	-1.907770	-1.961566	1.059489
H	-1.182539	-2.114459	1.690948
H	-1.612742	-1.186685	0.549397
O	-1.563471	3.656623	-0.826088
H	-1.104501	3.132547	-1.506597
H	-2.120867	3.006471	-0.365054
O	-2.757009	1.449448	0.471284
H	-1.989928	0.963127	0.089580
H	-2.567175	1.420868	1.424006
O	2.301852	2.502573	-1.034753
H	1.775355	2.847191	-0.291712
H	2.269436	1.541355	-0.909581
O	-0.463387	-3.581177	-0.834618
H	0.418251	-3.449056	-0.446291
H	-1.056882	-3.069897	-0.260409
C	0.475935	0.043455	0.009774
O	-2.569864	-1.333309	-2.126095
H	-1.750343	-0.969722	-1.756300
H	-3.226458	-1.186539	-1.426661
O	0.559104	-1.760220	-2.827875
H	0.909978	-1.145921	-2.155724
H	0.075487	-2.409296	-2.292720
O	4.305818	-0.192487	-0.396089
H	4.551558	0.550198	-0.957200
H	3.340161	-0.267954	-0.499425

M06_Radical_3_s1			Eopt -493.14955
O	-2.997331	-0.983208	-0.206606
O	-0.847783	-1.248260	-0.034225
O	-1.792204	0.803473	0.087135
O	0.484505	2.395467	-0.183766
H	0.732891	2.427552	-1.112625
H	-0.322708	1.849747	-0.156209
O	1.526420	-0.021340	0.881909
H	0.730932	-0.501969	0.592918
H	1.368559	0.881334	0.559696
O	3.735797	-0.968797	-0.517459

H	4.380933	-1.222282	0.148263
H	2.965664	-0.647358	-0.011855
C	-1.788584	-0.434283	-0.039349

M06_Radical_3_s2 Eopt -493.149309

C	1.318013	-0.243532	-0.010927
O	1.078268	-0.931270	-1.007759
O	1.185491	-0.605307	1.215446
O	1.727987	0.973737	-0.009293
O	-1.001728	1.644908	-1.064846
H	-0.052009	1.725752	-0.905790
H	-1.106106	0.763821	-1.444212
O	-1.707356	-1.563198	-0.559354
H	-1.799994	-0.950054	0.185479
H	-0.768814	-1.497315	-0.790485
O	-1.546364	0.507512	1.501889
H	-1.403576	1.049287	0.707556
H	-0.667970	0.158652	1.704348

M06_Radical_3_s3 Eopt -493.150619

C	-2.325103	0.153042	-0.118029
O	-1.789621	1.166988	0.459234
O	-3.432261	0.549475	-0.631790
O	-1.860216	-0.992776	-0.168975
O	0.580128	-0.940164	1.168679
H	-0.279723	-0.970023	0.705952
H	0.613844	-0.060109	1.557622
O	2.479113	-0.889196	-0.845905
H	1.813741	-0.939427	-0.131453
H	2.983708	-1.705378	-0.778647
O	4.196574	1.148303	0.017533
H	3.838704	1.964413	-0.342638
H	3.590601	0.451242	-0.292868

M06_Radical_6_s1 Eopt -722.410698

O	1.372293	0.141718	1.834385
O	0.515732	-1.576755	0.658689
O	-0.659522	0.157323	1.484937
O	-0.599114	2.799734	0.225796
O	1.935274	1.425663	-0.769378
O	2.692446	-1.258306	-1.126533
H	1.828129	1.420915	0.190230
H	0.109204	2.787558	-0.426598
H	3.533360	-1.419174	-0.687031
H	2.014551	-1.491653	-0.469748
H	2.317650	0.548445	-0.958429
H	-0.597878	1.902484	0.588994
O	-0.469741	0.315123	-1.897255
O	-2.961289	0.456407	-0.432931
O	-2.087262	-2.203460	-0.234831
H	-2.698622	0.909320	0.374915
H	-1.168632	-2.015968	0.030209
H	-1.249879	0.494798	-1.350060
H	-2.036669	-2.402276	-1.175478
H	-2.732297	-0.478719	-0.275260
H	0.274302	0.737698	-1.440106
C	0.416041	-0.508835	1.275888

M06_Radical_6_s2 Eopt -722.410351

O	0.041647	-1.579437	1.272755
O	0.267765	-0.444072	-0.621115
O	0.288937	0.516950	1.391960
O	-2.097300	2.392998	-0.135914
O	-2.970561	-0.168714	0.750400
O	-2.088762	-1.876574	-1.335325
H	-2.484022	-0.439704	1.534619
H	-2.306375	1.491081	0.163171
H	-2.015474	-2.764553	-0.973146
H	-1.199626	-1.496640	-1.234798
H	-2.721202	-0.813822	0.062081

H	-1.200811	2.346864	-0.506554
O	0.560876	2.297617	-1.254332
O	3.215036	0.760442	0.862946
O	2.917203	-1.552925	-0.814134
H	2.301452	0.881903	1.151753
H	1.987383	-1.310421	-0.948169
H	0.490102	2.427628	-2.204235
H	2.884811	-2.298944	-0.207472
H	3.183958	-0.037432	0.306987
H	0.561044	1.332161	-1.128290
C	0.197848	-0.491613	0.624606

M06_Radical_6_s3 Eopt -722.408678

O	-0.118906	-0.104462	0.823494
O	0.440661	0.579399	-1.242876
O	0.020203	-1.550125	-0.648082
O	3.015828	-1.843418	-0.610066
O	2.779729	-0.017554	1.554876
O	2.346589	2.270099	-0.038973
H	1.857177	-0.242987	1.726489
H	2.985647	-1.222202	0.138334
H	1.935849	2.920404	0.539149
H	1.606027	1.809010	-0.469282
H	2.718565	0.810762	1.044880
H	2.087470	-2.025203	-0.796468
O	-3.115918	-0.213931	1.961873
O	-2.948058	-1.015168	-0.766678
O	-2.234129	1.728460	-1.015844
H	-2.099028	-1.472428	-0.817997
H	-1.291615	1.569533	-1.174080
H	-3.051584	-0.539691	1.047772
H	-2.299079	1.848808	-0.062016
H	-2.743644	-0.089493	-0.988579
H	-4.052090	-0.268617	2.174378
C	0.143053	-0.294048	-0.417394

M06_Radical_9_s1 Eopt -951.671588

O	-0.725374	-1.300168	0.230504
O	-0.920447	-0.077027	-1.425935
O	-0.852367	0.917666	0.587031
O	0.825028	2.862913	-0.542182
H	0.098051	2.312967	-0.205899
H	0.482028	3.274461	-1.341714
O	-3.849100	0.663436	-1.227011
H	-2.947313	0.589049	-1.563295
H	-3.742859	0.955012	-0.308654
O	1.615362	-1.981784	-1.534004
H	1.775200	-1.018146	-1.555530
H	0.683149	-2.062777	-1.301259
O	2.542351	-1.787565	1.165743
H	2.211094	-1.952671	0.266427
H	2.088202	-0.974887	1.451306
O	-3.513544	0.717053	1.709550
H	-2.572171	0.882434	1.556498
H	-3.623309	-0.217655	1.476119
O	1.670554	0.795664	1.896611
H	2.243486	1.252741	1.270598
H	0.777291	0.894688	1.530399
O	-3.652356	-1.824605	0.263991
H	-3.796763	-1.147945	-0.416124
H	-2.691566	-1.919460	0.298990
O	2.387104	0.679804	-1.429187
H	1.849141	1.424890	-1.108350
H	3.125636	0.591926	-0.801697
O	4.456428	0.142253	0.430999
H	3.949116	-0.641833	0.709240
H	5.196765	-0.200326	-0.079438
C	-0.829051	-0.083929	-0.147747

M06_Radical_9_s2 Eopt -951.673428

O	0.391657	0.223565	-2.020253
O	1.931752	1.323287	-0.948955
O	1.817093	-0.928347	-0.842863
O	3.870586	-1.744756	0.959005
H	3.238182	-1.530556	0.254593
H	3.324796	-2.079727	1.678129
O	-0.203620	3.155874	-0.884307
H	0.626631	2.657625	-0.971532
H	-0.002764	3.878068	-0.280807
O	3.778183	1.124436	1.242171
H	3.896937	0.164084	1.297867
H	3.145535	1.232198	0.515125
O	-2.342030	-0.960946	-0.972859
H	-2.281044	-0.672627	-1.889393
H	-1.640716	-1.636611	-0.860166
O	0.810475	-0.445845	1.942173
H	1.350374	-0.760230	1.207306
H	0.121955	0.092895	1.512026
O	-0.302762	-2.737775	-0.508607
H	-0.267115	-3.375741	-1.228543
H	0.457660	-2.147477	-0.655645
O	-1.219566	1.020224	0.664754
H	-0.900038	1.775639	0.139010
H	-1.547412	0.368996	0.016941
O	-4.868513	-1.058829	0.215098
H	-4.003686	-1.135404	-0.225870
H	-4.892361	-1.784732	0.845959
C	1.454177	0.206854	-1.213916
O	-3.921129	1.273610	1.586385
H	-2.990130	1.269724	1.312937
H	-4.298885	0.486771	1.161610

M06_Radical_9_s3 Eopt -951.673748

O	0.506572	0.227917	-1.840744
O	1.724901	1.140268	-0.443852
O	1.637348	-1.108975	-0.430583
O	3.986440	-0.956852	1.154728
H	3.175135	-1.055371	0.627735
H	3.708885	-0.457757	1.929859
O	-0.463975	3.038300	-0.282726
H	0.367426	2.563693	-0.426501
H	-0.246984	3.736640	0.343192
O	4.663954	1.018963	-0.797458
H	4.577250	0.355002	-0.094297
H	3.755140	1.314171	-0.928744
O	-2.030306	-0.997844	-0.926820
H	-1.434123	-0.563578	-1.550141
H	-1.537169	-1.782334	-0.615288
O	0.714246	-0.532241	2.345662
H	1.139638	-0.924970	1.573692
H	-0.023753	-0.022880	1.965761
O	-0.384343	-3.015669	0.021350
H	-0.329720	-3.730375	-0.621069
H	0.378723	-2.443929	-0.169895
O	-1.455382	0.814546	1.148974
H	-1.137752	1.611584	0.687063
H	-1.638173	0.170252	0.439602
O	-4.802996	-0.623765	-0.934215
H	-3.855478	-0.840391	-0.982425
H	-5.218050	-1.400387	-0.547001
C	1.314549	0.006974	-0.864638
O	-4.307191	1.206152	1.210511
H	-3.340811	1.144727	1.266627
H	-4.541613	0.597650	0.491040

M06_Radical_12_sl Eopt -1180.936611

O	-0.319105	-0.040367	0.214754
O	1.178513	-1.005930	-1.040098
O	-0.133414	0.647352	-1.831210
O	-1.634423	-2.172306	-2.281747

H	-0.854066	-1.831315	-2.731699
H	-2.174720	-1.389124	-2.090982
O	-1.938924	0.831657	2.721492
H	-0.995297	0.687181	2.597586
H	-2.190629	1.458610	2.014636
O	4.037771	-0.827930	0.713042
H	3.681107	-1.711458	0.569145
H	3.905817	-0.359470	-0.131609
O	-3.083836	-1.181173	1.063513
H	-2.406204	-1.860165	0.887514
H	-2.665617	-0.556969	1.681652
O	2.259101	2.469240	0.138202
H	2.127204	1.840387	0.869410
H	1.368177	2.763353	-0.111397
O	1.974756	0.443945	2.102401
H	2.676881	-0.067893	1.655153
H	1.150268	0.108622	1.730490
O	-2.814627	2.460848	0.650969
H	-3.134718	1.797783	0.023430
H	-2.000899	2.799493	0.236773
O	3.452364	0.676523	-1.627995
H	3.015921	1.357513	-1.079096
H	2.741213	0.050711	-1.821397
O	-1.216402	-3.145138	0.332350
H	-1.199258	-2.812143	-0.582393
H	-0.331254	-2.977461	0.693207
O	1.481706	-2.650833	1.206492
H	1.468390	-1.976532	0.504041
H	1.593861	-2.157551	2.025682
O	-3.018615	0.232581	-1.332691
H	-2.996009	-0.256612	-0.483774
H	-2.123084	0.580526	-1.457051
O	-0.411909	3.155438	-0.630005
H	-0.406851	2.339104	-1.161575
H	-0.480722	3.877778	-1.263156
C	0.287806	-0.142603	-0.961724

M06_Radical_12_s2 Eopt -1180.935206

O	-0.008617	0.287994	0.427525
O	0.273661	-0.258386	-1.738486
O	1.633094	1.122243	-0.749908
O	-2.574618	0.310000	-1.608915
H	-1.659989	-0.011836	-1.623364
H	-2.695447	0.733656	-0.738666
O	0.164796	-2.507224	2.291589
H	0.868291	-1.847267	2.376712
H	-0.660397	-2.003453	2.370439
O	-0.350932	3.031956	0.985622
H	-0.196012	2.083225	1.109479
H	-0.471016	3.098731	0.020805
O	2.687472	-1.949204	-0.083206
H	1.843619	-2.407663	-0.191319
H	2.858597	-1.551390	-0.954451
O	-2.165684	-0.905661	1.710539
H	-2.652753	-1.482221	1.098207
H	-1.443414	-0.552603	1.161407
O	2.161730	-0.267539	2.120344
H	2.495762	-0.787098	1.365403
H	1.324226	0.080129	1.776082
O	-0.942953	2.848954	-1.785517
H	-1.554858	2.102072	-1.856709
H	-0.159113	2.570569	-2.271156
O	2.573438	2.663855	1.684779
H	1.679044	2.875691	1.383719
H	2.577271	1.701275	1.785694
O	2.912516	-0.873599	-2.723410
H	3.377026	-0.034938	-2.632554
H	1.976430	-0.640431	-2.625394
O	-3.097680	-2.366702	-0.570288
H	-3.069272	-1.500516	-1.007165

H	-2.176139	-2.673600	-0.598979
O	-0.248116	-2.849358	-0.498971
H	-0.168609	-1.991281	-0.943441
H	-0.145403	-2.665098	0.452882
O	-3.043050	1.685856	0.827483
H	-2.258878	2.239978	0.950817
H	-2.867773	0.886617	1.349301
C	0.563059	0.331995	-0.678530

M06_Radical_12_s3 Eopt -1180.938357

O	-0.517886	-0.262496	1.169234
O	0.428635	-0.310459	-0.873261
O	1.530653	-0.457045	1.086288
O	-1.195956	1.922678	-1.533267
H	-0.773875	1.058613	-1.387802
H	-1.434034	2.223990	-0.633253
O	1.039280	2.472311	1.628591
H	1.349655	1.572455	1.788964
H	1.233652	2.631261	0.688106
O	0.209404	-3.369945	0.284730
H	-0.532290	-3.081950	-0.261516
H	0.994664	-3.106824	-0.223839
O	-3.576482	0.435357	1.039771
H	-3.663054	0.451231	0.070480
H	-3.268565	-0.458476	1.245984
O	4.341749	-1.277408	0.234157
H	3.963057	-1.511287	1.087956
H	4.074865	-0.349236	0.096915
O	-2.510065	-2.218017	1.528241
H	-2.598302	-3.175053	1.584942
H	-1.566400	-2.030824	1.622374
O	1.462772	2.806176	-1.170996
H	0.541264	2.617667	-1.423036
H	1.614745	3.732077	-1.385427
O	2.327160	-2.382878	-1.401265
H	3.061567	-2.070541	-0.842380
H	1.738368	-1.614364	-1.450034
O	-3.633203	0.444357	-1.817993
H	-2.897683	1.077855	-1.852830
H	-3.181184	-0.415767	-1.776891
O	-2.008041	-1.831739	-1.280542
H	-1.229324	-1.252519	-1.242106
H	-2.312462	-1.895706	-0.359626
O	-1.766336	2.591978	1.118107
H	-2.273790	1.769623	1.238152
H	-0.858466	2.405485	1.412358
O	3.708712	1.443386	-0.073609
H	3.522723	1.669344	0.844441
H	2.928181	1.758638	-0.556244
C	0.473918	-0.342623	0.368139

M06_Radical_15_s1 Eopt -1410.197262

O	-0.483871	-0.786961	0.476473
O	0.977740	0.685628	-0.102062
O	-0.560242	-0.038657	-1.585184
O	2.908275	-0.077435	-2.141722
H	2.319073	0.582949	-1.754794
H	2.387786	-0.900904	-2.091900
O	-0.641290	-3.908525	0.591762
H	0.254806	-3.557705	0.665857
H	-1.077721	-3.368030	-0.092792
O	0.631418	3.008586	2.504047
H	1.272359	2.285636	2.591476
H	0.716465	3.300560	1.578321
O	1.932583	-2.453181	1.104134
H	2.732536	-1.932710	0.890722
H	1.329010	-1.810975	1.495903
O	-1.515967	3.765785	-1.855836
H	-2.062406	3.117501	-1.383605
H	-0.950795	3.224575	-2.434448

O	-1.673422	1.506735	2.013848
H	-0.849027	2.000579	2.191581
H	-1.407434	0.582259	1.942791
O	-2.225608	-2.407437	-1.200717
H	-1.697501	-1.670954	-1.542426
H	-2.798576	-1.983137	-0.537698
O	0.838914	3.522838	-0.255304
H	0.005915	3.744931	-0.704789
H	0.917664	2.562326	-0.367582
O	4.031917	-0.733974	0.427709
H	3.698448	-0.450358	-0.441555
H	3.658207	-0.103490	1.061620
O	2.306903	0.660961	2.331091
H	1.715009	0.517329	1.570892
H	2.111840	-0.053111	2.947434
O	1.465615	-2.460301	-1.720495
H	1.543125	-2.472964	-0.750810
H	0.531375	-2.305278	-1.899037
O	0.391214	2.109274	-3.167335
H	0.135145	1.326175	-2.649744
H	1.154842	2.467439	-2.701305
C	0.004984	0.002414	-0.477036
O	-3.701141	-0.875721	0.681443
H	-3.547183	-0.009243	0.266675
H	-4.655511	-1.000373	0.690313
O	-2.796508	1.546322	-0.519108
H	-2.336271	1.658677	0.337748
H	-2.192776	1.010837	-1.055573
O	-2.093812	-2.361347	2.536901
H	-2.614147	-1.793792	1.948618
H	-1.557842	-2.902737	1.934503

M06_Radical_15_s2 Eopt -1410.193559

O	-0.471372	0.048530	0.560889
O	0.062558	-0.007083	-1.623730
O	1.600021	0.196039	-0.086533
O	-2.279436	1.737502	-1.410245
H	-1.663371	0.996504	-1.509861
H	-2.306637	1.927443	-0.454244
O	-2.067664	-2.957203	1.242504
H	-1.175859	-2.821588	1.596798
H	-2.544047	-2.137149	1.449627
O	0.059072	1.830073	2.668351
H	-0.134345	1.109809	2.046211
H	0.655715	2.405471	2.154011
O	0.962686	-3.067527	-0.669288
H	0.069786	-2.964298	-1.026403
H	1.528767	-2.540962	-1.259455
O	-3.177641	-0.311844	1.198437
H	-3.730361	-0.384678	0.402339
H	-2.280564	-0.190263	0.842744
O	0.681078	-2.153142	1.975222
H	0.905703	-2.484448	1.084319
H	0.230372	-1.316166	1.787841
O	1.851132	3.098235	0.930486
H	1.240791	3.148481	0.170155
H	2.330820	2.272892	0.795769
O	2.484229	0.058090	2.813160
H	1.726821	0.654182	2.899531
H	2.096248	-0.780188	2.523369
O	2.407460	-1.402054	-2.530013
H	3.066466	-0.950557	-1.990121
H	1.615526	-0.847435	-2.452328
O	-4.186303	-0.460007	-1.478108
H	-3.703858	0.376422	-1.572532
H	-3.495643	-1.135996	-1.579900
O	-1.867633	-2.187144	-1.472690
H	-1.330076	-1.382783	-1.534513
H	-1.930180	-2.393324	-0.520847
O	-2.508495	2.496414	1.340786

H	-1.667018	2.448049	1.819812
H	-2.929729	1.640837	1.515321
C	0.310929	0.072832	-0.408235
O	3.591939	-2.013011	0.490150
H	2.873468	-1.381901	0.356549
H	3.160887	-2.871813	0.431681
O	2.595739	1.974848	-2.319166
H	2.784836	1.537647	-1.480573
H	2.450360	1.252180	-2.939405
O	0.257480	3.233164	-1.358247
H	-0.584198	2.760861	-1.440023
H	0.914949	2.704736	-1.842198

M06_Radical_15_s3 Eopt -1410.194984

O	0.686566	-0.204047	1.192935
O	-0.620200	0.228371	-0.596372
O	1.449229	-0.368878	-0.844263
O	0.462574	2.335463	-2.299591
H	0.008770	1.539163	-1.989036
H	1.327450	2.306546	-1.850280
O	3.587816	0.075858	1.545760
H	2.621887	0.053535	1.512850
H	3.864614	-0.231595	0.666450
O	-4.848098	-0.475996	0.257800
H	-4.428209	0.397821	0.310727
H	-4.229348	-1.043049	0.740975
O	1.236035	2.722497	1.433341
H	0.436613	3.008435	0.948952
H	1.079128	1.794501	1.647792
O	-0.289060	-2.383256	2.778715
H	0.149913	-1.616491	2.380975
H	-0.006424	-3.124304	2.230438
O	-1.510841	1.148229	2.495272
H	-1.077192	1.998122	2.635912
H	-0.813052	0.583197	2.125539
O	2.093201	-2.921408	0.635292
H	1.995229	-2.086320	1.109460
H	2.624858	-2.690413	-0.135314
O	-2.364230	-1.615146	1.004816
H	-1.803334	-1.848044	1.764885
H	-2.009800	-0.774241	0.681150
O	-0.873468	3.642260	-0.144006
H	-0.456557	3.293023	-0.951376
H	-1.664366	3.094426	-0.019738
O	-3.035738	1.734507	0.224571
H	-2.582533	1.227408	-0.461743
H	-2.560058	1.490139	1.043785
O	2.883538	2.328530	-0.815523
H	2.383836	2.447328	0.014898
H	3.144247	1.400073	-0.812030
O	-0.451535	-2.988206	-0.687648
H	0.374647	-2.949903	-0.175532
H	-1.126809	-2.557527	-0.138601
C	0.434919	-0.100711	-0.029171
O	-2.993746	-0.896098	-2.003548
H	-2.114755	-0.754223	-1.629412
H	-3.606306	-0.782489	-1.260700
O	-0.073095	-1.589927	-3.111521
H	-0.123902	-0.650425	-2.907646
H	-0.200849	-2.026946	-2.249393
O	4.381544	-0.819416	-1.043352
H	4.857930	-0.110094	-1.488298
H	3.549617	-0.895379	-1.523612

