

Lewis Acid Catalysis and Ligand Exchange in the Asymmetric Binaphthol-Catalyzed Propargylation of Ketones

Matthew N. Grayson and Jonathan M. Goodman*

Unilever Centre for Molecular Science Informatics, Department of Chemistry, University of Cambridge,
Lensfield Road, Cambridge CB2 1EW, United Kingdom

Supporting Information

List of contents:

- Full list of authors in the Gaussian03 reference. Page S2.
- Computational methods. Page S3.
- Comparison of reaction pathways. Page S4.
- Catalytic cycle. Page S5.
- Cartesian coordinates, absolute energies including zero-point energy corrections, free energies (in Hartrees) and number of imaginary frequencies of all the stationary points and values of imaginary frequencies of all transition structures. Pages S6-133.
- References. Page S134.

Full list of authors in the Gaussian03 reference

M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, J. A. Montgomery, Jr., T. Vreven, K. N. Kudin, J. C. Burant, J. M. Millam, S. S. Iyengar, J. Tomasi, V. Barone, B. Mennucci, M. Cossi, G. Scalmani, N. Rega, G. A. Petersson, H. Nakatsuji, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, M. Klene, X. Li, J. E. Knox, H. P. Hratchian, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, P. Y. Ayala, K. Morokuma, G. A. Voth, P. Salvador, J. J. Dannenberg, V. G. Zakrzewski, S. Dapprich, A. D. Daniels, M. C. Strain, O. Farkas, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. V. Ortiz, Q. Cui, A. G. Baboul, S. Clifford, J. Cioslowski, B. B. Stefanov, G. Liu, A. Liashenko, P. Piskorz, I. Komaromi, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, C. Gonzalez, and J. A. Pople, Gaussian, Inc., Wallingford CT, 2004.

Computational Methods

The B3LYP density functional,^{1,2} and split-valence polarized 6-31G** basis set,^{3,4} were used for all geometry optimizations in the study of ketone propargylation. All activation free energies are quoted relative to infinitely separated reagents. Quantum mechanical calculations were performed using Gaussian03 (Revision E.01).⁵ Single point energies were taken using the M06-2X density functional,⁶ and LACVP** basis set,⁷ using the Jaguar program (version 7.6).⁸ This energy was used to correct the gas phase energy obtained from the B3LYP calculations.^{9,10} All quoted energies are zero point energy (scaled by 0.9,¹¹) corrected.

Energy minima were located by first implementing an extensive conformational search in MacroModel using the OPLS-2005 force field.¹²⁻¹⁴ Selected structures were then optimized at the B3LYP/6-31G** level of theory. Single point energies were performed on the resulting structures using M06-2X/LACVP**. This energy was used to correct the gas phase energy obtained from the B3LYP calculations.

Free energies in solution were derived from gas phase optimized structures (B3LYP/6-31G**) by means of a single-point calculation using M06-2X/LACVP** with the polarizable continuum model (PCM),¹⁵ as implemented in the Jaguar program (version 7.6). These values were used to correct the Gibbs free energy derived from the B3LYP calculations.

Comparison of Reaction Pathways

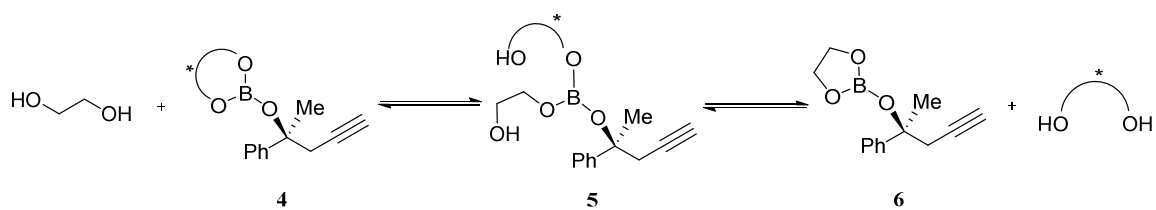
Table S1 Comparison of reaction pathways. Free energies in kcal mol⁻¹. Free energies of ligand exchange relative to free catalyst and achiral boronate.

	Uncatalyzed	Reaction with 1	Reaction with 2
M06-2X, LACVP** Gas Phase			
Relative Free Energy of Ligand Exchange	0.0	1.5	13.2
$\Delta G^\ddagger$	24.1	16.5	9.9
Summation	24.1	17.9	23.2
M06-2X, LACVP** Solvent = acetophenone			
Relative Free Energy of Ligand Exchange	0.0	7.0	12.6
$\Delta G^\ddagger$	27.0	21.7	13.2
Summation	27.0	28.7	25.8
M06-2X, LACV3P+** Gas Phase			
Relative Free Energy of Ligand Exchange	0.0	2.5	12.2
$\Delta G^\ddagger$	28.2	21.0	13.7
Summation	28.2	23.5	25.9
M06-2X, LACV3P+** Solvent = acetophenone			
Relative Free Energy of Ligand Exchange	0.0	8.2	11.0
$\Delta G^\ddagger$	31.9	27.4	18.0
Summation	31.9	35.6	29.1

Catalytic Cycle

Table S2 Thermodynamics of catalyst turnover. Free energies in kcal mol⁻¹.