M062X_3_s1 Eopt -493.384164

O	2.714854	0.227386	-0.119659
O	0.669920	0.908169	0.459242
O	0.974779	-1.138487	-0.396480
O	-1.605649	-1.344419	-0.871398
H	-1.862884	-0.427416	-1.041475

H	-0.630740	-1.262226	-0.670571
O	-1.329390	-0.291402	1.841300
H	-0.575302	0.147016	1.382117
H	-1.712930	-0.826939	1.134283
O	-1.558255	1.561952	-0.914507
H	-0.731959	1.310416	-0.435345
H	-2.206737	1.699883	-0.217247
C	1.465079	-0.004386	-0.023292

M062X_3_s2 Eopt -493.388048

C	-0.001557	-0.000060	0.060680
O	-0.395487	-1.233254	0.046500
O	-0.872698	0.957051	0.097460
O	1.262772	0.276150	0.037678
O	2.961781	-1.760499	-0.050678
H	2.274381	-1.033914	-0.018126
H	2.455472	-2.579132	-0.050141
O	-3.007409	-1.676072	-0.077838
H	-3.458846	-0.828471	-0.013191
H	-2.033427	-1.451121	-0.027345
O	0.051234	3.438107	-0.067398
H	1.010541	3.398568	-0.134009
H	-0.240324	2.482564	-0.007062

M062X_3_s3 Eopt -493.381905

C	-2.379550	0.221067	-0.132247
O	-2.008509	1.163412	0.668105
O	-3.516343	0.271333	-0.740423
O	-1.592117	-0.806759	-0.333422
O	0.546338	-0.943750	1.117823
H	-0.300226	-0.835135	0.562649
H	0.621503	-0.127479	1.623506
O	2.775618	-1.105637	-0.447621
H	1.943607	-1.036334	0.080755
H	2.489868	-1.165370	-1.365843
O	4.104090	1.335369	-0.201887
H	3.445678	2.029314	-0.312887
H	3.604260	0.496861	-0.295296

M062X_6_s1 Eopt -722.663588

O	1.150557	0.177126	-1.826540
O	-0.570756	1.070324	-0.726516
O	-0.629064	-1.075671	-1.345639
O	1.295453	-2.591704	0.010966
O	2.558109	0.158421	0.507620
O	1.143257	2.628441	0.648168
H	2.157793	0.113944	-0.387764
H	1.837228	-1.892641	0.394811
H	1.561922	3.243104	0.037478
H	0.534591	2.084664	0.090972
H	2.340074	1.066152	0.773727
H	0.624408	-2.111441	-0.511970
O	0.227968	-0.292045	2.251555
O	-2.002245	-1.415693	0.905756
O	-3.102138	1.106855	0.079128
H	-1.519369	-1.318118	0.044643
H	-2.176019	1.053339	-0.273104
H	-0.527496	-0.679174	1.775114
H	-3.664177	0.795395	-0.635969
H	-2.583897	-0.641494	0.903979
H	0.929485	-0.200119	1.590190
C	-0.013946	0.059659	-1.306348

M062X_6_s2 Eopt -722.667565

O	0.655477	1.286227	-0.129355
O	-1.485875	0.698779	-0.234803
O	0.075357	-0.859146	0.093414
O	2.145791	-0.965012	1.913239
O	3.258492	0.898202	0.034694
O	-1.754586	3.365611	-0.272347

H	2.275126	1.047760	-0.026612
H	2.785559	-0.358073	1.518918
H	-0.861298	3.719872	-0.257872
H	-1.629229	2.384984	-0.264561
H	3.666939	1.758120	-0.098535
H	1.397300	-0.940291	1.281999
O	-1.826985	-2.606904	-0.763113
O	-3.485147	-0.785477	0.732837
H	-1.118610	-1.987052	-0.480797
H	-2.708808	-0.260511	0.415494
H	-3.257312	-1.056436	1.626737
H	-2.610527	-2.227003	-0.342064
C	-0.246087	0.381666	-0.090501
O	2.308797	-1.346424	-1.467972
H	1.502235	-1.203473	-0.932702
H	2.904571	-0.654745	-1.149738

M062X_6_s3			Eopt -722.663791
O	0.918676	0.298710	-1.783752
O	-1.165094	0.592445	-1.052060
O	-0.252574	-1.441628	-1.011441
O	2.105646	-2.169550	0.171462
O	2.728524	0.660170	0.262014
O	-0.114666	2.796850	-0.014580
H	2.150136	0.581885	-0.524395
H	2.510820	-1.300458	0.306399
H	-0.841271	3.366189	0.255329
H	-0.540268	2.029966	-0.478849
H	2.089244	0.750376	0.988959
H	1.277094	-1.956048	-0.308829
O	0.518643	0.941065	2.037331
O	-1.036421	-1.379656	1.588664
O	-3.300658	-0.511381	0.084911
H	-0.740355	-1.482013	0.655179
H	-2.508337	-0.109666	-0.359873
H	-0.040334	0.160884	1.865035
H	-3.926553	0.210888	0.188673
H	-1.944178	-1.061889	1.479417
H	0.227993	1.615676	1.398619
C	-0.155098	-0.183667	-1.287677

M062X_9_s1			Eopt -951.939512
O	0.952024	1.719002	-0.978529
O	0.993813	-0.407715	-1.657753
O	0.042845	0.125496	0.283313
O	-0.463990	-2.340049	1.038181
H	-0.169492	-1.455257	0.695626
H	0.139111	-2.982235	0.651061
O	2.702614	-1.838856	0.012360
H	2.052090	-1.459968	-0.610708
H	2.523340	-1.377606	0.844527
O	-1.241678	-1.911629	-1.820745
H	-1.344477	-2.269962	-0.929735
H	-0.384499	-1.426318	-1.774212
O	-1.528469	2.788430	-0.403897
H	-0.609824	2.487052	-0.566649
H	-1.715193	2.496634	0.500722
O	2.173961	0.223240	2.099531
H	1.338850	0.237447	1.597175
H	2.796130	0.664110	1.501957
O	-1.625267	1.283839	2.091378
H	-2.298252	0.594887	1.983869
H	-0.910847	0.962670	1.503930
O	3.669702	1.065546	-0.290551
H	3.594247	0.109783	-0.417614
H	2.822147	1.417149	-0.613984
O	-3.086806	-1.046188	1.134467
H	-2.290264	-1.596205	1.123585
H	-3.047949	-0.545993	0.299417
O	-2.832707	0.385443	-1.307492

H	-2.306751	1.164170	-1.056794
H	-2.196972	-0.305193	-1.566200
C	0.660045	0.485393	-0.794680

M062X_9_s2			Eopt -951.940025
O	-1.428614	0.067034	-1.495756
O	0.580738	1.027289	-1.451329
O	0.134075	-0.683463	-0.091523
O	2.109158	-0.096373	1.597389
H	1.401894	-0.314154	0.940952
H	2.220465	0.857665	1.481318
O	1.421836	2.569082	0.677326
H	1.229425	2.035711	-0.121711
H	0.661187	2.367217	1.244339
O	3.137020	0.065188	-1.789473
H	3.425028	-0.506042	-1.061934
H	2.243379	0.381225	-1.548579
O	-3.281520	-0.435691	0.581858
H	-2.657851	-0.233755	-0.141636
H	-2.754134	-0.992527	1.174191
O	-0.958078	1.406790	1.848448
H	-0.640162	0.576203	1.464671
H	-1.501952	1.796671	1.140467
O	-1.231588	-2.106290	1.755546
H	-1.467002	-2.982671	1.435836
H	-0.774098	-1.669772	1.002569
O	-2.239245	2.542548	-0.461571
H	-1.516881	3.152741	-0.643110
H	-2.011618	1.734540	-0.960203
O	4.028551	-1.631107	0.388453
H	3.382247	-1.112020	0.911225
H	3.628466	-2.502678	0.294872
O	-2.144466	-2.616795	-1.369330
H	-2.651924	-2.589520	-0.549249
H	-1.856292	-1.688912	-1.484620
C	-0.230518	0.137394	-1.016616

M062X_9_s3			Eopt -951.941534
O	-1.391851	-0.155321	-1.373235
O	0.730448	0.506644	-1.502413
O	0.042697	-0.672629	0.258664
O	2.216781	0.362830	1.463380
H	1.456959	-0.049425	0.984821
H	2.230114	1.270611	1.132756
O	1.191969	2.764938	0.049451
H	1.102360	2.004518	-0.558885
H	0.529528	2.576682	0.732731
O	2.895695	-1.187404	-1.706616
H	3.449865	-1.145996	-0.912732
H	2.157427	-0.567475	-1.544625
O	-3.446089	-0.047792	0.490190
H	-2.716648	-0.066439	-0.160973
H	-3.132735	-0.647282	1.180501
O	-0.962764	1.673339	1.677301
H	-0.656666	0.796119	1.395577
H	-1.499735	1.977791	0.928311
O	-1.759267	-1.965697	1.781092
H	-1.302715	-2.217994	2.588950
H	-1.092998	-1.484135	1.233540
O	-1.849163	2.600250	-0.948615
H	-0.949535	2.948063	-0.974082
H	-1.757540	1.676903	-1.247190
O	4.466738	-0.991996	0.701206
H	3.685772	-0.505300	1.038648
H	4.417507	-1.860013	1.112519
O	-2.210215	-2.801432	-0.955886
H	-2.171937	-2.850430	0.008139
H	-1.934474	-1.883758	-1.142929
C	-0.202398	-0.109712	-0.878538

M062X_12_s1 Eopt -1181.219567

O	0.332772	-0.491408	1.369166
O	0.390483	0.456905	-0.655163
O	-1.248860	-0.975868	-0.144039
O	1.231025	-1.118255	-2.795434
H	0.903587	-0.488340	-2.117183
H	0.696940	-1.914849	-2.620686
O	-0.824256	-2.145422	3.237675
H	-0.394920	-1.559249	2.572854
H	-1.665808	-2.368188	2.805103
O	1.419175	3.776223	0.772868
H	2.039024	3.083914	0.478048
H	0.642066	3.642466	0.193678
O	2.637730	-2.134429	1.071528
H	3.031768	-1.827733	0.234333
H	1.854516	-1.563574	1.193597
O	-3.419824	2.737649	-0.761192
H	-3.654074	2.643587	0.168727
H	-3.332024	1.817928	-1.098978
O	0.545451	1.907801	2.803930
H	0.825613	2.585248	2.162232
H	0.497667	1.080517	2.281855
O	-3.007968	-2.413161	1.377623
H	-2.370924	-1.863713	0.860753
H	-3.706790	-1.805683	1.642733
O	-0.611575	3.028353	-1.039749
H	-1.574439	3.015256	-0.876287
H	-0.328544	2.095680	-0.934461
O	3.701733	-1.047845	-1.390400
H	2.897723	-1.179887	-1.931923
H	3.565750	-0.167247	-0.994901
O	2.849901	1.393983	-0.065637
H	1.935753	1.030244	-0.220164
H	3.082617	1.096204	0.821849
O	-0.667765	-3.079033	-1.897445
H	-0.237908	-3.773192	-1.385831
H	-0.890787	-2.381679	-1.243600
O	-3.049448	0.190104	-1.792139
H	-2.328477	-0.212287	-1.245029
H	-2.657481	0.340939	-2.659366
C	-0.176573	-0.335191	0.196651

M062X_12_s2 Eopt -1181.214757

O	-0.757504	0.178827	0.131728
O	1.249739	0.991054	-0.430862
O	-0.549897	2.310036	-0.539842
O	1.825892	0.387743	-3.069841
H	1.596170	0.665088	-2.153864
H	1.003820	0.462935	-3.567162
O	0.690076	-2.878404	1.745574
H	0.232878	-2.162581	2.226017
H	0.272930	-2.860395	0.862435
O	-3.437972	0.221481	-0.130581
H	-2.449240	0.224345	-0.030269
H	-3.613801	1.119311	-0.467613
O	4.248761	0.796316	1.874364
H	3.746836	0.049210	1.498741
H	3.859511	1.576942	1.436492
O	-0.439634	-2.359312	-0.846726
H	0.383726	-2.394016	-1.371845
H	-0.487194	-1.427877	-0.522022
O	-0.737368	-0.606251	2.747263
H	-0.212266	-0.014180	3.297542
H	-0.670590	-0.245562	1.830538
O	-3.143143	2.919907	-0.979109
H	-3.234857	2.976474	-1.936275
H	-2.196462	2.667495	-0.822888
O	-3.574766	-0.011196	2.720272
H	-3.644182	0.109391	1.754235
H	-2.631570	-0.210406	2.856734

O	2.961290	2.909880	0.426995
H	2.502435	3.489248	1.044810
H	2.271206	2.282541	0.095414
O	2.148398	-2.263101	-2.085689
H	2.034377	-1.409552	-2.548550
H	2.447677	-1.994348	-1.195525
O	2.643004	-1.150484	0.519234
H	2.062447	-0.410117	0.209191
H	2.052152	-1.738349	1.027672
O	-3.085118	-1.993763	-1.930957
H	-3.310024	-1.216708	-1.386464
H	-2.172510	-2.205565	-1.663021
C	-0.029588	1.174137	-0.281484

M062X_12_s3 Eopt -1181.216895

O	0.271374	-0.996173	0.830129
O	0.386532	0.618543	-0.724102
O	-0.988072	-1.112508	-1.023206
O	2.636721	0.192396	-2.362471
H	1.816026	0.329250	-1.844261
H	2.846783	-0.753014	-2.237981
O	-1.020476	-3.188788	1.837446
H	-0.530120	-2.415332	1.469416
H	-1.826775	-3.201532	1.298077
O	-0.210003	4.251750	0.317410
H	0.474999	3.636559	0.639933
H	-0.752618	3.694482	-0.275313
O	2.999360	-1.507223	0.878959
H	3.427718	-0.656671	0.661535
H	2.037373	-1.302787	0.875202
O	-3.987120	1.824742	0.023101
H	-3.739185	1.822927	0.954247
H	-4.333927	0.922869	-0.152052
O	0.807530	0.472435	3.088882
H	1.566556	0.036939	3.492041
H	0.618583	-0.051574	2.274420
O	-3.045099	-2.549045	-0.161604
H	-2.240511	-2.042860	-0.467570
H	-3.156491	-3.264791	-0.797429
O	-1.602705	2.441195	-1.375670
H	-2.407310	2.174706	-0.889241
H	-0.937797	1.741054	-1.189776
O	4.062697	1.020656	-0.008295
H	3.691276	0.789214	-0.882402
H	3.335798	1.514433	0.421287
O	1.695055	2.223923	0.999946
H	1.220711	1.614362	0.371809
H	1.512786	1.819400	1.867266
O	3.309010	-2.509631	-1.697822
H	3.172673	-2.251582	-0.758506
H	2.559844	-3.074552	-1.917171
O	-5.065667	-0.687032	-0.519970
H	-4.355644	-1.362443	-0.435879
H	-5.277676	-0.658025	-1.459682
C	-0.119363	-0.503826	-0.306638

M062X_15_s1 Eopt -1410.495422

O	0.025187	-0.913855	1.048454
O	1.166473	0.571592	-0.156074
O	-0.525177	-0.538242	-1.088775
O	2.792909	-0.528749	-2.166765
H	2.193544	0.019116	-1.622603
H	2.371550	-1.412183	-2.138352
O	-0.887729	-3.580037	0.591558
H	-0.488063	-2.703457	0.751105
H	-1.659689	-3.344923	0.050708
O	1.287136	3.272182	2.211884
H	1.875785	2.491019	2.229626
H	1.102376	3.406620	1.262744
O	2.291037	-2.635627	0.946103

H	3.064218	-2.083086	0.717856
H	1.589810	-1.987011	1.160345
O	-1.778164	3.334093	-1.967893
H	-2.138797	2.794540	-1.233638
H	-1.258340	2.680431	-2.476413
O	-0.896449	1.458417	2.350013
H	-0.184230	2.129027	2.332743
H	-0.457326	0.622144	2.094321
O	-2.737671	-2.170746	-1.097020
H	-1.975062	-1.567099	-1.040275
H	-3.455583	-1.699901	-0.657466
O	0.746729	3.281745	-0.538833
H	-0.121622	3.460216	-0.945662
H	0.807208	2.308374	-0.506975
O	4.354604	-0.770778	0.241108
H	3.894428	-0.648825	-0.610489
H	3.905462	-0.173690	0.851092
O	2.659534	0.763261	1.988308
H	2.044287	0.649680	1.223310
H	2.360620	0.143162	2.659371
O	1.199525	-2.862637	-1.695041
H	1.539278	-2.917097	-0.781766
H	0.441997	-2.251623	-1.628586
O	-0.013333	1.359599	-2.994634
H	-0.162316	0.671161	-2.312009
H	0.769667	1.882607	-2.682431
C	0.220601	-0.293678	-0.060857
O	-4.601575	-0.327265	0.171407
H	-3.957847	0.414858	0.142140
H	-5.276389	-0.068255	0.812608
O	-2.425200	1.388041	-0.023465
H	-1.945879	1.493747	0.828395
H	-1.896154	0.740601	-0.521453
O	-2.582575	-1.246850	2.110552
H	-3.287529	-1.009882	1.475780
H	-1.751111	-1.141365	1.613999

M062X_15_s2			Eopt -1410.492839
O	0.464545	-0.160893	0.650079
O	0.285296	-0.078473	-1.566811
O	-1.546710	-0.248032	-0.305256
O	2.253900	-2.029384	-1.348917
H	1.557958	-1.348015	-1.439922
H	2.184306	-2.338532	-0.430618
O	2.331627	2.647590	1.518555
H	1.381198	2.591253	1.710234
H	2.663771	1.745665	1.660693
O	-0.381123	-1.969595	2.426038
H	-0.098715	-1.267065	1.790634
H	-1.116106	-2.405270	1.964412
O	-0.604146	3.147878	-0.895273
H	0.331101	2.932369	-1.033266
H	-1.063053	2.596667	-1.552086
O	3.058934	-0.107781	1.332618
H	3.642711	-0.055803	0.558946
H	2.151219	-0.115792	0.949268
O	-0.504223	2.132818	1.770741
H	-0.716202	2.562350	0.923195
H	-0.162822	1.258393	1.484453
O	-2.598984	-2.530411	0.746655
H	-2.451318	-3.221716	0.094451
H	-2.226083	-1.715755	0.344908
O	-2.278538	0.205231	3.076864
H	-1.679877	-0.542975	2.933695
H	-1.840102	0.946750	2.634641
O	-1.538148	1.371560	-2.956675
H	-2.401801	1.068278	-2.660412
H	-0.901525	0.760242	-2.520557
O	4.199025	0.019880	-1.312495
H	3.611001	-0.752877	-1.397891

H	3.596278	0.777142	-1.396801
O	2.080804	1.976978	-1.256837
H	1.490078	1.194293	-1.318822
H	2.180619	2.164586	-0.306847
O	2.223862	-2.856188	1.434280
H	1.326933	-2.724398	1.780523
H	2.654211	-1.995641	1.564400
C	-0.283975	-0.168397	-0.409116
O	-2.850222	2.181979	0.722678
H	-2.013328	2.477661	0.356918
H	-3.537134	2.816228	0.504777
O	-4.116364	-1.165023	-1.431076
H	-3.279470	-0.869341	-1.796836
H	-4.803276	-0.530774	-1.648977
O	-0.276298	-2.623253	-2.155610
H	0.560596	-2.327570	-2.521370
H	-0.963209	-1.989003	-2.373511

M062X_15_s3			Eopt -1410.496085
O	0.548733	0.347560	1.185286
O	-0.703750	0.083543	-0.638339
O	1.493092	-0.234540	-0.748124
O	-0.051275	2.085702	-2.545429
H	-0.337247	1.297536	-2.050693
H	0.787446	2.329087	-2.119569
O	3.211546	0.525978	1.919158
H	2.279078	0.455158	1.633975
H	3.721784	0.307600	1.126515
O	-4.392399	-0.834741	0.064360
H	-3.951750	0.027209	0.176738
H	-3.860745	-1.423940	0.615855
O	0.421322	3.178574	1.179148
H	-0.278931	3.409385	0.542491
H	0.369005	2.211778	1.271190
O	0.491538	-2.081473	2.586872
H	0.619221	-1.190850	2.213782
H	1.031010	-2.638128	2.009540
O	-1.592433	0.824309	2.871277
H	-1.292184	1.617842	3.326210
H	-0.863527	0.604555	2.255215
O	2.220081	-2.703904	0.354868
H	2.051162	-1.821106	-0.026449
H	2.874857	-3.112320	-0.220837
O	-1.925467	-1.888320	1.081380
H	-1.213638	-2.008459	1.734259
H	-1.635187	-1.126289	0.550366
O	-1.561686	3.729261	-0.775987
H	-1.080965	3.234605	-1.463344
H	-2.132744	3.059169	-0.362662
O	-2.794910	1.471826	0.390484
H	-2.026441	0.993504	0.002335
H	-2.606259	1.427370	1.343025
O	2.290609	2.566091	-0.893369
H	1.739916	2.886787	-0.157359
H	2.250535	1.601376	-0.806566
O	-0.326643	-3.561650	-0.633805
H	0.537582	-3.348448	-0.242339
H	-0.962692	-3.038311	-0.119303
C	0.444566	0.062161	-0.066256
O	-2.557536	-1.481076	-2.096527
H	-1.754113	-1.061896	-1.750726
H	-3.231661	-1.277163	-1.428771
O	0.571237	-1.880324	-2.793866
H	0.915551	-1.212964	-2.170568
H	0.124725	-2.508266	-2.203959
O	4.327367	-0.203212	-0.687299
H	4.538382	0.663983	-1.049121
H	3.365046	-0.280605	-0.792399

M062X_24_s1			Eopt -2098.316852
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O	1.198123	0.234826	-0.716347
O	-0.851862	-0.363264	-0.093224
O	0.916726	-1.385046	0.776612
O	2.356806	-0.556226	2.903694
H	2.166704	0.399549	2.960097
H	1.869466	-0.836358	2.100592
O	-0.208918	-1.178681	4.080694
H	0.713615	-0.991375	3.839413
H	-0.444287	-1.929892	3.512046
O	-1.958641	1.364078	-1.780123
H	-1.439330	1.477702	-2.594846
H	-1.468315	0.704337	-1.234369
O	4.494417	-1.754156	1.413703
H	3.941480	-2.381960	0.921117
H	3.879498	-1.321334	2.028367
O	-2.181559	2.997197	0.449873
H	-1.887940	2.422995	1.166837
H	-2.039887	2.478947	-0.366815
O	-2.952384	-1.803935	1.038218
H	-3.399306	-1.143341	1.599242
H	-2.208440	-1.315003	0.635165
O	-0.686650	-3.151711	2.011227
H	-0.122759	-2.484178	1.554123
H	-1.589041	-2.848827	1.819305
O	-0.296711	1.599085	-4.063732
H	0.043546	0.694577	-3.961800
H	0.269277	2.115646	-3.462012
O	1.205060	2.669421	-1.974976
H	0.748853	3.340314	-1.431956
H	1.068018	1.824110	-1.501875
O	2.366148	3.909479	1.281431
H	2.868755	4.612844	1.698015
H	2.945874	3.530655	0.586676
O	0.097995	4.553092	-0.228647
H	-0.665366	4.058019	0.112992
H	0.828893	4.380056	0.390247
O	1.345361	2.024794	3.033681
H	1.693691	2.668234	2.391118
H	0.479156	1.743175	2.697227
O	2.602072	-3.226937	-0.245600
H	2.030818	-2.505399	0.094576
H	2.909451	-2.898039	-1.109316
O	-1.184752	0.850675	2.416465
H	-1.109977	0.413914	1.548361
H	-0.911637	0.160146	3.054025
O	-3.964778	0.321953	2.562122
H	-3.037864	0.614646	2.600751
H	-4.346186	0.831863	1.822786
O	3.877932	0.048281	-0.688739
H	2.895298	0.057728	-0.614185
H	4.181753	-0.495711	0.058260
O	-0.011441	-4.405612	-0.552037
H	0.915491	-4.113152	-0.547958
H	-0.341466	-4.127108	0.316779
O	-1.230560	-2.390528	-2.084559
H	-0.812116	-3.131217	-1.603725
H	-1.219632	-1.664664	-1.438196
O	0.877187	-0.876779	-3.254026
H	1.020728	-0.396028	-2.416674
H	0.170993	-1.504510	-3.022143
O	-4.484357	0.273862	-1.916695
H	-3.577216	0.631978	-1.967009
H	-4.363230	-0.680606	-1.765194
O	3.450787	-1.968209	-2.635010
H	2.573662	-1.697535	-2.953682
H	3.719503	-1.238224	-2.049211
O	3.756169	2.850232	-0.826068
H	2.928566	2.844557	-1.341852
H	3.937230	1.905370	-0.678022
O	-4.852517	1.841052	0.391351

H	-4.022815	2.343258	0.389282
H	-4.780675	1.247402	-0.379227
O	-4.012152	-2.470655	-1.430847
H	-3.134256	-2.552123	-1.837873
H	-3.791543	-2.284687	-0.499187
C	0.428823	-0.501840	-0.011299

	M062X_24_s2	Eopt -2098.314707
O	1.170442	0.612712
O	-0.843606	-0.293230
O	0.951288	-1.316943
O	2.146209	-0.715807
H	1.879251	0.215211
H	1.772201	-0.933253
O	-0.417451	-1.778223
H	0.491758	-1.459993
H	-0.542307	-2.424108
O	-1.942914	1.286946
H	-1.305651	1.608158
H	-1.429269	0.719535
O	4.568705	-1.379599
H	4.146151	-1.958547
H	3.838644	-1.118483
O	-2.856207	2.737046
H	-2.544769	2.202212
H	-2.504206	2.290352
O	-2.890859	-2.101957
H	-3.118890	-2.486800
H	-2.186975	-1.457777
O	-0.569929	-3.379736
H	-0.034671	-2.599563
H	-1.469355	-3.142410
O	0.085040	2.150544
H	0.533750	1.290914
H	0.438003	2.645953
O	0.945317	3.140140
H	0.226957	3.678675
H	0.827342	2.220893
O	2.144479	3.592147
H	1.860179	3.430025
H	1.730199	4.426058
O	-0.943366	4.752057
H	-1.650498	4.096232
H	-0.518028	4.859792
O	0.959466	1.801204
H	1.307816	2.375519
H	0.118772	1.438643
O	3.023686	-2.735953
H	2.325180	-2.124591
H	3.322364	-2.365495
O	-1.468685	0.459748
H	-1.338653	0.223798
H	-1.170822	-0.331151
O	-4.297534	0.293078
H	-3.327276	0.343038
H	-4.578151	0.410769
O	3.860435	0.735016
H	2.890344	0.598110
H	4.201323	0.066768
O	0.675914	-4.222165
H	1.541772	-3.816751
H	0.193326	-4.111301
O	-0.655535	-2.146230
H	-0.162285	-2.872808
H	-0.863509	-1.532730
O	1.398417	-0.269775
H	1.424574	0.115820
H	0.709429	-0.952853
O	-4.189477	-0.279502
H	-3.354886	0.221858

H	-3.931927	-1.214548	-2.242796
O	3.766448	-1.707335	-2.708969
H	2.938665	-1.208300	-2.852004
H	3.707812	-2.462014	-3.299459
O	3.740726	3.010190	-1.696139
H	2.797621	3.174184	-1.550643
H	3.933888	2.257912	-1.117386
O	-5.129204	0.958955	0.047415
H	-4.478265	1.675781	0.092998
H	-4.839541	0.425511	-0.715759
O	-3.292489	-2.945223	-2.110935
H	-2.346599	-2.806412	-2.308356
H	-3.567600	-3.725200	-2.596564
C	0.432046	-0.328581	0.165853

M062X_24_s3 Eopt -2098.311528

O	-0.915407	-0.266655	-0.326424
O	1.114167	0.553387	-0.726631
O	-0.330737	1.728137	0.486040
O	-2.134315	1.646138	2.528718
H	-1.884162	0.837670	2.992260
H	-1.527468	1.659008	1.760529
O	1.313617	1.918554	3.677746
H	1.514646	2.532545	2.942517
H	2.030615	2.031909	4.310902
O	1.388939	-1.960833	-1.688068
H	0.592513	-2.244168	-2.171240
H	1.233902	-1.025207	-1.418593
O	-4.251149	2.549550	0.889980
H	-3.638964	2.982995	0.274912
H	-3.674128	2.250981	1.609792
O	1.175742	-2.786892	0.958137
H	1.373810	-1.970872	1.436806
H	1.216200	-2.535731	0.008310
O	3.587607	1.732345	-0.320110
H	3.671868	2.406687	-1.004199
H	2.716070	1.326788	-0.488412
O	1.674587	3.266329	1.275917
H	0.967586	2.662470	0.939152
H	2.492155	2.920534	0.882386
O	-0.908651	-2.757635	-3.113192
H	-1.084490	-1.851179	-3.410734
H	-1.588039	-2.868543	-2.423265
O	-2.958971	-2.696911	-1.145246
H	-2.396112	-2.948559	-0.389413
H	-3.153433	-1.755008	-1.026790
O	-3.377432	-1.619487	1.975625
H	-3.510983	-1.003955	1.228746
H	-3.692755	-1.061825	2.815070
O	-1.524279	-3.536484	1.058771
H	-0.614286	-3.176926	1.094550
H	-2.059657	-2.969550	1.627934
O	-0.829060	-0.908166	3.056396
H	-1.561190	-1.166763	2.473904
H	-0.092339	-0.658935	2.469824
O	-2.093316	3.495236	-0.668952
H	-1.538045	2.815764	-0.235564
H	-1.998783	3.285695	-1.618120
O	1.830332	-0.204382	1.993841
H	1.792302	0.204025	1.115126
H	1.690390	0.521949	2.634270
O	4.463661	-1.253683	1.765386
H	3.572225	-0.879962	1.885555
H	4.305394	-2.156063	1.450520
O	-3.548391	0.041963	-0.233215
H	-2.566366	0.130569	-0.199670
H	-3.905604	0.888355	0.088219
O	0.332003	5.047923	-0.510201
H	-0.549763	4.639033	-0.515201
H	0.814105	4.595515	0.203044

O	1.236298	2.971916	-2.251973
H	0.994780	3.699899	-1.655697
H	1.206034	2.168417	-1.704497
O	-1.772036	-0.051533	-2.965337
H	-1.430264	-0.177821	-2.053324
H	-2.716682	-0.227672	-2.887505
O	4.121949	-2.565075	-1.745844
H	3.176288	-2.345176	-1.809530
H	4.573576	-1.728580	-1.543372
O	-1.383516	2.712832	-3.266324
H	-1.557381	1.757465	-3.196546
H	-0.451532	2.809096	-3.004058
O	-5.424027	-3.612048	-0.063676
H	-4.582414	-3.323019	-0.465158
H	-5.876412	-4.095365	-0.761085
O	3.813281	-3.853216	0.717236
H	2.882081	-3.620259	0.883908
H	3.987594	-3.479074	-0.163904
O	5.481091	-0.157030	-1.215988
H	5.722505	0.161220	-2.091491
H	4.820333	0.487650	-0.891247
C	-0.058604	0.669954	-0.190087

M062X_Radical_3_s1 Eopt -493.177688

O	-2.953345	-1.016747	-0.240436
O	-0.805530	-1.243848	0.002113
O	-1.789508	0.788660	0.102795
O	0.460296	2.420477	-0.216498
H	0.718074	2.430229	-1.143368
H	-0.334676	1.858275	-0.180885
O	1.532480	0.036553	0.917291
H	0.741638	-0.452002	0.626859
H	1.371560	0.934444	0.583818
O	3.670762	-0.983454	-0.538517
H	4.220706	-1.460015	0.089251
H	2.926902	-0.637670	-0.009771
C	-1.760907	-0.447733	-0.029982

M062X_Radical_3_s2 Eopt -493.176038

C	1.318344	-0.243831	-0.010307
O	1.078312	-0.933948	-1.005436
O	1.185039	-0.601799	1.216952
O	1.730187	0.973021	-0.012150
O	-1.004404	1.645618	-1.064880
H	-0.056324	1.742291	-0.906101
H	-1.094155	0.762897	-1.444078
O	-1.706359	-1.566927	-0.558444
H	-1.802106	-0.947527	0.180518
H	-0.768960	-1.494442	-0.793506
O	-1.547205	0.508056	1.500898
H	-1.403613	1.050560	0.707090
H	-0.669456	0.157041	1.702401

M062X_Radical_3_s3 Eopt -493.178291

C	-2.325146	0.152908	-0.118059
O	-1.789691	1.167181	0.458672
O	-3.432412	0.549006	-0.631887
O	-1.860134	-0.992881	-0.168580
O	0.580103	-0.939030	1.168944
H	-0.279737	-0.969264	0.706164
H	0.613709	-0.058675	1.557240
O	2.479132	-0.889855	-0.845476
H	1.813579	-0.939232	-0.131074
H	2.983255	-1.706295	-0.777515
O	4.196791	1.148138	0.017088
H	3.839192	1.964320	-0.343253
H	3.590569	0.451220	-0.293298

M062X_Radical_6_s1 Eopt -722.449853

O	1.372132	0.142292	1.834441
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O	0.515569	-1.576488	0.659192
O	-0.659705	0.157739	1.485099
O	-0.598760	2.799829	0.225200
O	1.935508	1.425260	-0.769659
O	2.692149	-1.258886	-1.126335
H	1.828341	1.420585	0.189950
H	0.109538	2.787068	-0.427207
H	3.533074	-1.419897	-0.686896
H	2.014267	-1.491890	-0.469410
H	2.317762	0.547972	-0.958631
H	-0.597859	1.902749	0.588818
O	-0.469604	0.314674	-1.897364
O	-2.961192	0.456445	-0.433151
O	-2.087244	-2.203387	-0.234625
H	-2.698553	0.909415	0.374672
H	-1.168649	-2.015842	0.030517
H	-1.249714	0.494544	-1.350194
H	-2.036495	-2.402513	-1.175212
H	-2.732252	-0.478679	-0.275380
H	0.274497	0.737235	-1.440297
C	0.415870	-0.508427	1.276146

M062X_Radical_6_s2 Eopt -722.451593

O	-0.087370	-1.327674	1.219127
O	0.120949	-0.183537	-0.707146
O	0.215888	0.715606	1.356294
O	-2.104205	2.191591	-0.235390
O	-2.995556	-0.272286	0.859588
O	-2.113600	-1.829338	-1.330168
H	-2.388130	-0.500135	1.573335
H	-2.377184	1.343619	0.156326
H	-1.972142	-2.731519	-1.011973
H	-1.245613	-1.394718	-1.259770
H	-2.746409	-0.863435	0.125156
H	-1.149472	2.215472	-0.118141
O	1.061681	2.445322	-1.242194
O	3.238317	0.313605	1.022327
O	2.563695	-1.687792	-0.933599
H	2.379972	0.707733	1.218381
H	1.696535	-1.277191	-1.068425
H	1.871952	2.419853	-1.760300
H	2.383017	-2.447813	-0.371446
H	3.049430	-0.360871	0.348578
H	0.813678	1.516309	-1.112335
C	0.080995	-0.258546	0.534984

M062X_Radical_6_s3 Eopt -722.448649

O	-0.118694	-0.104858	0.823284
O	0.440909	0.580577	-1.242554
O	0.020003	-1.549343	-0.649488
O	3.015628	-1.843227	-0.611229
O	2.779237	-0.019519	1.554662
O	2.346979	2.270051	-0.036810
H	1.856591	-0.244267	1.726683
H	2.985727	-1.221999	0.137179
H	1.936234	2.919955	0.541761
H	1.606424	1.809534	-0.467746
H	2.718488	0.809430	1.045609
H	2.087177	-2.024231	-0.797936
O	-3.115984	-0.216416	1.961976
O	-2.948136	-1.014210	-0.767464
O	-2.233997	1.730046	-1.014724
H	-2.099104	-1.471409	-0.819293
H	-1.291579	1.570683	-1.173102
H	-3.051591	-0.541221	1.047536
H	-2.298866	1.849610	-0.060788
H	-2.743823	-0.088405	-0.988936
H	-4.052132	-0.271587	2.174460
C	0.143150	-0.293484	-0.417775

M062X_Radical_9_s1 Eopt -951.719159

O	-0.622682	-1.334152	-0.925189
O	-0.619974	0.766540	-1.308494
O	-0.406367	0.066781	0.798587
O	0.579960	2.520482	1.839256
H	0.201182	1.722533	1.424549
H	-0.060406	3.220125	1.666423
O	-3.676229	1.320472	-0.983983
H	-2.760564	1.332495	-1.295353
H	-3.599268	1.072553	-0.045757
O	1.931002	2.063288	-2.103870
H	2.259690	2.445962	-1.266539
H	1.115232	1.602763	-1.858143
O	1.694796	-3.028479	-0.043940
H	1.029202	-2.549740	-0.559573
H	1.579839	-2.667994	0.858547
O	-3.308950	-0.048701	1.593029
H	-2.343771	0.029408	1.549305
H	-3.508687	-0.772682	0.976322
O	1.091813	-1.772638	2.415152
H	1.864343	-1.294436	2.737506
H	0.576037	-1.112925	1.916280
O	-3.699809	-1.669181	-0.883377
H	-3.822257	-0.742763	-1.149842
H	-2.743269	-1.801167	-0.949693
O	2.824662	3.194827	0.332475
H	2.058739	2.944806	0.893156
H	3.551641	2.640084	0.636450
O	4.229822	-2.118364	-0.811112
H	3.330813	-2.434242	-0.582484
H	4.355473	-2.369898	-1.732151
C	-0.538054	-0.158649	-0.427878

M062X_Radical_9_s2 Eopt -951.722651

O	0.474794	0.273550	-1.794896
O	1.747356	1.105890	-0.396392
O	1.610161	-1.139852	-0.465338
O	4.008774	-0.957343	1.011524
H	3.174515	-1.159344	0.554521
H	3.759335	-1.219055	1.903851
O	-0.275360	3.207551	-0.198016
H	0.407269	2.525037	-0.271111
H	0.008686	4.105617	0.000306
O	4.608896	0.935940	-0.834007
H	4.589323	0.247344	-0.149719
H	3.703897	1.255212	-0.930803
O	-2.205125	-0.774804	-0.931654
H	-1.615063	-0.329899	-1.553293
H	-1.721987	-1.580910	-0.662523
O	0.769200	-0.649771	2.353328
H	1.166491	-1.021775	1.556519
H	0.033523	-0.110716	2.011840
O	-0.441611	-3.018913	-0.033686
H	-0.340932	-3.658676	-0.745767
H	0.319838	-2.420334	-0.121037
O	-1.398932	0.787498	1.263996
H	-1.075201	1.594611	0.824352
H	-1.613530	0.174729	0.535849
O	-4.866887	-0.618307	-0.937549
H	-3.925907	-0.853058	-1.018105
H	-5.344259	-1.366032	-1.309529
C	1.301600	-0.001562	-0.848783
O	-4.227461	1.114545	1.272715
H	-3.272915	1.159741	1.450016
H	-4.493115	0.539018	0.537146

M062X_Radical_9_s3 Eopt -951.72094

O	0.735010	-0.365102	-1.851927
O	1.732489	1.194064	-0.776981
O	1.668764	-0.857159	0.106050

O	4.469260	-1.157420	0.713916
H	3.506468	-1.084854	0.586859
H	4.617614	-0.911185	1.634022
O	-0.449685	3.015413	-0.193302
H	0.322267	2.460582	-0.398955
H	-0.143828	3.620988	0.491955
O	4.744482	1.213505	-0.867491
H	4.770269	0.413436	-0.309680
H	3.796764	1.383154	-0.966206
O	-1.942624	-1.164250	-0.699235
H	-1.306791	-0.816700	-1.341136
H	-1.450424	-1.878806	-0.242207
O	0.341419	0.094148	2.603411
H	0.881687	-0.239406	1.871333
H	-0.467190	0.419454	2.162286
O	-0.229719	-2.972662	0.578369
H	-0.053707	-3.708457	-0.019200
H	0.487318	-2.334418	0.409088
O	-1.928064	1.003664	1.126940
H	-1.452243	1.726945	0.669235
H	-1.912008	0.253002	0.497937
O	-4.704669	-1.014381	-1.195350
H	-3.749372	-1.159149	-1.047261
H	-5.141984	-1.748927	-0.750670
C	1.389421	-0.036634	-0.802810
O	-4.740409	1.266684	0.555528
H	-3.799342	1.274706	0.809620
H	-4.812052	0.497403	-0.039576

M062X_Radical_12_s1

Eopt -1180.992947

O	-0.174764	0.301114	0.999499
O	0.018616	-0.676089	-0.950101
O	-0.174997	1.525438	-0.815857
O	-2.632416	-0.967134	-2.379705
H	-1.702802	-1.020467	-2.113168
H	-2.861153	-0.031291	-2.210421
O	-0.890380	2.601325	2.963268
H	-0.729814	1.729282	2.580724
H	-0.799126	3.202733	2.199991
O	2.440258	-3.326590	0.576969
H	1.481626	-3.472186	0.504574
H	2.645661	-2.723017	-0.167411
O	-2.967996	-0.612007	1.810816
H	-3.124554	-1.303463	1.137196
H	-2.084319	-0.275087	1.607914
O	4.352387	0.699838	-0.762170
H	4.555727	0.611309	0.175732
H	3.704124	1.434080	-0.817268
O	2.021799	-1.199328	2.435888
H	2.197076	-1.944995	1.828963
H	1.337336	-0.681978	1.988595
O	-0.615788	4.098297	0.550259
H	-0.454633	3.271416	0.066905
H	0.241197	4.540131	0.568470
O	2.801456	-1.494921	-1.533521
H	3.360365	-0.743133	-1.242854
H	1.891612	-1.174332	-1.434394
O	-3.311994	-2.617809	-0.173869
H	-3.178260	-2.042963	-0.954310
H	-2.425811	-2.978918	0.004373
O	-0.507498	-3.223429	0.408625
H	-0.336269	-2.355335	0.003285
H	-0.595056	-3.031532	1.350877
O	-2.971014	1.800701	-1.861674
H	-3.601232	1.937604	-1.144887
H	-2.098313	1.859327	-1.442090
O	2.491244	2.768790	-1.013851
H	1.604792	2.372893	-0.986973
H	2.589233	3.098481	-1.914754
C	-0.108120	0.382648	-0.270944

M062X_Radical_12_s2

Eopt -1180.989646

O	0.582072	-0.451002	0.199529
O	-1.220890	-1.041763	-0.968875
O	0.522938	-2.347350	-0.886263
O	-1.436982	0.658924	-3.347387
H	-1.303161	0.029103	-2.619493
H	-0.570280	0.750273	-3.759672
O	-0.869330	2.199362	2.331599
H	-0.399099	1.425198	2.691763
H	-0.338686	2.454129	1.553647
O	3.474407	-0.216349	-0.056972
H	2.506813	-0.233027	0.041962
H	3.646231	-0.983292	-0.637593
O	-4.644207	-0.901077	1.399838
H	-4.054879	-0.152068	1.196754
H	-4.238285	-1.647873	0.920974
O	0.564894	2.482916	-0.168793
H	-0.222678	2.681971	-0.717882
H	0.584030	1.512667	-0.124198
O	0.679552	-0.140501	3.042198
H	0.228476	-0.803339	3.578102
H	0.565427	-0.431785	2.120720
O	3.432188	-2.534761	-1.699431
H	3.565084	-2.283044	-2.620767
H	2.470668	-2.531160	-1.577978
O	3.562374	-0.546954	2.826611
H	3.645431	-0.483503	1.858609
H	2.610720	-0.429189	2.990278
O	-3.300252	-2.931830	-0.117140
H	-2.916937	-3.577902	0.486888
H	-2.553512	-2.375060	-0.393851
O	-1.855571	2.836705	-1.571105
H	-1.712615	2.155924	-2.258491
H	-2.292529	2.347252	-0.848891
O	-2.753776	1.083622	0.544122
H	-2.244166	0.387941	0.098206
H	-2.145742	1.432819	1.230866
O	3.226122	2.381106	-1.282615
H	3.429530	1.492305	-0.938449
H	2.317817	2.543052	-0.971910
C	-0.047664	-1.254965	-0.543686

M062X_Radical_12_s3

Eopt -1180.990989

O	-0.441726	0.581440	1.462006
O	0.695875	-0.007421	-0.358169
O	1.664501	0.991716	1.374214
O	-1.577717	-0.029318	-2.240788
H	-0.851590	0.043317	-1.599808
H	-2.356838	0.357356	-1.785904
O	-2.533812	2.550428	0.968795
H	-1.757417	1.989894	1.125536
H	-2.203562	3.319377	0.463064
O	2.914810	-3.436651	0.135764
H	1.947934	-3.385062	0.231335
H	3.136088	-2.629372	-0.367716
O	-4.225500	-1.693921	0.200597
H	-3.523436	-2.098655	-0.355744
H	-3.867546	-1.695029	1.095677
O	5.319982	0.736899	-0.650152
H	5.747098	0.359687	0.127090
H	4.771150	1.474343	-0.307955
O	-1.080323	-2.056467	2.604237
H	-2.033381	-2.190389	2.541288
H	-0.940316	-1.134005	2.333449
O	-1.645420	4.818391	-0.461617
H	-1.235772	4.495727	-1.273151
H	-2.439223	5.280052	-0.757185
O	3.257634	-1.042201	-1.365246
H	3.982093	-0.440063	-1.097857

H	2.447574	-0.630850	-1.021280
O	-2.253840	-2.685390	-1.512520
H	-2.028455	-1.797851	-1.860791
H	-1.498642	-2.899349	-0.931913
O	0.061992	-2.896116	0.158551
H	0.306224	-2.005567	-0.142815
H	-0.331636	-2.734604	1.040504
O	-3.850769	0.909179	-0.889431
H	-4.018405	0.057415	-0.439891
H	-3.427058	1.483340	-0.217913
O	3.618628	2.787072	0.194398
H	4.021557	3.254443	0.935380
H	2.905571	2.259156	0.590663
C	0.642242	0.507596	0.785138

M062X_Radical_15_s1

Eopt -1410.264548

O	-0.501433	-0.787863	0.487307
O	0.957652	0.686156	-0.095191
O	-0.569521	-0.055639	-1.580053
O	2.900727	-0.067419	-2.126086
H	2.298593	0.581646	-1.739842
H	2.392222	-0.899567	-2.083893
O	-0.627755	-3.934053	0.560570
H	0.265012	-3.580545	0.642556
H	-1.065844	-3.390616	-0.120237
O	0.676969	3.067065	2.480587
H	1.296740	2.327116	2.580474
H	0.767679	3.338646	1.549351
O	1.922440	-2.459378	1.101978
H	2.721783	-1.938377	0.897002
H	1.318764	-1.822822	1.499164
O	-1.510993	3.767487	-1.834569
H	-2.061503	3.124466	-1.357930
H	-0.960413	3.220191	-2.420406
O	-1.622004	1.547381	2.012081
H	-0.804916	2.057212	2.180137
H	-1.341454	0.627251	1.953389
O	-2.230356	-2.421574	-1.204374
H	-1.700047	-1.686543	-1.548249
H	-2.792873	-1.995753	-0.534501
O	0.878050	3.527000	-0.286786
H	0.033254	3.750043	-0.714206
H	0.942703	2.564185	-0.385944
O	4.010076	-0.718671	0.454289
H	3.678826	-0.435600	-0.417176
H	3.619921	-0.098059	1.088515
O	2.261355	0.659695	2.349006
H	1.674185	0.522979	1.584707
H	2.036790	-0.037603	2.974024
O	1.467527	-2.464033	-1.728174
H	1.547209	-2.476482	-0.759071
H	0.539686	-2.268837	-1.903785
O	0.360639	2.093727	-3.173618
H	0.111886	1.312321	-2.650236
H	1.134164	2.450255	-2.722398
C	-0.010044	-0.003479	-0.469656
O	-3.694926	-0.884898	0.688590
H	-3.531899	-0.015122	0.283277
H	-4.649176	-1.009129	0.674539
O	-2.796754	1.548089	-0.495487
H	-2.323043	1.665541	0.353438
H	-2.199308	1.016507	-1.042506
O	-2.111235	-2.435375	2.512201
H	-2.617462	-1.845077	1.933595
H	-1.557774	-2.951432	1.902600

M062X_Radical_15_s2

Eopt -1410.260807

O	-0.453597	-0.055422	0.690313
O	-0.032256	0.049024	-1.491086
O	1.622444	0.319187	-0.021870

O	-2.067684	1.901175	-1.313365
H	-1.411171	1.177611	-1.386121
H	-2.163620	2.066678	-0.358813
O	-2.107645	-3.029158	1.202092
H	-1.195663	-2.892042	1.504063
H	-2.551326	-2.180120	1.362105
O	0.026751	1.618431	2.752099
H	-0.125277	0.952849	2.042512
H	0.598211	2.271488	2.313892
O	0.991553	-3.182184	-0.888651
H	0.059757	-3.034572	-1.109786
H	1.466736	-2.576241	-1.484441
O	-3.107409	-0.353863	1.066597
H	-3.596593	-0.368245	0.228426
H	-2.168140	-0.248202	0.794408
O	0.662983	-2.304498	1.804098
H	0.923180	-2.661270	0.936034
H	0.262103	-1.444075	1.567116
O	1.792450	2.946855	0.985837
H	1.237347	3.300792	0.270488
H	1.882572	2.009186	0.738384
O	2.301768	-0.246208	3.168674
H	1.593419	0.410931	3.095554
H	1.973390	-1.002769	2.661977
O	2.080185	-1.248444	-2.690608
H	2.849266	-0.956726	-2.188079
H	1.346198	-0.694226	-2.349879
O	-3.926535	-0.269109	-1.697849
H	-3.409564	0.552926	-1.663896
H	-3.252941	-0.966752	-1.764275
O	-1.728398	-2.127900	-1.500752
H	-1.169260	-1.323159	-1.460360
H	-1.890969	-2.385240	-0.576476
O	-2.510506	2.407771	1.493845
H	-1.671978	2.295876	1.969189
H	-2.903315	1.519418	1.503613
C	0.383472	0.106568	-0.273839
O	3.529928	-1.688739	0.213721
H	2.796268	-1.049076	0.152315
H	3.105800	-2.549995	0.150270
O	2.549434	1.833059	-2.082347
H	2.264337	1.213245	-1.373185
H	2.431937	1.338608	-2.899817
O	0.359357	3.512907	-1.419155
H	-0.472576	3.013984	-1.421571
H	1.028449	2.906637	-1.783355

M062X_Radical_15_s3

Eopt -1410.257261

O	0.687349	-0.202942	1.192387
O	-0.620260	0.228311	-0.596574
O	1.448909	-0.369576	-0.845073
O	0.461958	2.335337	-2.300073
H	0.007846	1.538932	-1.990264
H	1.326522	2.306048	-1.850173
O	3.588488	0.074790	1.545690
H	2.622533	0.054418	1.512140
H	3.865239	-0.232628	0.666356
O	-4.847820	-0.475830	0.257302
H	-4.428177	0.398088	0.310453
H	-4.228994	-1.042801	0.740479
O	1.235801	2.722974	1.435288
H	0.436743	3.009088	0.950395
H	1.078860	1.794772	1.648831
O	-0.288521	-2.381698	2.778541
H	0.150712	-1.615265	2.380458
H	-0.005624	-3.123167	2.230985
O	-1.511192	1.147070	2.495187
H	-1.078015	1.997022	2.636901
H	-0.813008	0.582824	2.125004
O	2.093409	-2.920698	0.635909

H	1.996584	-2.085030	1.109306
H	2.625042	-2.691129	-0.135127
O	-2.363922	-1.614766	1.004440
H	-1.802741	-1.847052	1.764494
H	-2.009630	-0.774105	0.679976
O	-0.872827	3.642072	-0.143407
H	-0.456241	3.292544	-0.950817
H	-1.663930	3.094588	-0.018926
O	-3.035763	1.734939	0.224737
H	-2.582815	1.228159	-0.461979
H	-2.560059	1.489922	1.043746
O	2.881925	2.327707	-0.814651
H	2.382704	2.446953	0.015979
H	3.142306	1.399164	-0.811030
O	-0.451170	-2.988562	-0.687111
H	0.374935	-2.949594	-0.174915
H	-1.126654	-2.557747	-0.138433
C	0.435101	-0.100506	-0.029672
O	-2.993577	-0.895226	-2.004251
H	-2.114500	-0.753189	-1.630379
H	-3.605951	-0.781808	-1.261220
O	-0.073259	-1.591319	-3.111640
H	-0.123544	-0.651679	-2.908282
H	-0.200909	-2.027840	-2.249242
O	4.381780	-0.819875	-1.043913
H	4.855717	-0.109150	-1.489254
H	3.549296	-0.897639	-1.522995

M062X_Radical_24_s1

Eopt -2098.074433

O	-0.806205	1.249846	-0.465950
O	1.029341	0.168449	-0.050969
O	-0.950718	-0.905505	-0.158583
O	-2.374992	-0.852642	-2.706487
H	-2.098920	0.031673	-3.024985
H	-1.992535	-0.911849	-1.818047
O	0.105399	-1.950896	-3.596175
H	-0.801070	-1.647877	-3.416331
H	0.333957	-2.484369	-2.816568
O	2.044340	1.446526	2.373719
H	1.490404	1.568545	3.166092
H	1.491429	0.958480	1.746677
O	-4.700710	-1.909233	-1.409175
H	-4.178117	-2.511301	-0.856034
H	-4.051395	-1.542452	-2.030172
O	2.166186	2.865215	-0.140334
H	1.698010	2.042458	-0.350034
H	2.254193	2.810634	0.823678
O	3.081445	-1.720334	-0.945600
H	3.523753	-1.355502	-1.732290
H	2.598936	-0.970620	-0.566823
O	0.688290	-3.140583	-1.065168
H	0.129877	-2.431460	-0.706836
H	1.586435	-2.760441	-1.055101
O	0.177036	1.817658	4.469014
H	-0.342858	1.117636	4.033226
H	-0.156543	2.630612	4.069586
O	-0.900233	3.101260	2.041500
H	-0.589589	3.665487	1.303749
H	-0.473604	2.249641	1.886531
O	-2.144545	3.535976	-1.812174
H	-2.690082	4.217909	-2.217042
H	-2.631553	3.241429	-1.012158
O	-0.088033	4.569083	-0.172736
H	0.709701	4.026543	-0.295229
H	-0.736628	4.236172	-0.817162
O	-1.274815	1.532415	-3.580784
H	-1.553701	2.215301	-2.945331
H	-0.367317	1.291512	-3.330153
O	-2.752727	-3.192689	0.356518
H	-2.165133	-2.539122	-0.045307

H	-3.039010	-2.768162	1.188567
O	1.344581	0.461615	-3.031636
H	1.474448	0.476990	-2.074073
H	0.962894	-0.422524	-3.216576
O	4.168468	-0.106255	-3.003022
H	3.253774	0.120308	-3.234259
H	4.352547	0.439419	-2.214575
O	-3.696965	-0.006814	0.456934
H	-2.789605	-0.296266	0.272688
H	-4.234610	-0.517604	-0.173559
O	-0.253410	-4.215227	1.389022
H	-1.169571	-3.988189	1.159911
H	0.211814	-4.136768	0.540839
O	0.990617	-1.816728	2.135082
H	0.492865	-2.622196	1.888231
H	1.151364	-1.348973	1.301820
O	-1.142290	-0.184064	2.993626
H	-1.551659	0.215138	2.216614
H	-0.414185	-0.741090	2.655531
O	4.294695	-0.151432	1.791411
H	3.509179	0.309696	2.129714
H	4.065032	-1.094326	1.775471
O	-3.541752	-1.783712	2.663696
H	-2.696691	-1.448037	2.999191
H	-3.807050	-1.099202	2.026521
O	-3.321109	2.773493	0.547773
H	-2.537736	2.838202	1.121324
H	-3.503989	1.820296	0.476005
O	4.536058	1.284224	-0.611030
H	3.800400	1.908776	-0.513617
H	4.464343	0.699614	0.166306
O	3.578862	-2.944773	1.563581
H	2.701499	-2.719301	1.910967
H	3.512446	-2.731442	0.619703
C	-0.208444	0.092936	-0.212184

M062X_Radical_24_s2

Eopt -2098.073563

O	-0.928360	1.143408	-0.583369
O	0.988260	0.225122	-0.174197
O	-0.911093	-0.920018	0.004312
O	-2.536186	-1.171501	-2.421798
H	-2.279748	-0.337958	-2.859081
H	-2.110617	-1.122176	-1.552717
O	-0.094691	-2.399682	-3.320113
H	-0.994534	-2.066921	-3.121888
H	0.195367	-2.817918	-2.485277
O	2.137312	1.891573	1.968220
H	1.907772	2.769015	1.702241
H	1.563309	1.299763	1.424858
O	-4.746694	-2.107246	-0.869549
H	-4.141603	-2.708369	-0.365605
H	-4.179876	-1.793202	-1.583923
O	1.769719	2.987983	-0.897816
H	1.459778	2.085140	-0.757156
H	2.345592	3.146832	-0.158247
O	3.074318	-1.745895	-0.890922
H	3.449725	-1.493671	-1.750685
H	2.591677	-0.952064	-0.599628
O	0.718790	-3.181332	-0.721171
H	0.173417	-2.422781	-0.413178
H	1.624937	-2.796405	-0.826268
O	0.419126	2.618873	4.525856
H	0.027353	1.905440	4.062946
H	-0.036985	3.396481	4.185141
O	-0.819676	3.463484	1.589451
H	-0.736299	3.893571	0.704797
H	-0.263898	2.678616	1.512837
O	-2.915801	2.943132	-2.100340
H	-3.494796	3.292097	-2.788894
H	-3.057101	2.073375	-2.106792

O	-0.522554	4.477913	-0.969503
H	0.302438	4.003962	-1.003236
H	-1.160598	3.950113	-1.434992
O	-1.477040	1.045075	-3.692233
H	-1.702558	1.821545	-3.150389
H	-0.568857	0.839492	-3.472476
O	-2.633802	-3.374224	0.630973
H	-2.050311	-2.757125	0.148436
H	-2.612354	-4.157549	0.123426
O	1.142214	0.083854	-3.131079
H	1.329854	0.262125	-2.194717
H	0.762287	-0.823774	-3.147155
O	3.965726	-0.450312	-3.227537
H	3.038238	-0.267463	-3.402806
H	4.182866	0.198628	-2.545440
O	-3.526521	-0.265123	0.989061
H	-2.637072	-0.420352	0.652816
H	-4.082620	-0.784059	0.398094
O	-0.051756	-3.876811	1.889230
H	-0.965549	-3.843098	1.676377
H	0.374368	-3.919720	1.016928
O	1.256127	-1.405766	2.289897
H	0.712824	-2.192443	2.192397
H	1.357121	-1.041107	1.386211
O	-0.672949	0.357457	3.245560
H	-1.190453	0.647045	2.502856
H	0.009094	-0.193307	2.870363
O	4.411364	0.206051	1.543579
H	3.618680	0.706796	1.854445
H	4.210796	-0.760551	1.655676
O	-2.676038	-1.701640	3.341339
H	-1.878632	-1.158295	3.553587
H	-3.097327	-1.194156	2.661210
O	-3.457686	2.569208	0.717994
H	-2.586645	2.824197	1.106875
H	-3.540692	1.598177	0.824609
O	4.435468	1.251585	-1.058604
H	3.691773	1.839077	-1.054894
H	4.428413	0.819916	-0.182219
O	3.762318	-2.615309	1.729157
H	2.925505	-2.347727	2.097941
H	3.626119	-2.520071	0.770364
C	-0.236558	0.073666	-0.229822

M062X_Radical_24_s3

Eopt -2098.076239

O	1.915851	0.075707	0.048419
O	-0.215222	0.455110	0.666920
O	1.473574	1.015673	1.948365
O	-1.380778	1.913123	2.899347
H	-1.594227	2.798091	2.564487
H	-1.101495	1.423909	2.110367
O	-3.945740	0.450772	1.521173
H	-3.280645	-0.234188	1.733110
H	-4.070896	0.946446	2.337186
O	-0.644890	-1.003749	-1.733529
H	0.173654	-1.068342	-2.267935
H	-0.472528	-0.364118	-1.022702
O	6.044218	-0.028769	-0.068097
H	5.560871	-0.492544	0.637179
H	6.981446	-0.167987	0.096767
O	-2.896071	0.519971	-2.594204
H	-2.917972	1.031133	-1.763574
H	-2.123283	-0.059225	-2.477900
O	-1.938545	-1.387907	1.977975
H	-2.013485	-2.325359	1.726496
H	-1.251178	-1.011601	1.406316
O	-0.386383	-0.464212	4.150636
H	-0.470369	0.483571	3.980044
H	-1.038144	-0.861475	3.547599
O	1.599995	-1.307239	-3.364284

H	2.335037	-1.759343	-2.931632
H	1.859243	-0.372985	-3.344920
O	1.880357	1.414492	-2.488895
H	1.568778	0.877787	-1.744445
H	2.768965	1.678279	-2.202777
O	0.972076	3.881752	1.334326
H	1.719282	4.488296	1.361934
H	1.282888	3.059617	1.734135
O	-1.700050	3.022047	-3.404125
H	-2.097538	2.151407	-3.256089
H	-1.152276	3.175118	-2.620215
O	-1.851757	4.304027	1.353056
H	-0.883749	4.316134	1.302770
H	-2.122840	3.634873	0.701440
O	4.020974	-1.199884	1.509768
H	3.445903	-0.572432	1.043128
H	3.893240	-2.023437	1.003077
O	-2.493141	2.032623	-0.249045
H	-1.584302	1.707551	-0.167352
H	-2.996210	1.518528	0.414356
O	-5.975176	-1.063785	0.201186
H	-5.335668	-0.523033	0.688908
H	-5.538226	-1.261793	-0.645978
O	4.038982	1.983555	-0.575662
H	3.327954	1.490023	-0.142892
H	4.820479	1.422532	-0.454629
O	1.402519	-1.983812	2.598601
H	2.283680	-1.618894	2.433633
H	0.922159	-1.327069	3.132491
O	0.514113	-2.930502	0.184405
H	0.736756	-2.454764	1.011154
H	0.138461	-2.273460	-0.421560
O	4.074337	-1.004829	-1.817944
H	3.408144	-0.454216	-1.386276
H	4.910042	-0.754852	-1.390170
O	-2.453385	-3.201709	-1.655280
H	-1.821534	-2.464084	-1.645996
H	-2.402649	-3.584412	-0.765358
O	3.293183	-3.266584	-0.321930
H	3.552251	-2.575267	-0.956347
H	2.331563	-3.169384	-0.223086
O	0.216490	3.434984	-1.351984
H	0.855391	2.818389	-1.743594
H	0.488297	3.550779	-0.426419
O	-4.701753	-1.632178	-2.243757
H	-4.198131	-0.815032	-2.406047
H	-4.008185	-2.272979	-2.005511
O	-1.885170	-4.017183	1.006823
H	-1.889692	-4.825341	1.528568
H	-0.955064	-3.839140	0.771908
C	1.021156	0.477058	0.814706

M06L_3_s1

Eopt -493.490829

O	2.715138	0.227492	-0.118502
O	0.669317	0.909359	0.455949
O	0.975519	-1.138924	-0.395427
O	-1.605006	-1.347592	-0.866511
H	-1.862969	-0.431580	-1.040688
H	-0.629842	-1.263890	-0.667171
O	-1.329278	-0.285570	1.842016
H	-0.575120	0.151679	1.381847
H	-1.712160	-0.823455	1.136407
O	-1.559430	1.558797	-0.918536
H	-0.732908	1.308304	-0.439176
H	-2.208423	1.695034	-0.221423
C	1.465224	-0.004097	-0.023618

M06L_3_s2

Eopt -493.495851

C	-0.006555	-0.002948	0.042191
O	-0.337780	-1.247429	0.070471

O	-0.918092	0.907008	0.025240
O	1.236767	0.332919	0.031336
O	2.804026	-1.770266	-0.055906
H	2.178283	-0.991867	-0.019167
H	2.234257	-2.541346	0.005761
O	-2.941858	-1.516208	-0.053203
H	-3.300569	-0.624576	-0.052532
H	-1.951810	-1.383660	-0.008034
O	0.155805	3.296402	-0.033169
H	1.108407	3.169926	-0.046729
H	-0.220190	2.369801	-0.010601

M06L_3_s3 Eopt -493.488892

C	-1.595662	-0.146190	-0.099980
O	-1.310788	0.852333	0.669080
O	-2.751127	-0.257363	-0.630619
O	-0.684589	-1.043920	-0.331665
O	1.237436	-0.980312	1.348555
H	0.444475	-0.969305	0.707426
H	1.261101	-0.091211	1.716420
O	2.688672	-0.396741	-0.949306
H	2.279537	-0.712395	-0.119800
H	2.086290	-0.691786	-1.639695
O	1.033881	1.910429	-0.086513
H	0.199730	1.466520	0.204457
H	1.594958	1.199902	-0.425174

M06L_6_s1 Eopt -722.829847

O	1.263842	0.196284	-1.574831
O	-0.509926	1.123816	-0.575962
O	-0.657314	-0.941085	-1.424304
O	1.019551	-2.838749	-0.213247
O	2.457084	0.665223	0.844759
O	1.091008	3.146051	0.205913
H	2.118285	0.465387	-0.058052
H	1.015165	-2.382060	0.643545
H	1.731448	3.298460	-0.494083
H	0.526678	2.408302	-0.142891
H	2.143006	1.573949	0.965765
H	0.472574	-2.243889	-0.764432
O	0.677170	-1.129592	2.128794
O	-1.901194	-1.398659	0.961004
O	-3.137085	1.068246	0.022942
H	-1.498211	-1.280863	0.067507
H	-2.183799	1.058141	-0.249861
H	-0.222600	-1.054296	1.762097
H	-3.574184	0.527163	-0.639333
H	-2.472933	-0.620089	1.017743
H	1.199265	-0.430265	1.692170
C	0.037872	0.127328	-1.196373

M06L_6_s2 Eopt -722.833148

O	0.655348	1.286551	-0.127168
O	-1.485918	0.698812	-0.232664
O	0.075659	-0.859113	0.093906
O	2.147892	-0.967590	1.911414
O	3.258539	0.898927	0.034863
O	-1.755462	3.365353	-0.272712
H	2.275095	1.048339	-0.025549
H	2.787353	-0.360144	1.517389
H	-0.862288	3.719906	-0.258381
H	-1.629803	2.384745	-0.264010
H	3.666738	1.758965	-0.098335
H	1.398771	-0.941816	1.280951
O	-1.826403	-2.606727	-0.763438
O	-3.486359	-0.786251	0.731479
H	-1.118189	-1.986871	-0.480722
H	-2.709624	-0.261054	0.415538
H	-3.260146	-1.057011	1.625850
H	-2.610185	-2.226964	-0.342699

C	-0.246046	0.381794	-0.088881
O	2.308281	-1.344208	-1.469682
H	1.501960	-1.202172	-0.933831
H	2.903977	-0.652701	-1.150903

M06L_6_s3 Eopt -722.829638

O	0.918627	0.298938	-1.783761
O	-1.165300	0.591145	-1.051868
O	-0.251017	-1.442099	-1.010580
O	2.107977	-2.168554	0.171505
O	2.727686	0.661748	0.262399
O	-0.117973	2.797561	-0.015893
H	2.149796	0.582801	-0.524305
H	2.512267	-1.299091	0.306681
H	-0.845376	3.366001	0.253755
H	-0.542456	2.029679	-0.479536
H	2.087908	0.752029	0.988908
H	1.279138	-1.955660	-0.308569
O	0.517434	0.943085	2.036914
O	-1.035032	-1.379559	1.589373
O	-3.300107	-0.514770	0.084475
H	-0.738739	-1.481965	0.655963
H	-2.508051	-0.112277	-0.360074
H	-0.040948	0.162375	1.865105
H	-3.926918	0.206786	0.187614
H	-1.943128	-1.062866	1.479912
H	0.226057	1.617219	1.398044
C	-0.154654	-0.184165	-1.287336

M06L_9_s1 Eopt -952.163791

O	0.951454	1.720216	-0.977927
O	0.993547	-0.406130	-1.658281
O	0.042636	0.125889	0.283142
O	-0.461805	-2.340524	1.036949
H	-0.168264	-1.455226	0.694880
H	0.142563	-2.981704	0.650161
O	2.702863	-1.837813	0.010719
H	2.052027	-1.458806	-0.611951
H	2.522891	-1.377999	0.843521
O	-1.240825	-1.911633	-1.821053
H	-1.342887	-2.270429	-0.930131
H	-0.383998	-1.425659	-1.774680
O	-1.529891	2.788290	-0.404015
H	-0.611026	2.487502	-0.566603
H	-1.716498	2.496553	0.500646
O	2.173150	0.221877	2.100005
H	1.338252	0.236592	1.597322
H	2.795655	0.662945	1.502925
O	-1.625752	1.283630	2.091256
H	-2.298224	0.594120	1.984153
H	-0.911252	0.962813	1.503711
O	3.669165	1.066327	-0.289215
H	3.593547	0.110655	-0.416889
H	2.821753	1.418300	-0.612580
O	-3.085489	-1.048090	1.135180
H	-2.288738	-1.597785	1.123885
H	-3.047169	-0.547738	0.300210
O	-2.833090	0.384201	-1.306563
H	-2.307397	1.163212	-1.056208
H	-2.197128	-0.306070	-1.565698
C	0.659699	0.486466	-0.794708

M06L_9_s2 Eopt -952.165304

O	-1.391877	-0.111577	-1.390557
O	0.732154	0.544646	-1.513739
O	0.057743	-0.711212	0.199136
O	2.217512	0.285077	1.457827
H	1.462790	-0.111315	0.957624
H	2.244475	1.199425	1.146329

O	1.237606	2.738555	0.105103
H	1.129335	1.997260	-0.524130
H	0.571402	2.545874	0.783346
O	2.920712	-1.114400	-1.749309
H	3.447650	-1.135356	-0.936279
H	2.173916	-0.510291	-1.566486
O	-3.420106	-0.105444	0.551033
H	-2.731902	-0.037381	-0.137585
H	-3.015126	-0.710864	1.190802
O	-0.928761	1.622100	1.698350
H	-0.625411	0.751253	1.396662
H	-1.462637	1.947786	0.956026
O	-1.636627	-1.845581	1.977561
H	-1.831994	-2.752227	1.722418
H	-1.054100	-1.498942	1.263795
O	-1.818111	2.625574	-0.897142
H	-0.917320	2.970678	-0.918880
H	-1.731590	1.709273	-1.219519
O	4.446948	-1.101638	0.702617
H	3.672903	-0.604356	1.041075
H	4.349087	-1.989432	1.059065
O	-2.361893	-2.679271	-1.054371
H	-2.944497	-2.596180	-0.293047
H	-2.001621	-1.776828	-1.171436
C	-0.196293	-0.095502	-0.906974

M06L_9_s3 Eopt -952.163787

O	-1.392021	-0.155520	-1.372989
O	0.730272	0.506388	-1.502558
O	0.042728	-0.672558	0.258819
O	2.217046	0.363113	1.462960
H	1.457136	-0.049221	0.984609
H	2.230286	1.270854	1.132221
O	1.191806	2.765001	0.048830
H	1.102226	2.004434	-0.559326
H	0.529562	2.576743	0.732300
O	2.895330	-1.187903	-1.706793
H	3.449666	-1.146300	-0.913035
H	2.157136	-0.567878	-1.544830
O	-3.446039	-0.047761	0.490658
H	-2.716684	-0.066476	-0.160599
H	-3.132582	-0.647159	1.181002
O	-0.962567	1.673539	1.677226
H	-0.656505	0.796291	1.395551
H	-1.499677	1.977894	0.928297
O	-1.759044	-1.965465	1.781616
H	-1.302452	-2.217471	2.589543
H	-1.092842	-1.483974	1.233920
O	-1.849301	2.600138	-0.948705
H	-0.949659	2.947908	-0.974270
H	-1.757734	1.676745	-1.247156
O	4.466988	-0.991668	0.700621
H	3.686011	-0.504984	1.038056
H	4.417914	-1.859594	1.112146
O	-2.210245	-2.801595	-0.955206
H	-2.171849	-2.850500	0.008819
H	-1.934550	-1.883932	-1.142370
C	-0.202504	-0.109841	-0.878453

M06L_12_s1 Eopt -1181.500334

O	-0.924289	-0.935502	1.377328
O	0.702478	-0.193168	0.061230
O	-0.937125	1.182518	0.665895
O	0.222148	0.296090	-2.614856
H	0.489595	0.167623	-1.681716
H	-0.743644	0.378850	-2.543683
O	-3.690272	-0.716302	1.363733
H	-2.716187	-0.795912	1.389676
H	-3.833822	0.241330	1.364998
O	3.646172	-1.175748	1.292778

H	3.147186	-1.779142	0.719512
H	3.541707	-0.306275	0.873838
O	-1.898004	-2.305589	-0.921756
H	-1.156764	-2.451569	-1.534739
H	-1.488484	-1.990409	-0.097331
O	2.399485	3.956523	-0.038025
H	2.206066	4.170721	0.879503
H	1.555020	3.625365	-0.407480
O	1.300551	-1.636405	2.959902
H	2.074475	-1.397872	2.427200
H	0.534938	-1.458385	2.384853
O	-3.384557	2.145822	1.358361
H	-2.481946	1.797219	1.198626
H	-3.394677	2.407640	2.283687
O	3.032688	1.183194	-0.225079
H	2.954279	2.139166	-0.076553
H	2.120432	0.840699	-0.149130
O	0.349130	-2.571593	-2.658507
H	0.350656	-1.607831	-2.786607
H	0.877859	-2.706653	-1.852643
O	1.613074	-2.647356	-0.131935
H	1.198341	-1.751837	0.010137
H	1.195306	-3.225075	0.515094
O	-2.501819	0.389745	-1.671884
H	-2.412002	-0.554712	-1.449812
H	-2.128501	0.841816	-0.899166
O	0.113656	2.870905	-1.129728
H	-0.240462	2.241204	-0.454344
H	0.354584	2.299252	-1.869915
C	-0.391748	0.021617	0.709389

M06L_12_s2 Eopt -1181.497731

O	-0.260647	-0.363209	0.250598
O	0.453110	0.617185	-1.615656
O	-1.676845	0.830940	-0.987869
O	1.485367	-1.931403	-2.025635
H	1.123206	-1.031911	-1.896657
H	0.979608	-2.495468	-1.417584
O	1.901139	0.744351	2.746157
H	0.982207	1.054744	2.696659
H	1.858741	-0.189148	2.480126
O	-2.231595	-2.114550	0.685058
H	-1.526932	-1.433996	0.553386
H	-2.830637	-1.962975	-0.064132
O	0.415594	3.378625	0.390446
H	1.217107	2.834719	0.346687
H	0.096006	3.385621	-0.528057
O	1.757361	-1.745047	1.354093
H	2.577056	-1.675182	0.839034
H	1.109636	-1.198705	0.851171
O	-0.825689	1.509829	2.155320
H	-0.555273	2.271627	1.612820
H	-0.688317	0.755398	1.542868
O	-3.697936	-0.938974	-1.441351
H	-3.533640	-1.320357	-2.308894
H	-2.968872	-0.296146	-1.302213
O	-3.463808	0.256948	1.954418
H	-3.117818	-0.564884	1.575488
H	-2.684718	0.826232	2.035498
O	-0.160352	3.135034	-2.417755
H	-1.119542	3.167041	-2.485420
H	0.040185	2.189333	-2.231660
O	3.798360	-1.161306	-0.596881
H	3.080266	-1.490289	-1.168134
H	3.538265	-0.244834	-0.406389
O	2.533354	1.356898	0.018424
H	1.800928	1.012295	-0.538527
H	2.316207	1.106976	0.933863
O	0.144126	-3.633219	-0.092869
H	-0.729112	-3.252619	0.092424

H 0.734764 -3.178923 0.529574
C -0.511939 0.365771 -0.792318

M06L_12_s3 Eopt -1181.499046

O -0.450651 -0.271469 0.576061
O 0.476341 0.400841 -1.338564
O -0.692301 -1.492813 -1.272779
O 2.502122 -1.513791 -2.005182
H 1.832790 -0.810259 -1.936394
H 2.129781 -2.238217 -1.474618
O -1.530468 -2.480630 1.811407
H -1.097846 -1.715528 1.379537
H -2.320260 -2.605509 1.271372
O 0.986151 4.357829 -0.487574
H 1.597208 3.618143 -0.344546
H 0.124282 3.914082 -0.515483
O 1.864825 -1.393476 1.779372
H 2.622425 -1.053140 1.271170
H 1.094718 -0.912785 1.429737
O -2.774127 1.028330 1.484779
H -2.051982 0.457138 1.168158
H -3.379639 1.071138 0.733664
O 0.390245 1.813780 2.146399
H 0.674331 1.358837 2.945758
H 0.068734 1.099680 1.555055
O -3.218573 -1.794102 -0.471662
H -2.271730 -1.771496 -0.758053
H -3.670031 -2.339354 -1.123556
O -1.219385 2.539503 -0.631296
H -1.518799 2.306810 0.259074
H -0.545763 1.867257 -0.851828
O 3.963288 -0.380105 0.141353
H 3.585333 -0.819524 -0.641125
H 3.508137 0.481659 0.155888
O 2.292795 1.861890 0.070603
H 1.635819 1.341427 -0.448892
H 1.870668 1.927039 0.943970
O 1.150669 -3.335882 -0.213543
H 1.436851 -2.811028 0.553483
H 0.372765 -2.850445 -0.542375
O -3.526705 0.897108 -1.402005
H -3.372681 -0.025523 -1.136726
H -2.682333 1.356162 -1.277020
C -0.226096 -0.457111 -0.685866

M06L_15_s1 Eopt -1410.837224

O 0.005440 -0.963851 1.101398
O 1.120357 0.549336 -0.083709
O -0.568113 -0.552998 -1.018858
O 2.800192 -0.325100 -2.112910
H 2.178790 0.137541 -1.519796
H 2.404751 -1.210455 -2.177451
O -0.904605 -3.591570 0.524125
H -0.519616 -2.723095 0.736620
H -1.691679 -3.350497 0.013452
O 1.261298 3.256963 2.164447
H 1.855830 2.490592 2.222468
H 1.112947 3.375078 1.209016
O 2.300208 -2.629459 0.852877
H 3.062582 -2.052429 0.673061
H 1.589118 -2.021206 1.116757
O -1.676087 3.262935 -2.010213
H -2.056275 2.766780 -1.266301
H -1.177262 2.581367 -2.496646
O -0.910340 1.453015 2.384547
H -0.198451 2.115610 2.327032
H -0.487040 0.610984 2.149768
O -2.806937 -2.145968 -1.082891
H -2.028468 -1.555941 -1.010881
H -3.518703 -1.676387 -0.627955

O 0.840150 3.231825 -0.618230
H -0.017935 3.426729 -1.027111
H 0.863035 2.257488 -0.551404
O 4.347049 -0.731342 0.265880
H 3.906738 -0.553776 -0.583682
H 3.900771 -0.149588 0.903514
O 2.648176 0.750637 2.044317
H 2.014312 0.623836 1.286642
H 2.351734 0.139309 2.726585
O 1.246501 -2.722150 -1.811462
H 1.597108 -2.814188 -0.907209
H 0.477871 -2.141086 -1.702865
O -0.040486 1.197192 -3.028460
H -0.190928 0.559890 -2.292495
H 0.818013 1.589321 -2.836282
C 0.184289 -0.326123 0.000917
O -4.611738 -0.285655 0.235537
H -3.970688 0.448978 0.192363
H -5.281546 -0.020556 0.873175
O -2.430649 1.409335 0.001093
H -1.959582 1.506653 0.851810
H -1.917192 0.738615 -0.481531
O -2.612076 -1.284239 2.137889
H -3.298842 -1.015812 1.511579
H -1.771864 -1.177163 1.659526

M06L_15_s2 Eopt -1410.83368

O 0.453597 0.055422 0.690313
O 0.032256 -0.049024 -1.491086
O -1.622444 -0.319188 -0.021870
O 2.067685 -1.901174 -1.313365
H 1.411172 -1.177610 -1.386121
H 2.163621 -2.066677 -0.358813
O 2.107644 3.029159 1.202092
H 1.195662 2.892043 1.504063
H 2.551325 2.180121 1.362105
O -0.026750 -1.618431 2.752099
H 0.125278 -0.952849 2.042512
H -0.598210 -2.271488 2.313892
O -0.991554 3.182184 -0.888651
H -0.059758 3.034572 -1.109786
H -1.466737 2.576240 -1.484441
O 3.107409 0.353864 1.066597
H 3.596593 0.368247 0.228426
H 2.168140 0.248203 0.794408
O -0.662984 2.304498 1.804098
H -0.923181 2.661270 0.936034
H -0.262103 1.444075 1.567116
O -1.792449 -2.946856 0.985837
H -1.237346 -3.300792 0.270488
H -1.882571 -2.009187 0.738384
O -2.301768 0.246207 3.168674
H -1.593419 -0.410932 3.095554
H -1.973390 1.002768 2.661977
O -2.080185 1.248443 -2.690608
H -2.849266 0.956725 -2.188079
H -1.346198 0.694226 -2.349879
O 3.926535 0.269111 -1.697849
H 3.409564 -0.552925 -1.663896
H 3.252941 0.966753 -1.764275
O 1.728397 2.127901 -1.500752
H 1.169260 1.323160 -1.460360
H 1.890968 2.385241 -0.576476
O 2.510507 -2.407770 1.493845
H 1.671979 -2.295875 1.969189
H 2.903316 -1.519417 1.503613
C -0.383472 -0.106568 -0.273839
O -3.529929 1.688738 0.213721
H -2.796268 1.049075 0.152315
H -3.105801 2.549994 0.150270

O	-2.549433	-1.833060	-2.082347
H	-2.264336	-1.213246	-1.373185
H	-2.431936	-1.338609	-2.899817
O	-0.359355	-3.512907	-1.419155
H	0.472577	-3.013984	-1.421571
H	-1.028448	-2.906637	-1.783355

M06L_15_s3 Eopt -1410.835548

O	0.584543	0.352233	1.254301
O	-0.675168	0.053778	-0.557643
O	1.519991	-0.268231	-0.673461
O	-0.090214	1.954355	-2.573758
H	-0.350615	1.187331	-2.033418
H	0.760184	2.223018	-2.187772
O	3.157927	1.060378	1.967358
H	2.258690	0.785934	1.698987
H	3.725180	0.723040	1.259823
O	-4.369925	-0.833724	0.102866
H	-3.923442	0.021044	0.245065
H	-3.837159	-1.448019	0.625079
O	0.494787	3.194565	1.073632
H	-0.231626	3.391425	0.455065
H	0.431276	2.239274	1.240856
O	0.519100	-2.155173	2.542447
H	0.622592	-1.235092	2.242036
H	1.060880	-2.651989	1.912711
O	-1.538913	0.826654	2.947029
H	-1.246525	1.609400	3.424749
H	-0.805870	0.625811	2.328494
O	2.071812	-2.868890	0.223348
H	1.978494	-1.961210	-0.121873
H	2.865208	-3.227519	-0.186544
O	-1.907770	-1.961566	1.059489
H	-1.182539	-2.114459	1.690948
H	-1.612742	-1.186685	0.549397
O	-1.563471	3.656623	-0.826088
H	-1.104501	3.132547	-1.506597
H	-2.120867	3.006471	-0.365054
O	-2.757009	1.449448	0.471284
H	-1.989928	0.963127	0.089580
H	-2.567175	1.420868	1.424006
O	2.301852	2.502573	-1.034753
H	1.775355	2.847191	-0.291712
H	2.269436	1.541355	-0.909581
O	-0.463387	-3.581177	-0.834618
H	0.418251	-3.449056	-0.446291
H	-1.056882	-3.069897	-0.260409
C	0.475935	0.043455	0.009774
O	-2.569864	-1.333309	-2.126095
H	-1.750343	-0.969722	-1.756300
H	-3.226458	-1.186539	-1.426661
O	0.559104	-1.760220	-2.827875
H	0.909978	-1.145921	-2.155724
H	0.075487	-2.409296	-2.292720
O	4.305818	-0.192487	-0.396089
H	4.551558	0.550198	-0.957200
H	3.340161	-0.267954	-0.499425

M06L_Radical_3_s1 Eopt -493.314794

O	-2.997331	-0.983208	-0.206606
O	-0.847783	-1.248260	-0.034225
O	-1.792204	0.803473	0.087135
O	0.484505	2.395467	-0.183766
H	0.732891	2.427552	-1.112625
H	-0.322708	1.849747	-0.156209
O	1.526420	-0.021340	0.881909
H	0.730932	-0.501969	0.592918
H	1.368559	0.881334	0.559696
O	3.735797	-0.968797	-0.517459
H	4.380933	-1.222282	0.148263

H	2.965664	-0.647358	-0.011855
C	-1.788584	-0.434283	-0.039349

M06L_Radical_3_s2 Eopt -493.313835

C	1.318013	-0.243532	-0.010927
O	1.078268	-0.931270	-1.007759
O	1.185491	-0.605307	1.215446
O	1.727987	0.973737	-0.009293
O	-1.001728	1.644908	-1.064846
H	-0.052009	1.725752	-0.905790
H	-1.106106	0.763821	-1.444212
O	-1.707356	-1.563198	-0.559354
H	-1.799994	-0.950054	0.185479
H	-0.768814	-1.497315	-0.790485
O	-1.546364	0.507512	1.501889
H	-1.403576	1.049287	0.707556
H	-0.667970	0.158652	1.704348

M06L_Radical_3_s3 Eopt -493.316394

C	-2.325103	0.153042	-0.118029
O	-1.789621	1.166988	0.459234
O	-3.432261	0.549475	-0.631790
O	-1.860216	-0.992776	-0.168975
O	0.580128	-0.940164	1.168679
H	-0.279723	-0.970023	0.705952
H	0.613844	-0.060109	1.557622
O	2.479113	-0.889196	-0.845905
H	1.813741	-0.939427	-0.131453
H	2.983708	-1.705378	-0.778647
O	4.196574	1.148303	0.017533
H	3.838704	1.964413	-0.342638
H	3.590601	0.451242	-0.292868

M06L_Radical_6_s1 Eopt -722.644285

O	1.406701	0.480748	1.890128
O	0.296526	-1.247600	1.115944
O	-0.768511	0.545427	1.878350
O	-0.503203	3.020910	0.293489
O	1.973982	1.297470	-0.895035
O	2.018018	-1.524083	-1.185304
H	1.904432	1.318593	0.068610
H	0.144334	2.744795	-0.362994
H	2.850683	-1.904553	-0.891520
H	1.463852	-1.527966	-0.388158
H	2.150977	0.355016	-1.072828
H	-0.640715	2.221858	0.822198
O	-0.576061	0.561567	-2.065346
O	-2.758475	0.155494	-0.197316
O	-1.566223	-2.402676	-0.732604
H	-2.210676	0.344523	0.578872
H	-0.907590	-2.068090	-0.103128
H	-1.280717	0.529459	-1.398011
H	-1.206766	-2.147811	-1.588055
H	-2.552382	-0.776644	-0.384836
H	0.211791	0.855884	-1.581188
C	0.298099	-0.090281	1.619137

M06L_Radical_6_s2 Eopt -722.645498

O	-0.089814	-1.459713	1.275525
O	0.191954	-0.350768	-0.658175
O	0.196615	0.584536	1.390202
O	-2.044995	2.316437	-0.217236
O	-2.915044	-0.221795	0.737627
O	-2.035908	-2.031491	-1.271312
H	-2.422796	-0.477281	1.524887
H	-2.217847	1.416746	0.105803
H	-1.900362	-2.862674	-0.804640
H	-1.175799	-1.583633	-1.229796
H	-2.680357	-0.889592	0.069006
H	-1.115684	2.325944	-0.491306

O	0.710587	2.382794	-1.135291
O	3.156376	0.743818	0.805138
O	2.784465	-1.558872	-0.878795
H	2.254321	0.902750	1.108062
H	1.857694	-1.294346	-0.983030
H	0.648655	2.569502	-2.077320
H	2.756346	-2.305648	-0.271856
H	3.086959	-0.046147	0.244495
H	0.667276	1.413710	-1.065876
C	0.101286	-0.401483	0.581684

M06L_Radical_6_s3 Eopt -722.642006

O	-0.118906	-0.104462	0.823494
O	0.440661	0.579399	-1.242876
O	0.020203	-1.550125	-0.648082
O	3.015828	-1.843418	-0.610066
O	2.779729	-0.017554	1.554876
O	2.346589	2.270099	-0.038973
H	1.857177	-0.242987	1.726489
H	2.985647	-1.222202	0.138334
H	1.935849	2.920404	0.539149
H	1.606027	1.809010	-0.469282
H	2.718565	0.810762	1.044880
H	2.087470	-2.025203	-0.796468
O	-3.115918	-0.213931	1.961873
O	-2.948058	-1.015168	-0.766678
O	-2.234129	1.728460	-1.015844
H	-2.099028	-1.472428	-0.817997
H	-1.291615	1.569533	-1.174080
H	-3.051584	-0.539691	1.047772
H	-2.299079	1.848808	-0.062016
H	-2.743644	-0.089493	-0.988579
H	-4.052090	-0.268617	2.174378
C	0.143053	-0.294048	-0.417394

M06L_Radical_9_sl Eopt -951.972334

O	-0.725374	-1.300168	0.230504
O	-0.920447	-0.077027	-1.425935
O	-0.852367	0.917666	0.587031
O	0.825028	2.862913	-0.542182
H	0.098051	2.312967	-0.205899
H	0.482028	3.274461	-1.341714
O	-3.849100	0.663436	-1.227011
H	-2.947313	0.589049	-1.563295
H	-3.742859	0.955012	-0.308654
O	1.615362	-1.981784	-1.534004
H	1.775200	-1.018146	-1.555530
H	0.683149	-2.062777	-1.301259
O	2.542351	-1.787565	1.165743
H	2.211094	-1.952671	0.266427
H	2.088202	-0.974887	1.451306
O	-3.513544	0.717053	1.709550
H	-2.572171	0.882434	1.556498
H	-3.623309	-0.217655	1.476119
O	1.670554	0.795664	1.896611
H	2.243486	1.252741	1.270598
H	0.777291	0.894688	1.530399
O	-3.652356	-1.824605	0.263991
H	-3.796763	-1.147945	-0.416124
H	-2.691566	-1.919460	0.298990
O	2.387104	0.679804	-1.429187
H	1.849141	1.424890	-1.108350
H	3.125636	0.591926	-0.801697
O	4.456428	0.142253	0.430999
H	3.949116	-0.641833	0.709240
H	5.196765	-0.200326	-0.079438
C	-0.829051	-0.083929	-0.147747

M06L_Radical_9_s2 Eopt -951.975977

O	0.391657	0.223565	-2.020253
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O	1.931752	1.323287	-0.948955
O	1.817093	-0.928347	-0.842863
O	3.870586	-1.744756	0.959005
H	3.238182	-1.530556	0.254593
H	3.324796	-2.079727	1.678129
O	-0.203620	3.155874	-0.884307
H	0.626631	2.657625	-0.971532
H	-0.002764	3.878068	-0.280807
O	3.778183	1.124436	1.242171
H	3.896937	0.164084	1.297867
H	3.145535	1.232198	0.515125
O	-2.342030	-0.960946	-0.972859
H	-2.281044	-0.672627	-1.889393
H	-1.640716	-1.636611	-0.860166
O	0.810475	-0.445845	1.942173
H	1.350374	-0.760230	1.207306
H	0.121955	0.092895	1.512026
O	-0.302762	-2.737775	-0.508607
H	-0.267115	-3.375741	-1.228543
H	0.457660	-2.147477	-0.655645
O	-1.219566	1.020224	0.664754
H	-0.900038	1.775639	0.139010
H	-1.547412	0.368996	0.016941
O	-4.868513	-1.058829	0.215098
H	-4.003686	-1.135404	-0.225870
H	-4.892361	-1.784732	0.845959
C	1.454177	0.206854	-1.213916
O	-3.921129	1.273610	1.586385
H	-2.990130	1.269724	1.312937
H	-4.298885	0.486771	1.161610

M06L_Radical_9_s3 Eopt -951.973091

O	0.506572	0.227917	-1.840744
O	1.724901	1.140268	-0.443852
O	1.637348	-1.108975	-0.430583
O	3.986440	-0.956852	1.154728
H	3.175135	-1.055371	0.627735
H	3.708885	-0.457757	1.929859
O	-0.463975	3.038300	-0.282726
H	0.367426	2.563693	-0.426501
H	-0.246984	3.736640	0.343192
O	4.663954	1.018963	-0.797458
H	4.577250	0.355002	-0.094297
H	3.755140	1.314171	-0.928744
O	-2.030306	-0.997844	-0.926820
H	-1.434123	-0.563578	-1.550141
H	-1.537169	-1.782334	-0.615288
O	0.714246	-0.532241	2.345662
H	1.139638	-0.924970	1.573692
H	-0.023753	-0.022880	1.965761
O	-0.384343	-3.015669	0.021350
H	-0.329720	-3.730375	-0.621069
H	0.378723	-2.443929	-0.169895
O	-1.455382	0.814546	1.148974
H	-1.137752	1.611584	0.687063
H	-1.638173	0.170252	0.439602
O	-4.802996	-0.623765	-0.934215
H	-3.855478	-0.840391	-0.982425
H	-5.218050	-1.400387	-0.547001
C	1.314549	0.006974	-0.864638
O	-4.307191	1.206152	1.210511
H	-3.340811	1.144727	1.266627
H	-4.541613	0.597650	0.491040

M06L_Radical_12_sl Eopt -1181.304365

O	-0.319105	-0.040367	0.214754
O	1.178513	-1.005930	-1.040098
O	-0.133414	0.647352	-1.831210
O	-1.634423	-2.172306	-2.281747
H	-0.854066	-1.831315	-2.731699

H	-2.174720	-1.389124	-2.090982
O	-1.938924	0.831657	2.721492
H	-0.995297	0.687181	2.597586
H	-2.190629	1.458610	2.014636
O	4.037771	-0.827930	0.713042
H	3.681107	-1.711458	0.569145
H	3.905817	-0.359470	-0.131609
O	-3.083836	-1.181173	1.063513
H	-2.406204	-1.860165	0.887514
H	-2.665617	-0.556969	1.681652
O	2.259101	2.469240	0.138202
H	2.127204	1.840387	0.869410
H	1.368177	2.763353	-0.111397
O	1.974756	0.443945	2.102401
H	2.676881	-0.067893	1.655153
H	1.150268	0.108622	1.730490
O	-2.814627	2.460848	0.650969
H	-3.134718	1.797783	0.023430
H	-2.000899	2.799493	0.236773
O	3.452364	0.676523	-1.627995
H	3.015921	1.357513	-1.079096
H	2.741213	0.050711	-1.821397
O	-1.216402	-3.145138	0.332350
H	-1.199258	-2.812143	-0.582393
H	-0.331254	-2.977461	0.693207
O	1.481706	-2.650833	1.206492
H	1.468390	-1.976532	0.504041
H	1.593861	-2.157551	2.025682
O	-3.018615	0.232581	-1.332691
H	-2.996009	-0.256612	-0.483774
H	-2.123084	0.580526	-1.457051
O	-0.411909	3.155438	-0.630005
H	-0.406851	2.339104	-1.161575
H	-0.480722	3.877778	-1.263156
C	0.287806	-0.142603	-0.961724

M06L_Radical_12_s2			Eopt -1181.304236
O	-0.008617	0.287994	0.427525
O	0.273661	-0.258386	-1.738486
O	1.633094	1.122243	-0.749908
O	-2.574618	0.310000	-1.608915
H	-1.659989	-0.011836	-1.623364
H	-2.695447	0.733656	-0.738666
O	0.164796	-2.507224	2.291589
H	0.868291	-1.847267	2.376712
H	-0.660397	-2.003453	2.370439
O	-0.350932	3.031956	0.985622
H	-0.196012	2.083225	1.109479
H	-0.471016	3.098731	0.020805
O	2.687472	-1.949204	-0.083206
H	1.843619	-2.407663	-0.191319
H	2.858597	-1.551390	-0.954451
O	-2.165684	-0.905661	1.710539
H	-2.652753	-1.482221	1.098207
H	-1.443414	-0.552603	1.161407
O	2.161730	-0.267539	2.120344
H	2.495762	-0.787098	1.365403
H	1.324226	0.080129	1.776082
O	-0.942953	2.848954	-1.785517
H	-1.554858	2.102072	-1.856709
H	-0.159113	2.570569	-2.271156
O	2.573438	2.663855	1.684779
H	1.679044	2.875691	1.383719
H	2.577271	1.701275	1.785694
O	2.912516	-0.873599	-2.723410
H	3.377026	-0.034938	-2.632554
H	1.976430	-0.640431	-2.625394
O	-3.097680	-2.366702	-0.570288
H	-3.069272	-1.500516	-1.007165
H	-2.176139	-2.673600	-0.598979

O	-0.248116	-2.849358	-0.498971
H	-0.168609	-1.991281	-0.943441
H	-0.145403	-2.665098	0.452882
O	-3.043050	1.685856	0.827483
H	-2.258878	2.239978	0.950817
H	-2.867773	0.886617	1.349301
C	0.563059	0.331995	-0.678530

M06L_Radical_12_s3			Eopt -1181.30292
O	-0.517886	-0.262496	1.169234
O	0.428635	-0.310459	-0.873261
O	1.530653	-0.457045	1.086288
O	-1.195956	1.922678	-1.533267
H	-0.773875	1.058613	-1.387802
H	-1.434034	2.223990	-0.633253
O	1.039280	2.472311	1.628591
H	1.349655	1.572455	1.788964
H	1.233652	2.631261	0.688106
O	0.209404	-3.369945	0.284730
H	-0.532290	-3.081950	-0.261516
H	0.994664	-3.106824	-0.223839
O	-3.576482	0.435357	1.039771
H	-3.663054	0.451231	0.070480
H	-3.268565	-0.458476	1.245984
O	4.341749	-1.277408	0.234157
H	3.963057	-1.511287	1.087956
H	4.074865	-0.349236	0.096915
O	-2.510065	-2.218017	1.528241
H	-2.598302	-3.175053	1.584942
H	-1.566400	-2.030824	1.622374
O	1.462772	2.806176	-1.170996
H	0.541264	2.617667	-1.423036
H	1.614745	3.732077	-1.385427
O	2.327160	-2.382878	-1.401265
H	3.061567	-2.070541	-0.842380
H	1.738368	-1.614364	-1.450034
O	-3.633203	0.444357	-1.817993
H	-2.897683	1.077855	-1.852830
H	-3.181184	-0.415767	-1.776891
O	-2.008041	-1.831739	-1.280542
H	-1.229324	-1.252519	-1.242106
H	-2.312462	-1.895706	-0.359626
O	-1.766336	2.591978	1.118107
H	-2.273790	1.769623	1.238152
H	-0.858466	2.405485	1.412358
O	3.708712	1.443386	-0.073609
H	3.522723	1.669344	0.844441
H	2.928181	1.758638	-0.556244
C	0.473918	-0.342623	0.368139

M06L_Radical_15_sl			Eopt -1410.634466
O	-0.483871	-0.786961	0.476473
O	0.977740	0.685628	-0.102062
O	-0.560242	-0.038657	-1.585184
O	2.908275	-0.077435	-2.141722
H	2.319073	0.582949	-1.754794
H	2.387786	-0.900904	-2.091900
O	-0.641290	-3.908525	0.591762
H	0.254806	-3.557705	0.665857
H	-1.077721	-3.368030	-0.092792
O	0.631418	3.008586	2.504047
H	1.272359	2.285636	2.591476
H	0.716465	3.300560	1.578321
O	1.932583	-2.453181	1.104134
H	2.732536	-1.932710	0.890722
H	1.329010	-1.810975	1.495903
O	-1.515967	3.765785	-1.855836
H	-2.062406	3.117501	-1.383605
H	-0.950795	3.224575	-2.434448
O	-1.673422	1.506735	2.013848

H	-0.849027	2.000579	2.191581
H	-1.407434	0.582259	1.942791
O	-2.225608	-2.407437	-1.200717
H	-1.697501	-1.670954	-1.542426
H	-2.798576	-1.983137	-0.537698
O	0.838914	3.522838	-0.255304
H	0.005915	3.744931	-0.704789
H	0.917664	2.562326	-0.367582
O	4.031917	-0.733974	0.427709
H	3.698448	-0.450358	-0.441555
H	3.658207	-0.103490	1.061620
O	2.306903	0.660961	2.331091
H	1.715009	0.517329	1.570892
H	2.111840	-0.053111	2.947434
O	1.465615	-2.460301	-1.720495
H	1.543125	-2.472964	-0.750810
H	0.531375	-2.305278	-1.899037
O	0.391214	2.109274	-3.167335
H	0.135145	1.326175	-2.649744
H	1.154842	2.467439	-2.701305
C	0.004984	0.002414	-0.477036
O	-3.701141	-0.875721	0.681443
H	-3.547183	-0.009243	0.266675
H	-4.655511	-1.000373	0.690313
O	-2.796508	1.546322	-0.519108
H	-2.336271	1.658677	0.337748
H	-2.192776	1.010837	-1.055573
O	-2.093812	-2.361347	2.536901
H	-2.614147	-1.793792	1.948618
H	-1.557842	-2.902737	1.934503

M06L_Radical_15_s2

Eopt -1410.634884

O	-0.471372	0.048530	0.560889
O	0.062558	-0.007083	-1.623730
O	1.600021	0.196039	-0.086533
O	-2.279436	1.737502	-1.410245
H	-1.663371	0.996504	-1.509861
H	-2.306637	1.927443	-0.454244
O	-2.067664	-2.957203	1.242504
H	-1.175859	-2.821588	1.596798
H	-2.544047	-2.137149	1.449627
O	0.059072	1.830073	2.668351
H	-0.134345	1.109809	2.046211
H	0.655715	2.405471	2.154011
O	0.962686	-3.067527	-0.669288
H	0.069786	-2.964298	-1.026403
H	1.528767	-2.540962	-1.259455
O	-3.177641	-0.311844	1.198437
H	-3.730361	-0.384678	0.402339
H	-2.280564	-0.190263	0.842744
O	0.681078	-2.153142	1.975222
H	0.905703	-2.484448	1.084319
H	0.230372	-1.316166	1.787841
O	1.851132	3.098235	0.930486
H	1.240791	3.148481	0.170155
H	2.330820	2.272892	0.795769
O	2.484229	0.058090	2.813160
H	1.726821	0.654182	2.899531
H	2.096248	-0.780188	2.523369
O	2.407460	-1.402054	-2.530013
H	3.066466	-0.950557	-1.990121
H	1.615526	-0.847435	-2.452328
O	-4.186303	-0.460007	-1.478108
H	-3.703858	0.376422	-1.572532
H	-3.495643	-1.135996	-1.579900
O	-1.867633	-2.187144	-1.472690
H	-1.330076	-1.382783	-1.534513
H	-1.930180	-2.393324	-0.520847
O	-2.508495	2.496414	1.340786
H	-1.667018	2.448049	1.819812

H	-2.929729	1.640837	1.515321
C	0.310929	0.072832	-0.408235
O	3.591939	-2.013011	0.490150
H	2.873468	-1.381901	0.356549
H	3.160887	-2.871813	0.431681
O	2.595739	1.974848	-2.319166
H	2.784836	1.537647	-1.480573
H	2.450360	1.252180	-2.939405
O	0.257480	3.233164	-1.358247
H	-0.584198	2.760861	-1.440023
H	0.914949	2.704736	-1.842198

M06L_Radical_15_s3

Eopt -1410.630565

O	0.686566	-0.204047	1.192935
O	-0.620200	0.228371	-0.596372
O	1.449229	-0.368878	-0.844263
O	0.462574	2.335463	-2.299591
H	0.008770	1.539163	-1.989036
H	1.327450	2.306546	-1.850280
O	3.587816	0.075858	1.545760
H	2.621887	0.053535	1.512850
H	3.864614	-0.231595	0.666450
O	-4.848098	-0.475996	0.257800
H	-4.428209	0.397821	0.310727
H	-4.229348	-1.043049	0.740975
O	1.236035	2.722497	1.433341
H	0.436613	3.008435	0.948952
H	1.079128	1.794501	1.647792
O	-0.289060	-2.383256	2.778715
H	0.149913	-1.616491	2.380975
H	-0.006424	-3.124304	2.230438
O	-1.510841	1.148229	2.495272
H	-1.077192	1.998122	2.635912
H	-0.813052	0.583197	2.125539
O	2.093201	-2.921408	0.635292
H	1.995229	-2.086320	1.109460
H	2.624858	-2.690413	-0.135314
O	-2.364230	-1.615146	1.004816
H	-1.803334	-1.848044	1.764885
H	-2.009800	-0.774241	0.681150
O	-0.873468	3.642260	-0.144006
H	-0.456557	3.293023	-0.951376
H	-1.664366	3.094426	-0.019738
O	-3.035738	1.734507	0.224571
H	-2.582533	1.227408	-0.461743
H	-2.560058	1.490139	1.043785
O	2.883538	2.328530	-0.815523
H	2.383836	2.447328	0.014898
H	3.144247	1.400073	-0.812030
O	-0.451535	-2.988206	-0.687648
H	0.374647	-2.949903	-0.175532
H	-1.126809	-2.557527	-0.138601
C	0.434919	-0.100711	-0.029171
O	-2.993746	-0.896098	-2.003548
H	-2.114755	-0.754223	-1.629412
H	-3.606306	-0.782489	-1.260700
O	-0.073095	-1.589927	-3.111521
H	-0.123902	-0.650425	-2.907646
H	-0.200849	-2.026946	-2.249393
O	4.381544	-0.819416	-1.043352
H	4.857930	-0.110094	-1.488298
H	3.549617	-0.895379	-1.523612

w97BXD_6_s1

Eopt -722.738428

O	0.174788	-1.655318	-0.115524
O	-1.707356	-0.471689	-0.064530
O	0.252967	0.571212	-0.261974
O	2.861789	-1.671983	0.127792
H	1.876572	-1.686450	0.058006
H	3.094195	-0.955154	-0.479554

O	2.628261	0.652578	-1.567928
H	1.751658	0.589985	-1.123265
H	2.482872	0.318225	-2.455214
O	-2.967778	1.914020	-0.339271
H	-2.260759	2.539348	-0.125475
H	-2.514834	1.044765	-0.255172
O	-2.921882	-2.855241	0.170791
H	-2.441300	-1.996614	0.083849
H	-2.229985	-3.519236	0.164759
O	2.055409	0.542844	1.861422
H	2.545570	-0.225322	1.537896
H	1.378758	0.650283	1.166540
O	-0.436677	3.106911	0.304921
H	-0.213915	2.163511	0.125142
H	-0.429205	3.186424	1.260888
C	-0.425968	-0.529407	-0.147333

w97BXD_6_s2 Eopt -722.73567

O	0.165465	-0.495196	0.799543
O	-1.002715	-1.053228	-1.021767
O	1.120881	-1.692679	-0.823627
O	2.671293	-0.381272	1.863317
H	1.753288	-0.484354	1.526551
H	3.154971	-0.142628	1.063171
O	1.054561	2.039877	-0.125475
H	0.293099	2.119405	-0.719629
H	0.839510	1.224528	0.360219
O	-1.960960	1.063530	1.527606
H	-2.683295	0.493818	1.224202
H	-1.169339	0.531390	1.286430
O	3.104316	0.201015	-1.026443
H	2.555612	0.979978	-0.851779
H	2.455324	-0.532041	-0.968555
O	-3.415831	-0.998967	0.170681
H	-3.453644	-1.736383	0.783128
H	-2.512389	-1.040512	-0.225754
O	-1.564956	1.647417	-1.319107
H	-1.364198	0.689268	-1.322854
H	-1.839483	1.784814	-0.401533
C	0.099018	-1.088543	-0.351903

w97BXD_6_s3 Eopt -722.735446

O	0.119316	0.647314	0.058628
O	-0.941189	-0.127158	1.868314
O	1.274133	-0.363654	1.682272
O	2.365322	-0.009606	-1.441891
H	1.610347	0.297543	-0.900696
H	2.414552	-0.945101	-1.214373
O	-0.662428	-1.537008	-1.508598
H	-1.516503	-1.728800	-1.107352
H	-0.388089	-0.715891	-1.057899
O	1.452610	3.041476	0.124180
H	0.975640	2.186942	0.120549
H	2.378929	2.796412	0.079632
O	-2.096654	1.597374	-1.194323
H	-1.976145	1.250449	-2.081069
H	-1.306228	1.284773	-0.698115
O	-3.104982	-0.657204	0.330033
H	-2.322857	-0.492655	0.905046
H	-3.012660	0.036621	-0.337509
O	1.581020	-2.585859	-0.053645
H	0.784517	-2.424333	-0.583415
H	1.553993	-1.872801	0.610117
C	0.151219	0.046906	1.224222

w97BXD_12_s1 Eopt -1181.360714

O	0.332772	-0.491408	1.369166
O	0.390483	0.456905	-0.655163
O	-1.248860	-0.975868	-0.144039
O	1.231025	-1.118255	-2.795434

H	0.903587	-0.488340	-2.117183
H	0.696940	-1.914849	-2.620686
O	-0.824256	-2.145422	3.237675
H	-0.394920	-1.559249	2.572854
H	-1.665808	-2.368188	2.805103
O	1.419175	3.776223	0.772868
H	2.039024	3.083914	0.478048
H	0.642066	3.642466	0.193678
O	2.637730	-2.134429	1.071528
H	3.031768	-1.827733	0.234333
H	1.854516	-1.563574	1.193597
O	-3.419824	2.737649	-0.761192
H	-3.654074	2.643587	0.168727
H	-3.332024	1.817928	-1.098978
O	0.545451	1.907801	2.803930
H	0.825613	2.585248	2.162232
H	0.497667	1.080517	2.281855
O	-3.007968	-2.413161	1.377623
H	-2.370924	-1.863713	0.860753
H	-3.706790	-1.805683	1.642733
O	-0.611575	3.028353	-1.039749
H	-1.574439	3.015256	-0.876287
H	-0.328544	2.095680	-0.934461
O	3.701733	-1.047845	-1.390400
H	2.897723	-1.179887	-1.931923
H	3.565750	-0.167247	-0.994901
O	2.849901	1.393983	-0.065637
H	1.935753	1.030244	-0.220164
H	3.082617	1.096204	0.821849
O	-0.667765	-3.079033	-1.897445
H	-0.237908	-3.773192	-1.385831
H	-0.890787	-2.381679	-1.243600
O	-3.049448	0.190104	-1.792139
H	-2.328477	-0.212287	-1.245029
H	-2.657481	0.340939	-2.659366
C	-0.176573	-0.335191	0.196651

w97BXD_12_s2 Eopt -1181.356451

O	-0.757504	0.178827	0.131728
O	1.249739	0.991054	-0.430862
O	-0.549897	2.310036	-0.539842
O	1.825892	0.387743	-3.069841
H	1.596170	0.665088	-2.153864
H	1.003820	0.462935	-3.567162
O	0.690076	-2.878404	1.745574
H	0.232878	-2.162581	2.226017
H	0.272930	-2.860395	0.862435
O	-3.437972	0.221481	-0.130581
H	-2.449240	0.224345	-0.030269
H	-3.613801	1.119311	-0.467613
O	4.248761	0.796316	1.874364
H	3.746836	0.049210	1.498741
H	3.859511	1.576942	1.436492
O	-0.439634	-2.359312	-0.846726
H	0.383726	-2.394016	-1.371845
H	-0.487194	-1.427877	-0.522022
O	-0.737368	-0.606251	2.747263
H	-0.212266	-0.014180	3.297542
H	-0.670590	-0.245562	1.830538
O	-3.143143	2.919907	-0.979109
H	-3.234857	2.976474	-1.936275
H	-2.196462	2.667495	-0.822888
O	-3.574766	-0.011196	2.720272
H	-3.644182	0.109391	1.754235
H	-2.631570	-0.210406	2.856734
O	2.961290	2.909880	0.426995
H	2.502435	3.489248	1.044810
H	2.271206	2.282541	0.095414
O	2.148398	-2.263101	-2.085689
H	2.034377	-1.409552	-2.548550

H	2.447677	-1.994348	-1.195525
O	2.643004	-1.150484	0.519234
H	2.062447	-0.410117	0.209191
H	2.052152	-1.738349	1.027672
O	-3.085118	-1.993763	-1.930957
H	-3.310024	-1.216708	-1.386464
H	-2.172510	-2.205565	-1.663021
C	-0.029588	1.174137	-0.281484

w97BXD_12_s3 Eopt -1181.358849

O	0.271374	-0.996173	0.830129
O	0.386532	0.618543	-0.724102
O	-0.988072	-1.112508	-1.023206
O	2.636721	0.192396	-2.362471
H	1.816026	0.329250	-1.844261
H	2.846783	-0.753014	-2.237981
O	-1.020476	-3.188788	1.837446
H	-0.530120	-2.415332	1.469416
H	-1.826775	-3.201532	1.298077
O	-0.210003	4.251750	0.317410
H	0.474999	3.636559	0.639933
H	-0.752618	3.694482	-0.275313
O	2.999360	-1.507223	0.878959
H	3.427718	-0.656671	0.661535
H	2.037373	-1.302787	0.875202
O	-3.987120	1.824742	0.023101
H	-3.739185	1.822927	0.954247
H	-4.333927	0.922869	-0.152052
O	0.807530	0.472435	3.088882
H	1.566556	0.036939	3.492041
H	0.618583	-0.051574	2.274420
O	-3.045099	-2.549045	-0.161604
H	-2.240511	-2.042860	-0.467570
H	-3.156491	-3.264791	-0.797429
O	-1.602705	2.441195	-1.375670
H	-2.407310	2.174706	-0.889241
H	-0.937797	1.741054	-1.189776
O	4.062697	1.020656	-0.008295
H	3.691276	0.789214	-0.882402
H	3.335798	1.514433	0.421287
O	1.695055	2.223923	0.999946
H	1.220711	1.614362	0.371809
H	1.512786	1.819400	1.867266
O	3.309010	-2.509631	-1.697822
H	3.172673	-2.251582	-0.758506
H	2.559844	-3.074552	-1.917171
O	-5.065667	-0.687032	-0.519970
H	-4.355644	-1.362443	-0.435879
H	-5.277676	-0.658025	-1.459682
C	-0.119363	-0.503826	-0.306638

w97BXD_18_s1 Eopt -1639.975385

O	-0.948536	0.156731	0.354576
O	1.256812	0.111621	0.005334
O	0.024166	-1.729363	-0.343427
O	2.604424	-1.146838	2.075931
H	2.190793	-0.675430	1.317751
H	1.925517	-1.807924	2.311322
O	-0.812549	3.714599	1.567382
H	-1.196055	3.400411	0.723763
H	-0.893682	2.945508	2.160018
O	-3.298544	-1.008219	0.952855
H	-2.407033	-0.678946	0.670006
H	-3.536925	-1.711124	0.317229
O	-0.073496	3.222691	-2.936123
H	0.841649	3.084473	-2.604039
H	-0.187464	2.576256	-3.641601
O	-4.592731	-0.734978	-2.788919
H	-5.520363	-0.737279	-3.050088
H	-4.513346	-0.021164	-2.117005

O	2.497327	2.950434	-1.887606
H	2.263327	2.982325	-0.938758
H	2.796740	2.030448	-2.018275
O	-0.808058	1.128235	2.958079
H	0.137923	1.164719	3.203260
H	-0.809828	0.804388	2.028910
O	2.623882	-1.855730	-3.725124
H	1.793980	-1.630319	-4.159776
H	2.366292	-2.381331	-2.932984
O	-1.764133	2.479891	-0.805784
H	-1.199094	2.722965	-1.567994
H	-1.374860	1.649555	-0.442900
O	-4.161959	-2.862923	-1.023744
H	-3.392943	-3.354694	-1.332730
H	-4.307708	-2.164028	-1.697171
O	4.389247	-1.928367	-0.091395
H	4.168332	-1.180274	-0.675777
H	3.885864	-1.749515	0.723787
O	-4.288193	1.116254	-0.740556
H	-4.029128	0.430209	-0.094543
H	-3.474283	1.638038	-0.875355
O	3.271424	0.174171	-1.826867
H	3.067230	-0.428952	-2.567669
H	2.509575	0.073754	-1.208799
O	2.015119	1.332999	3.423080
H	2.261023	0.443633	3.104939
H	2.041545	1.880947	2.615631
O	1.758373	2.641153	0.853472
H	1.481804	1.735998	0.560583
H	0.922476	3.100808	1.063747
O	0.304376	-2.898357	2.251578
H	-0.427289	-2.444546	2.715845
H	0.196545	-2.617933	1.321827
O	-1.894656	-1.499966	3.442195
H	-2.468942	-1.485875	2.653816
H	-1.494626	-0.609550	3.440627
O	2.080087	-3.180183	-1.352147
H	1.363127	-2.614168	-0.968046
H	2.892331	-2.876260	-0.907464
C	0.111408	-0.494328	-0.005735

w97BXD_18_s2 Eopt -1639.976022

O	1.092520	0.133692	0.282492
O	-1.103155	0.375873	-0.052413
O	-0.132243	-1.605358	-0.415037
O	-1.298998	2.039550	-2.231047
H	-1.157382	1.439768	-1.464037
H	-0.490648	1.948980	-2.777757
O	1.074108	2.573832	3.122865
H	1.218411	1.612350	3.217641
H	1.396420	2.767206	2.222300
O	3.565312	-0.485501	-0.665976
H	2.631350	-0.355116	-0.371797
H	3.554421	-1.307093	-1.193799
O	-0.974458	-1.621065	3.445246
H	-1.711411	-0.996748	3.262572
H	-0.931874	-2.185359	2.664309
O	1.760531	-3.440718	0.253191
H	1.098481	-2.739328	0.032805
H	2.368498	-3.014705	0.885349
O	-3.066396	0.174440	2.951339
H	-2.547480	0.968596	2.714785
H	-3.396274	-0.141446	2.087940
O	1.685771	2.796110	0.299227
H	0.896580	3.313429	0.046231
H	1.382733	1.854102	0.288339
O	-3.794974	-3.226637	-0.596157
H	-4.634905	-3.355204	-1.050789
H	-3.159863	-2.959867	-1.298170
O	1.470191	-0.264918	2.973644

H	0.649441	-0.730667	3.235033
H	1.344224	-0.109467	2.009738
O	3.431010	-3.044476	-1.927565
H	2.899351	-2.994354	-2.729562
H	2.796747	-3.269795	-1.209481
O	-3.496574	0.206880	-2.679230
H	-3.718266	0.065365	-1.742034
H	-2.775536	0.863586	-2.655801
O	3.608615	-1.920709	1.911023
H	3.752181	-1.406906	1.095706
H	2.925374	-1.417577	2.391375
O	-3.670607	-0.471890	0.212144
H	-3.763916	-1.423757	0.017791
H	-2.709239	-0.273178	0.091832
O	-0.804394	4.103972	-0.306192
H	-1.000111	3.496847	-1.046637
H	-1.142943	3.630863	0.476684
O	-1.497153	2.293345	1.859819
H	-1.272236	1.615231	1.176935
H	-0.674493	2.408500	2.374155
O	1.044267	1.818189	-3.779042
H	1.810446	1.844723	-3.162857
H	1.044230	0.925782	-4.142747
O	3.180632	2.031859	-2.000492
H	3.403369	1.138026	-1.676184
H	2.699151	2.430336	-1.248090
O	-1.922911	-2.220368	-2.392130
H	-1.290770	-1.966165	-1.676849
H	-2.416126	-1.401897	-2.588083
C	-0.047783	-0.373983	-0.063752

w97BXD_18_s3 Eopt -1639.967542

O	-0.984386	0.292968	-0.114673
O	1.194634	0.061310	0.351038
O	0.185565	-1.368767	-1.039971
O	1.179569	-0.246294	3.049052
H	1.152176	-0.101377	2.073340
H	0.370692	-0.766000	3.217761
O	-0.654331	4.032865	-0.506982
H	-0.876283	3.404227	-1.223128
H	-1.085547	3.637238	0.270696
O	-4.506496	-0.484461	0.256859
H	-5.467162	-0.544606	0.311769
H	-4.187670	-1.413600	0.189508
O	1.077783	1.477162	-3.695814
H	1.831633	1.627621	-3.083549
H	1.187890	2.131286	-4.394767
O	-2.081263	-2.186079	-2.244071
H	-1.260573	-1.838268	-1.806063
H	-2.632574	-1.396739	-2.402736
O	3.211161	1.922396	-1.936442
H	2.733694	2.345332	-1.194888
H	3.493627	1.068187	-1.558194
O	-1.845032	2.272959	1.504795
H	-2.703145	2.470307	1.110385
H	-1.456639	1.563074	0.929028
O	4.022237	-3.007019	-1.582931
H	4.700756	-3.452178	-1.063310
H	3.166663	-3.295556	-1.190531
O	-1.342603	1.911517	-2.290826
H	-0.537079	1.775297	-2.830997
H	-1.210527	1.320664	-1.512948
O	-3.420223	-3.019312	0.013472
H	-2.778429	-3.046567	0.733031
H	-2.899195	-2.780115	-0.790043
O	3.895787	-1.189397	2.467112
H	3.918282	-0.955231	1.521769
H	2.995805	-0.954449	2.751269
O	-3.729719	0.176663	-2.470841
H	-3.983661	0.069282	-1.535415

H	-2.985566	0.803287	-2.470522
O	3.745196	-0.448558	-0.372023
H	3.859667	-1.309422	-0.820046
H	2.778041	-0.371462	-0.175553
O	1.636477	2.601747	3.245015
H	1.419944	1.655193	3.317024
H	1.679678	2.755679	2.283250
O	1.734952	2.744300	0.354292
H	1.456150	1.796642	0.369223
H	0.949016	3.233326	0.038661
O	-1.249508	-1.791328	3.028761
H	-1.971426	-1.134058	2.916252
H	-1.063340	-2.104189	2.135445
O	-3.282648	0.104368	2.771382
H	-3.761741	-0.123336	1.950233
H	-2.751680	0.880348	2.515031
O	1.580614	-3.592383	-0.458109
H	1.090514	-2.752038	-0.653900
H	1.124803	-4.275184	-0.962511
C	0.126844	-0.339976	-0.266224

w97BXD_24_s1 Eopt -2098.59186

O	1.221770	0.195054	-0.865412
O	-0.783143	-0.350722	-0.027208
O	1.074868	-1.229323	0.849619
O	2.479181	-0.139495	2.940615
H	2.230314	0.806839	2.974556
H	1.995930	-0.483571	2.155933
O	0.033521	-0.954023	4.274892
H	0.924857	-0.694992	3.973168
H	-0.170029	-1.739421	3.734186
O	-2.136518	1.041669	-1.888653
H	-1.623349	1.122759	-2.716301
H	-1.566638	0.516949	-1.268961
O	4.700682	-1.335545	1.468983
H	4.177074	-2.013125	1.003876
H	4.064453	-0.904229	2.067096
O	-2.538725	3.053753	-0.022641
H	-2.186505	2.648388	0.780038
H	-2.364846	2.393178	-0.730777
O	-2.794478	-1.857423	1.277192
H	-3.284754	-1.185239	1.793497
H	-2.085362	-1.347792	0.829124
O	-0.386245	-3.026843	2.264664
H	0.118531	-2.350772	1.744606
H	-1.316070	-2.793651	2.092539
O	-0.453163	1.197952	-4.194607
H	-0.056627	0.321825	-4.035366
H	0.104897	1.798048	-3.660961
O	1.104591	2.592159	-2.286254
H	0.572545	3.267629	-1.814580
H	1.035136	1.778078	-1.741604
O	1.924636	4.269875	1.029002
H	2.321404	5.078836	1.371425
H	2.575577	3.899529	0.388094
O	-0.232413	4.580184	-0.808161
H	-1.015900	4.108247	-0.468227
H	0.438192	4.530673	-0.100253
O	1.313812	2.431413	3.063273
H	1.536481	3.057696	2.346285
H	0.452040	2.045827	2.819514
O	2.867807	-3.072714	-0.070760
H	2.250341	-2.355739	0.204410
H	3.073184	-2.881468	-1.008072
O	-1.149341	0.987836	2.548019
H	-1.047752	0.574388	1.669126
H	-0.812487	0.311531	3.173547
O	-3.942303	0.331763	2.648731
H	-3.026817	0.670888	2.673256
H	-4.353559	0.765653	1.872498

O	3.956036	0.435615	-0.686918
H	2.984777	0.268001	-0.703296
H	4.290105	-0.095376	0.058955
O	0.319998	-4.504493	-0.175635
H	1.224679	-4.142734	-0.226592
H	-0.014183	-4.155724	0.671000
O	-1.114994	-2.723643	-1.861564
H	-0.623489	-3.377371	-1.319403
H	-1.143748	-1.930384	-1.298995
O	0.896399	-1.206658	-3.254312
H	1.042148	-0.651137	-2.457014
H	0.216318	-1.839479	-2.952923
O	-4.636012	-0.188899	-1.825322
H	-3.751974	0.217739	-1.941997
H	-4.444792	-1.117350	-1.585162
O	3.368372	-2.509260	-2.814255
H	2.514783	-2.075637	-3.024516
H	3.996498	-1.782133	-2.730974
O	3.535885	3.199681	-0.937154
H	2.757242	3.074643	-1.515622
H	3.804107	2.282332	-0.725580
O	-5.062998	1.570732	0.369574
H	-4.312986	2.174810	0.229801
H	-4.977760	0.911731	-0.349653
O	-3.923229	-2.848423	-1.072755
H	-3.064961	-2.946167	-1.521647
H	-3.658533	-2.539080	-0.181313
C	0.508257	-0.457572	-0.015064

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Eopt -2098.59078

O	1.169204	0.610324	-0.282431
O	-0.842414	-0.301400	-0.026872
O	0.952805	-1.310577	0.806865
O	2.132267	-0.673687	3.155417
H	1.858699	0.256619	3.267755
H	1.763260	-0.902259	2.276250
O	-0.435071	-1.732285	3.955572
H	0.474414	-1.413987	3.828051
H	-0.553957	-2.386805	3.247858
O	-1.938543	1.271399	-1.864253
H	-1.300628	1.585977	-2.528594
H	-1.426391	0.706068	-1.238442
O	4.563692	-1.334781	1.817260
H	4.148530	-1.927818	1.168611
H	3.828581	-1.068138	2.394617
O	-2.857257	2.738911	0.262047
H	-2.554251	2.207792	1.004966
H	-2.501227	2.285377	-0.530769
O	-2.887561	-2.110060	0.580177
H	-3.114489	-2.499756	-0.277542
H	-2.184967	-1.465591	0.376024
O	-0.565290	-3.371566	1.569188
H	-0.031023	-2.593054	1.279319
H	-1.464038	-3.140277	1.279390
O	0.091386	2.117424	-3.645272
H	0.540935	1.259002	-3.568954
H	0.441891	2.619590	-2.888869
O	0.941996	3.129743	-1.163628
H	0.225632	3.670655	-0.778708
H	0.825678	2.212733	-0.832805
O	2.145866	3.591768	1.453985
H	1.858340	3.427960	0.542641
H	1.754317	4.439003	1.680878
O	-0.936807	4.748341	0.083445
H	-1.646335	4.094624	0.229097
H	-0.505834	4.845612	0.936224
O	0.933285	1.838736	3.269529
H	1.290367	2.402688	2.560625
H	0.096530	1.471587	2.938146
O	3.034340	-2.735719	-0.166374

H	2.332912	-2.122856	0.139548
H	3.332511	-2.375923	-1.022370
O	-1.485724	0.486600	2.588101
H	-1.349117	0.238639	1.656239
H	-1.188783	-0.297376	3.090427
O	-4.313778	0.310869	2.663263
H	-3.343615	0.364328	2.637451
H	-4.592824	0.424820	1.740271
O	3.864580	0.716675	-0.053005
H	2.893023	0.588419	-0.064531
H	4.204524	0.082453	0.597127
O	0.691952	-4.233156	-0.894640
H	1.555788	-3.823958	-0.714922
H	0.205312	-4.117298	-0.062075
O	-0.644147	-2.172742	-2.225319
H	-0.150148	-2.895115	-1.786760
H	-0.852778	-1.553603	-1.506273
O	1.408028	-0.297530	-2.917481
H	1.430398	0.096469	-2.025040
H	0.720050	-0.981082	-2.838740
O	-4.180512	-0.299653	-2.293630
H	-3.346595	0.202939	-2.241521
H	-3.922479	-1.234143	-2.242091
O	3.772011	-1.741066	-2.683533
H	2.946527	-1.239509	-2.830780
H	3.707147	-2.503494	-3.263328
O	3.740084	3.013272	-1.709768
H	2.795358	3.172900	-1.570063
H	3.931712	2.258704	-1.133246
O	-5.135197	0.964387	0.017958
H	-4.482872	1.679911	0.062834
H	-4.840731	0.423326	-0.738094
O	-3.283077	-2.964519	-2.096253
H	-2.336039	-2.828633	-2.290407
H	-3.558154	-3.745670	-2.580025
C	0.432648	-0.329920	0.169634

w97BXD_24_s3

Eopt -2098.587187

O	-0.986050	0.336895	-0.384977
O	1.191233	0.343921	-0.798339
O	0.313326	1.898474	0.528569
O	-0.922436	2.152949	2.933879
H	-0.880691	1.240256	3.264778
H	-0.503926	2.079644	2.051548
O	2.862297	1.074662	3.295330
H	2.878688	1.755943	2.595272
H	3.781744	0.832588	3.429067
O	0.520177	-2.081744	-1.781137
H	-0.358537	-2.051929	-2.205060
H	0.718700	-1.164018	-1.484165
O	-3.068957	3.384638	1.590302
H	-2.513916	3.710287	0.862119
H	-2.427023	2.957017	2.185337
O	0.209888	-3.141575	0.736877
H	0.659528	-2.489582	1.291548
H	0.262374	-2.763494	-0.167003
O	3.846409	0.909972	-0.682229
H	3.975170	1.469017	-1.453649
H	2.883685	0.712474	-0.682605
O	2.724592	2.832211	1.135232
H	1.840608	2.449114	0.904326
H	3.332752	2.335169	0.567195
O	-2.024902	-2.000071	-2.939296
H	-2.023545	-1.052386	-3.146699
H	-2.603547	-2.036185	-2.155264
O	-3.740605	-1.847601	-0.726737
H	-3.298817	-2.377127	-0.030821
H	-3.730722	-0.939313	-0.395591
O	-3.198635	-0.921228	2.656077
H	-3.344218	-0.264066	1.941286

H	-3.821203	-0.713051	3.355261
O	-2.517908	-3.248740	1.309484
H	-1.559754	-3.176010	1.142089
H	-2.732646	-2.515326	1.910070
O	-0.558046	-0.615091	3.469021
H	-1.444038	-0.801890	3.112083
H	0.068919	-0.742978	2.741717
O	-1.053335	4.082454	-0.330738
H	-0.617888	3.274026	0.011967
H	-1.163446	3.892330	-1.281537
O	1.766339	-0.922629	1.745805
H	1.722895	-0.536874	0.856624
H	2.160181	-0.226794	2.312524
O	3.782199	-2.908334	1.761442
H	3.102546	-2.213854	1.748401
H	3.409948	-3.610009	1.201643
O	-3.408489	0.795797	0.552210
H	-2.467180	0.724591	0.264023
H	-3.483977	1.707337	0.885344
O	1.752993	4.778225	-0.734699
H	0.800187	4.690091	-0.570216
H	2.167348	4.245540	-0.035965
O	1.676640	2.625272	-2.579186
H	1.783419	3.350257	-1.936955
H	1.552226	1.831236	-2.037172
O	-2.175818	0.824831	-2.773068
H	-1.729165	0.645419	-1.916747
H	-3.107058	0.902372	-2.549365
O	2.944288	-3.349792	-2.257500
H	2.089226	-2.889680	-2.183037
H	3.613386	-2.688337	-2.003690
O	-1.011404	3.349309	-3.035498
H	-1.483746	2.498725	-2.991720
H	-0.073220	3.100694	-2.945699
O	-6.395148	-2.630418	-1.032659
H	-5.464789	-2.358691	-0.928411
H	-6.536772	-2.661846	-1.980710
O	2.446730	-4.785082	0.094961
H	1.626814	-4.339127	0.366956
H	2.679213	-4.343584	-0.743974
O	4.943533	-1.519020	-1.538358
H	5.387840	-1.306131	-2.362232
H	4.557390	-0.675298	-1.236196
C	0.160624	0.864529	-0.215809

w97BXD_Radical_6_s1

Eopt -722.532758

O	2.275855	-1.167587	0.563015
O	0.885462	-1.623080	-0.969559
O	1.864564	0.395600	-0.936087
O	-0.717316	0.503127	2.213955
H	-0.594934	-0.408932	1.904760
H	0.012712	1.023248	1.835306
O	1.323874	2.177341	1.211648
H	1.621289	1.627787	0.469296
H	2.022455	2.104594	1.866324
O	-1.761778	-0.536590	-1.860985
H	-1.342330	0.337218	-1.963989
H	-1.034598	-1.091255	-1.554044
O	-0.966185	-2.147185	1.189089
H	-0.340278	-2.104173	0.451888
H	-1.805878	-1.879334	0.804845
O	-2.960874	0.572323	0.484355
H	-2.208764	0.636473	1.097020
H	-2.591289	0.133144	-0.298871
O	-0.370385	1.890771	-1.792695
H	0.426935	1.396330	-1.538174
H	-0.729277	2.210857	-0.960620
C	1.663036	-0.750620	-0.489269

w97BXD_Radical_6_s2

Eopt -722.533085

O	1.356064	0.069790	-1.373186
O	0.027756	-1.715085	-1.161458
O	-0.752919	-0.004735	-2.092850
O	0.939979	2.666502	-0.375507
H	1.130107	1.813287	-0.801060
H	0.098608	2.938987	-0.751067
O	-0.308642	1.430409	1.926976
H	0.015937	0.510857	1.928881
H	0.211805	1.889801	1.245106
O	3.003079	-0.665251	0.760773
H	3.475956	-1.472428	0.545612
H	2.499908	-0.448407	-0.044320
O	-2.505692	1.187380	0.208293
H	-1.732343	1.297820	0.802129
H	-2.129705	0.983970	-0.657609
O	-2.568593	-1.626200	0.598490
H	-2.663605	-0.659520	0.545698
H	-1.931419	-1.818758	-0.098517
O	0.544103	-1.249925	1.962084
H	0.059356	-1.559391	1.192572
H	1.450239	-1.110877	1.629557
C	0.272344	-0.518070	-1.527648

w97BXD_Radical_6_s3

Eopt -722.532285

O	1.014041	-0.906040	-0.637518
O	-0.358469	-0.059736	-2.187534
O	1.112263	1.195873	-1.386554
O	0.664779	-0.069202	2.119095
H	0.815943	-0.415330	1.227338
H	1.149629	0.760443	2.131784
O	-1.936399	0.868989	1.582544
H	-2.255299	0.328735	0.837433
H	-1.074217	0.483094	1.817540
O	3.610875	-0.436071	0.524248
H	2.769297	-0.583115	0.067195
H	3.350476	-0.141500	1.400059
O	-0.941151	-2.653355	0.418334
H	-0.905504	-2.411160	1.347344
H	-0.234025	-2.130359	0.004734
O	-2.748938	-0.744897	-0.583057
H	-2.151698	-0.363045	-1.238118
H	-2.242520	-1.500813	-0.234275
O	-0.632669	2.945508	0.208332
H	-1.131241	2.257376	0.684413
H	-0.013264	2.447575	-0.338842
C	0.607962	0.023259	-1.361620

w97BXD_Radical_12_s1

Eopt -1181.140775

O	-0.174764	0.301114	0.999499
O	0.018616	-0.676089	-0.950101
O	-0.174997	1.525438	-0.815857
O	-2.632416	-0.967134	-2.379705
H	-1.702802	-1.020467	-2.113168
H	-2.861153	-0.031291	-2.210421
O	-0.890380	2.601325	2.963268
H	-0.729814	1.729282	2.580724
H	-0.799126	3.202733	2.199991
O	2.440258	-3.326590	0.576969
H	1.481626	-3.472186	0.504574
H	2.645661	-2.723017	-0.167411
O	-2.967996	-0.612007	1.810816
H	-3.124554	-1.303463	1.137196
H	-2.084319	-0.275087	1.607914
O	4.352387	0.699838	-0.762170
H	4.555727	0.611309	0.175732
H	3.704124	1.434080	-0.817268
O	2.021799	-1.199328	2.435888
H	2.197076	-1.944995	1.828963
H	1.337336	-0.681978	1.988595
O	-0.615788	4.098297	0.550259

H	-0.454633	3.271416	0.066905
H	0.241197	4.540131	0.568470
O	2.801456	-1.494921	-1.533521
H	3.360365	-0.743133	-1.242854
H	1.891612	-1.174332	-1.434394
O	-3.311994	-2.617809	-0.173869
H	-3.178260	-2.042963	-0.954310
H	-2.425811	-2.978918	0.004373
O	-0.507498	-3.223429	0.408625
H	-0.336269	-2.355335	0.003285
H	-0.595056	-3.031532	1.350877
O	-2.971014	1.800701	-1.861674
H	-3.601232	1.937604	-1.144887
H	-2.098313	1.859327	-1.442090
O	2.491244	2.768790	-1.013851
H	1.604792	2.372893	-0.986973
H	2.589233	3.098481	-1.914754
C	-0.108120	0.382648	-0.270944

w97BXD_Radical_12_s2

Eopt -1181.141484

O	0.582072	-0.451002	0.199529
O	-1.220890	-1.041763	-0.968875
O	0.522938	-2.347350	-0.886263
O	-1.436982	0.658924	-3.347387
H	-1.303161	0.029103	-2.619493
H	-0.570280	0.750273	-3.759672
O	-0.869330	2.199362	2.331599
H	-0.399099	1.425198	2.691763
H	-0.338686	2.454129	1.553647
O	3.474407	-0.216349	-0.056972
H	2.506813	-0.233027	0.041962
H	3.646231	-0.983292	-0.637593
O	-4.644207	-0.901077	1.399838
H	-4.054879	-0.152068	1.196754
H	-4.238285	-1.647873	0.920974
O	0.564894	2.482916	-0.168793
H	-0.222678	2.681971	-0.717882
H	0.584030	1.512667	-0.124198
O	0.679552	-0.140501	3.042198
H	0.228476	-0.803339	3.578102
H	0.565427	-0.431785	2.120720
O	3.432188	-2.534761	-1.699431
H	3.565084	-2.283044	-2.620767
H	2.470668	-2.531160	-1.577978
O	3.562374	-0.546954	2.826611
H	3.645431	-0.483503	1.858609
H	2.610720	-0.429189	2.990278
O	-3.300252	-2.931830	-0.117140
H	-2.916937	-3.577902	0.486888
H	-2.553512	-2.375060	-0.393851
O	-1.855571	2.836705	-1.571105
H	-1.712615	2.155924	-2.258491
H	-2.292529	2.347252	-0.848891
O	-2.753776	1.083622	0.544122
H	-2.244166	0.387941	0.098206
H	-2.145742	1.432819	1.230866
O	3.226122	2.381106	-1.282615
H	3.429530	1.492305	-0.938449
H	2.317817	2.543052	-0.971910
C	-0.047664	-1.254965	-0.543686

w97BXD_Radical_12_s3

Eopt -1181.14389

O	-0.441726	0.581440	1.462006
O	0.695875	-0.007421	-0.358169
O	1.664501	0.991716	1.374214
O	-1.577717	-0.029318	-2.240788
H	-0.851590	0.043317	-1.599808
H	-2.356838	0.357356	-1.785904
O	-2.533812	2.550428	0.968795
H	-1.757417	1.989894	1.125536

H	-2.203562	3.319377	0.463064
O	2.914810	-3.436651	0.135764
H	1.947934	-3.385062	0.231335
H	3.136088	-2.629372	-0.367716
O	-4.225500	-1.693921	0.200597
H	-3.523436	-2.098655	-0.355744
H	-3.867546	-1.695029	1.095677
O	5.319982	0.736899	-0.650152
H	5.747098	0.359687	0.127090
H	4.771150	1.474343	-0.307955
O	-1.080323	-2.056467	2.604237
H	-2.033381	-2.190389	2.541288
H	-0.940316	-1.134005	2.333449
O	-1.645420	4.818391	-0.461617
H	-1.235772	4.495727	-1.273151
H	-2.439223	5.280052	-0.757185
O	3.257634	-1.042201	-1.365246
H	3.982093	-0.440063	-1.097857
H	2.447574	-0.630850	-1.021280
O	-2.253840	-2.685390	-1.512520
H	-2.028455	-1.797851	-1.860791
H	-1.498642	-2.899349	-0.931913
O	0.061992	-2.896116	0.158551
H	0.306224	-2.005567	-0.142815
H	-0.331636	-2.734604	1.040504
O	-3.850769	0.909179	-0.889431
H	-4.018405	0.057415	-0.439891
H	-3.427058	1.483340	-0.217913
O	3.618628	2.787072	0.194398
H	4.021557	3.254443	0.935380
H	2.905571	2.259156	0.590663
C	0.642242	0.507596	0.785138

w97BXD_Radical_18_s1

Eopt -1639.752217

O	0.960344	0.604615	-0.050795
O	-1.216907	0.127945	0.111931
O	0.280155	-1.424371	0.254454
O	-1.966407	0.945702	-2.473235
H	-1.810492	0.776317	-1.531321
H	-1.138996	0.624830	-2.883861
O	0.405439	3.747022	1.916269
H	0.853156	2.975187	2.297815
H	0.679449	3.739798	0.985080
O	3.509357	-0.034226	-0.942427
H	2.632423	0.204434	-0.598701
H	3.376744	-0.958081	-1.226585
O	-0.250946	-0.457930	3.486743
H	-1.148748	-0.118860	3.304061
H	-0.132164	-1.189391	2.875440
O	2.746066	-3.047114	1.359922
H	3.409008	-3.700944	1.589234
H	3.139424	-2.186197	1.605918
O	-2.842313	0.498154	3.025722
H	-2.653804	1.284005	2.488551
H	-3.158644	-0.161234	2.391123
O	0.963251	3.255144	-0.887444
H	0.064732	3.473308	-1.199238
H	0.880019	2.341874	-0.566492
O	-2.258365	-3.925986	0.769921
H	-1.553070	-3.844144	1.417142
H	-1.838489	-3.714944	-0.085215
O	1.744432	1.270188	2.592185
H	1.046355	0.703621	2.975988
H	1.608365	1.161677	1.639533
O	2.812743	-2.707352	-1.411269
H	1.907313	-2.630913	-1.725237
H	2.736202	-2.874860	-0.451569
O	-3.420236	-1.526944	-2.134356
H	-3.607540	-1.461401	-1.185403
H	-3.007177	-0.678742	-2.360557

O	3.889013	-0.562206	1.865632
H	3.906262	-0.334147	0.921633
H	3.215508	0.023869	2.244369
O	-3.434861	-1.371985	0.799853
H	-3.138850	-2.294229	0.897890
H	-2.621459	-0.903439	0.550374
O	-1.739707	3.646029	-1.534142
H	-1.843131	2.803700	-2.007135
H	-1.963864	3.423754	-0.616076
O	-2.043677	2.590653	1.162690
H	-1.711088	1.785536	0.734138
H	-1.239554	3.018112	1.513897
O	0.453673	-0.113009	-3.376131
H	1.140091	0.560305	-3.209179
H	0.627930	-0.810136	-2.736369
O	2.441897	1.807896	-2.917606
H	2.963791	1.229075	-2.339982
H	1.978546	2.405312	-2.308357
O	-1.174841	-3.139695	-1.706990
H	-0.500116	-2.551171	-1.353756
H	-1.928993	-2.557228	-1.916540
C	-0.005672	-0.170816	0.096995

w97BXD_Radical_18_s2

O	0.879883	0.115987	-0.167837
O	-1.326694	-0.022585	0.101865
O	-0.197336	-1.679468	-0.768205
O	-2.160211	1.902731	-1.889275
H	-1.915059	1.289355	-1.175820
H	-1.393053	1.857917	-2.500313
O	0.831106	2.450773	3.097953
H	1.153068	1.528703	3.061873
H	1.022195	2.795102	2.206327
O	3.574459	0.302463	-1.135786
H	2.657531	0.063301	-0.924514
H	3.953561	-0.482182	-1.586889
O	-0.390479	-1.980701	3.232142
H	-1.245992	-1.498048	3.240510
H	-0.411618	-2.509493	2.426106
O	5.211014	-2.976319	0.389387
H	4.576663	-3.675345	0.583421
H	4.874210	-2.182502	0.860168
O	-2.828573	-0.587810	3.316184
H	-2.514539	0.308702	3.094418
H	-3.291267	-0.878597	2.510084
O	1.111495	3.031999	0.258891
H	0.212117	3.409267	0.155807
H	0.978683	2.073471	0.167486
O	-3.884331	-3.726590	-0.515144
H	-4.768675	-3.961571	-0.817643
H	-3.437151	-3.344648	-1.300571
O	1.709709	-0.228841	2.619045
H	1.002447	-0.848281	2.902272
H	1.507970	-0.071387	1.681885
O	4.792090	-1.982002	-2.190225
H	4.140100	-2.525013	-2.647169
H	4.922507	-2.413394	-1.317903
O	-4.197573	-0.152987	-2.200326
H	-4.277818	-0.377114	-1.257630
H	-3.571667	0.594087	-2.219704
O	4.391119	-0.556296	1.492284
H	4.146978	-0.182409	0.623087
H	3.555080	-0.582140	1.988419
O	-3.913145	-1.136155	0.635160
H	-3.970855	-2.063218	0.326485
H	-3.007272	-0.863489	0.409882
O	-1.576259	3.900938	0.093627
H	-1.822992	3.329478	-0.658903
H	-1.781206	3.358603	0.876359
O	-1.806980	1.896051	2.232741

Eopt -1639.753281

H	-1.596246	1.298970	1.494518
H	-0.933071	2.100168	2.627941
O	0.099900	1.621203	-3.525962
H	0.906774	1.972001	-3.088763
H	0.199861	0.662616	-3.498749
O	2.387338	2.683174	-2.290768
H	2.902847	1.896212	-2.036191
H	1.971799	2.965574	-1.454032
O	-2.535223	-2.407958	-2.599213
H	-1.725102	-2.194248	-2.114305
H	-3.081115	-1.596330	-2.534605
C	-0.218359	-0.499162	-0.265941

w97BXD_Radical_18_s3

O	-1.108318	0.232528	0.262787
O	1.108732	0.221026	0.081115
O	-0.139288	-0.570228	-1.572934
O	2.072875	-0.781331	2.361104
H	1.636816	-0.366784	1.583603
H	1.693340	-1.675134	2.360651
O	-1.041590	3.767847	1.245021
H	-1.508850	3.413888	0.467664
H	-1.054699	3.023558	1.870775
O	-3.686302	-1.326442	1.292873
H	-4.466431	-1.733547	1.677026
H	-3.295512	-2.008009	0.707151
O	-0.749462	2.547885	-3.150447
H	0.170026	2.532744	-2.816788
H	-0.855315	3.417487	-3.542668
O	-2.596430	-1.244509	-2.396384
H	-1.714646	-0.911631	-2.102256
H	-3.242298	-0.675526	-1.944790
O	1.870707	2.628357	-2.229802
H	1.758436	2.832246	-1.285319
H	2.306329	1.760770	-2.226659
O	-0.975303	1.300352	2.681350
H	-1.892722	1.272371	2.964778
H	-0.978616	0.910077	1.768439
O	3.070058	-2.451180	-2.839225
H	3.871312	-2.830545	-2.470971
H	2.357580	-2.737687	-2.238161
O	-2.330001	2.355577	-0.852792
H	-1.835791	2.478435	-1.685235
H	-1.893261	1.575556	-0.445093
O	-2.396715	-3.111293	-0.364705
H	-1.499025	-2.995789	-0.038971
H	-2.456342	-2.519360	-1.143047
O	4.439658	-0.872066	0.763370
H	4.091420	-0.530290	-0.075291
H	3.668778	-0.879405	1.355214
O	-4.410587	0.380354	-0.891279
H	-4.172918	-0.112340	-0.087503
H	-3.803635	1.137919	-0.914053
O	3.144841	0.121149	-1.623154
H	3.113115	-0.710198	-2.126066
H	2.356501	0.089965	-1.026748
O	2.468349	1.966280	3.193564
H	2.324640	1.015279	3.099011
H	2.156331	2.335881	2.351963
O	1.537911	2.831767	0.598602
H	1.329600	1.879997	0.469320
H	0.675026	3.244403	0.783433
O	0.603028	-3.143163	1.754861
H	-0.174776	-2.624846	2.030977
H	0.687416	-3.024940	0.794257
O	-1.421507	-1.652544	2.980062
H	-2.217605	-1.513992	2.438354
H	-1.018905	-0.776315	3.033304
O	0.955332	-2.986620	-1.091474
H	0.539000	-2.122802	-1.317056

Eopt -1639.751062

H	0.350782	-3.652555	-1.428702
C	-0.055502	-0.038145	-0.410105

w97BXD_Radical_24_s1

O	1.090595	0.765464	0.220785
O	-0.991240	0.133898	0.115280
O	0.693314	-1.338517	0.093310
O	2.085440	-2.264632	2.379995
H	1.949030	-1.473518	2.940101
H	1.644853	-2.015648	1.553428
O	-0.536560	-3.274437	3.002770
H	0.401543	-3.040666	2.905227
H	-0.802658	-3.535532	2.106289
O	-1.755061	2.474064	-1.442148
H	-1.188004	2.785278	-2.173995
H	-1.335439	1.666125	-1.116547
O	4.240727	-2.593581	0.501903
H	3.665392	-2.892200	-0.220134
H	3.641452	-2.501759	1.259922
O	-1.811126	2.773634	1.348534
H	-1.407820	1.896685	1.352186
H	-1.855572	2.977013	0.399460
O	-3.182563	-1.768957	0.127511
H	-3.670641	-1.561379	0.947173
H	-2.492166	-1.089641	0.092196
O	-1.083389	-3.588151	0.198448
H	-0.422278	-2.879526	0.169313
H	-1.925651	-3.096507	0.205765
O	-0.047275	3.147549	-3.523780
H	0.453831	2.320716	-3.393485
H	0.541085	3.847054	-3.229141
O	1.844865	3.716601	-0.752712
H	1.357971	3.886631	0.079663
H	1.354694	3.011810	-1.184684
O	2.406428	2.332456	2.871079
H	2.886471	2.727837	3.602591
H	3.026929	2.336043	2.110225
O	0.639126	4.154707	1.700441
H	-0.220864	3.706368	1.636682
H	1.213076	3.532636	2.182754
O	1.287500	-0.044620	3.805984
H	1.642913	0.772481	3.413670
H	0.363276	-0.110022	3.515820
O	2.288440	-2.926471	-1.641408
H	1.796472	-2.329718	-1.058957
H	2.718303	-2.327116	-2.280409
O	-1.423958	-0.634339	3.015491
H	-1.415391	-0.354078	2.092365
H	-1.167067	-1.578858	2.992074
O	-4.261425	-0.798937	2.509471
H	-3.358524	-0.772392	2.863027
H	-4.364563	0.061799	2.056304
O	3.988301	-0.040512	-0.594587
H	3.028511	0.025122	-0.543374
H	4.184468	-0.887031	-0.146911
O	-0.353549	-3.471277	-2.593165
H	0.593958	-3.360783	-2.404674
H	-0.735630	-3.661895	-1.721797
O	-1.171865	-0.838111	-2.796730
H	-0.876864	-1.771242	-2.731904
H	-1.333947	-0.568244	-1.885117
O	1.156513	0.678928	-2.990160
H	1.409840	0.824975	-2.072872
H	0.353497	0.121461	-2.942581
O	-4.348750	1.448490	-1.648278
H	-3.449005	1.817477	-1.689053
H	-4.260799	0.530811	-1.962288
O	3.477434	-0.957349	-3.253751
H	2.664079	-0.434516	-3.348621
H	3.860295	-0.613130	-2.430298

Eopt -2098.363149

O	3.982163	2.505956	0.639986
H	3.284190	2.902489	0.086202
H	4.107004	1.612483	0.280182
O	-4.444968	1.606135	1.148759
H	-3.587870	2.028960	1.314986
H	-4.461272	1.473308	0.181755
O	-4.033622	-1.233737	-2.476664
H	-3.137643	-1.138505	-2.832032
H	-3.876668	-1.505742	-1.554977
C	0.219877	-0.179989	0.142264

w97BXD_Radical_24_s2

O	0.830326	1.015746	-0.641504
O	-0.767985	-0.418603	0.009570
O	1.254576	-0.330209	0.911699
O	2.495173	0.162375	3.804181
H	1.712802	0.745544	3.711220
H	2.884778	0.139735	2.926760
O	0.827464	-2.104877	3.647048
H	1.456694	-1.364052	3.714614
H	1.162131	-2.658935	2.920201
O	-2.453815	1.120625	-1.689432
H	-1.991379	1.524200	-2.449697
H	-1.803039	0.537831	-1.269305
O	5.035414	-0.520541	0.658963
H	4.419345	-1.197928	0.332141
H	4.778872	-0.368804	1.571618
O	-2.771685	2.224507	0.830024
H	-2.088001	1.754588	1.318000
H	-2.661873	1.930493	-0.095722
O	-0.946396	-3.280308	0.635855
H	-1.031060	-3.625769	-0.257064
H	-0.898492	-2.320820	0.517843
O	1.614887	-3.825578	1.541930
H	2.236889	-3.428329	0.923082
H	0.737869	-3.681450	1.138049
O	-0.986229	2.235478	-3.782394
H	-0.368335	1.487932	-3.823722
H	-0.560504	2.855713	-3.165474
O	0.285592	3.619691	-1.673507
H	-0.331821	4.071049	-1.072435
H	0.377479	2.736171	-1.288753
O	0.848876	3.630923	1.761797
H	0.083743	4.008900	1.296978
H	1.571314	3.639112	1.110063
O	-1.389328	4.573943	0.348578
H	-1.998968	3.843636	0.565717
H	-1.843014	5.390237	0.567473
O	0.200181	1.664344	3.567844
H	0.379860	2.271587	2.825813
H	-0.391623	0.970162	3.232779
O	3.014849	-2.128703	-0.533396
H	2.398745	-1.501880	-0.131078
H	3.156509	-1.799776	-1.447587
O	-1.364993	-0.595010	2.854513
H	-1.305967	-0.534616	1.891223
H	-0.631754	-1.193972	3.106438
O	-4.006019	-1.628060	2.693212
H	3.086144	-1.349661	2.827552
H	-4.367180	-0.962706	2.080440
O	3.718524	1.362325	-0.977973
H	2.807753	1.044088	-0.939611
H	4.204502	0.785829	-0.361850
O	1.182569	-3.893058	-1.887875
H	1.796926	-3.361844	-1.354635
H	0.844520	-4.558469	-1.283195
O	-0.811991	-2.048943	-2.431922
H	-0.131523	-2.730261	-2.255576
H	-0.841776	-1.526673	-1.618527
O	0.857816	0.051292	-3.370698

Eopt -2098.365086

H	0.965360	0.470892	-2.505029
H	0.250925	-0.688846	-3.188669
O	-4.643396	-0.593610	-1.681227
H	-3.898213	0.019532	-1.809804
H	-4.233472	-1.477256	-1.685105
O	3.282640	-1.356700	-3.153587
H	2.449978	-0.870012	-3.300414
H	3.161230	-2.196117	-3.604514
O	2.792524	3.919395	-0.272907
H	2.032557	3.963939	-0.873880
H	3.194141	3.051703	-0.457821
O	-4.981679	0.339818	0.940850
H	-4.274636	1.001536	0.989441
H	-4.899236	-0.037044	0.044577
O	-3.355763	-3.094386	-1.735102
H	-2.464181	-2.800561	-1.994255
H	-3.276409	-3.330319	-0.807252
C	0.369438	0.084447	0.072104

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Eopt -2098.368023

O	1.450226	1.325355	0.148079
O	0.096778	-0.458855	0.178648
O	1.857984	-0.257571	1.491485
O	0.540159	0.316010	4.152915
H	-0.199790	0.899110	3.897232
H	1.001831	0.128247	3.329583
O	-3.542924	-1.690623	2.143979
H	-2.677478	-2.132886	2.023177
H	-3.718344	-1.696046	3.087469
O	-0.973747	0.008121	-2.418315
H	-0.374393	0.580470	-2.936169
H	-0.550788	-0.095685	-1.551987
O	5.959856	0.810774	-0.442268
H	5.474183	0.011653	-0.165318
H	6.714443	0.863382	0.148736
O	-3.341324	1.119153	-1.441200
H	-3.139044	0.969866	-0.498553
H	-2.522100	0.836452	-1.889681
O	-1.065245	-2.675976	1.564268
H	-1.188075	-3.301557	0.827114
H	-0.675507	-1.891796	1.145156
O	1.178271	-3.118201	3.150648
H	1.381604	-2.229862	3.454623
H	0.363686	-3.016590	2.623666
O	0.727038	1.760301	-3.748907
H	1.585749	1.427669	-3.441371
H	0.540278	2.472057	-3.114728
O	0.505410	3.481273	-1.510719
H	0.744941	2.745225	-0.928943
H	1.304296	4.011734	-1.574944
O	-0.819235	4.505558	2.645311
H	-1.238446	5.171852	3.196389
H	0.124773	4.628587	2.776398
O	-3.660582	3.921760	-1.271428
H	-3.508268	2.965515	-1.353081
H	-2.873316	4.269773	-0.818158
O	-1.618401	1.937148	3.481539
H	-1.321340	2.824089	3.218844
H	-1.926090	1.519358	2.657030
O	4.361479	-1.371126	0.275213
H	3.619638	-0.874116	0.642509
H	4.092396	-1.570477	-0.645228
O	-2.431523	0.642033	1.142534
H	-1.584333	0.297727	0.825252
H	-2.889513	-0.135124	1.516919
O	-5.340940	-2.652987	0.186554
H	-4.742402	-2.344030	0.884301
H	-5.061358	-2.175077	-0.615414
O	4.059169	2.646832	0.540288
H	3.226338	2.162035	0.510532

H	4.721073	2.022984	0.194177
O	2.864366	-3.727568	1.021556
H	3.484353	-2.993269	0.892755
H	2.332186	-3.482824	1.802624
O	1.213584	-2.918931	-1.035436
H	1.761435	-3.250314	-0.291940
H	0.825659	-2.098260	-0.701456
O	3.008233	0.912664	-2.315246
H	2.574199	1.077613	-1.466744
H	3.835295	1.400043	-2.273018
O	-2.165016	-2.471203	-2.973035
H	-1.672144	-1.644421	-2.829286
H	-1.886722	-3.063511	-2.255114
O	3.470190	-1.838609	-2.311499
H	3.285914	-0.887485	-2.405497
H	2.637205	-2.225467	-1.989022
O	-1.358104	5.020849	-0.091363
H	-0.688586	4.496764	-0.563975
H	-1.202712	4.838483	0.849512
O	-4.583636	-1.319531	-2.153244
H	-4.251890	-0.446345	-1.880015
H	-3.782093	-1.787607	-2.452928
O	-1.247054	-4.101825	-0.833083
H	-1.291267	-5.057695	-0.907527
H	-0.310491	-3.858316	-0.975176
C	1.080824	0.199917	0.567180