	Free Catalyst + Reagents	2 + Acetophenone + Ethylene Glycol	4 + Ethylene Glycol	5	Free Catalyst + 6
ΔG (M06-2X)	0.0	13.2	-6.1	-20.5	-17.5
ΔG_{sol} (M06-2X)	0.0	12.6	-2.9	-10.4	-14.0



Uncatalyzed Reaction**Acetophenone**

B3LYP/6-31G** Energy = -384.783817
B3LYP/6-31G** Free Energy = -384.802631
M06-2X/LACVP** Derived Free Energy = -384.746889
M06-2X/LACVP** Derived Solution Free Energy = -384.757264
M06-2X/LACV3P+** Derived Free Energy = -384.846905
M06-2X/LACV3P+** Derived Solution Free Energy = -384.859087
Number of Imaginary Frequencies = 0

B3LYP/6-31G** Geometry

C	1.697744	-0.202741	-0.000008
O	2.212018	-1.311008	0.000019
C	-2.592543	0.110915	0.000003
C	-1.965126	-1.138628	-0.000005
C	-0.576463	-1.219476	-0.000007
C	0.205027	-0.053308	-0.000008
C	-0.433044	1.196292	0.000001
C	-1.825298	1.277127	0.000008
H	-3.676850	0.175198	0.000004
H	-2.561308	-2.046413	-0.000010
H	-0.065188	-2.176212	-0.000012
H	0.152373	2.110137	0.000005
H	-2.310662	2.248582	0.000017
C	2.562000	1.047048	-0.000008
H	2.361181	1.664359	-0.882406
H	2.361207	1.664324	0.882422
H	3.609317	0.744717	-0.000027

2-(propa-1,2-dien-1-yl)-1,3,2-dioxaborolane

B3LYP/6-31G** Energy = -369.986575
B3LYP/6-31G** Free Energy = -370.008703
M06-2X/LACVP** Derived Free Energy = -369.948341
M06-2X/LACVP** Derived Solution Free Energy = -369.959445
M06-2X/LACV3P+** Derived Free Energy = -370.053168
M06-2X/LACV3P+** Derived Solution Free Energy = -370.065913
Number of Imaginary Frequencies = 0

B3LYP/6-31G** Geometry

C	1.256122	-0.955147	-0.011769
C	2.343762	-0.218654	-0.001100
B	-0.173096	-0.357675	-0.004887
C	3.420917	0.517864	0.009952
O	-1.293926	-1.154044	-0.030064
O	-0.455804	0.986452	0.027223
H	3.883095	0.829500	0.943164

H	3.886842	0.852026	-0.913533
C	-2.445072	-0.301009	0.047931
H	-2.963739	-0.489042	0.994783
H	-3.128822	-0.539682	-0.772737
C	-1.880215	1.141095	-0.041314
H	-2.215337	1.778161	0.783201
H	-2.140430	1.633504	-0.985152
H	1.368637	-2.040251	-0.024765

TS-1

B3LYP/6-31G** Energy = -754.734109
B3LYP/6-31G** Free Energy = -754.750834
M06-2X/LACVP** Derived Free Energy = -754.656799
M06-2X/LACVP** Derived Solution Free Energy = -754.673643
M06-2X/LACV3P+** Derived Free Energy = -754.855142
M06-2X/LACV3P+** Derived Solution Free Energy = -754.874168
Number of Imaginary Frequencies = 1 (-375.61)

B3LYP/6-31G** Geometry

C	-0.462669	1.892271	1.265766
C	0.834147	1.637628	1.599604
B	1.950218	-0.147026	0.205774
C	3.718069	-0.500444	-1.224038
C	3.840947	-1.424356	0.000163
H	4.655135	0.009777	-1.475537
H	3.383718	-1.062284	-2.109916
H	4.079499	-2.460492	-0.266188
H	4.620490	-1.063390	0.690766
O	2.562955	-1.364441	0.615540
O	2.729979	0.451144	-0.841995
H	-1.245780	1.506228	1.914489
H	-0.712969	2.816761	0.750469
C	-0.409533	0.518120	-0.347443
O	0.502306	-0.379533	-0.059422
C	-4.408895	-1.044171	0.046870
C	-3.316187	-1.743445	0.564497
C	-2.027982	-1.231018	0.435482
C	-1.810696	-0.005083	-0.214713
C	-2.914294	0.690694	-0.732191
C	-4.202399	0.173544	-0.602511
H	-5.412734	-1.446377	0.146153
H	-3.467040	-2.694756	1.066237
H	-1.174020	-1.773530	0.823658
H	-2.777230	1.639114	-1.240044
H	-5.044856	0.723161	-1.011836
C	-0.087293	1.477486	-1.480544
H	-0.798687	2.300446	-1.552202
H	0.924676	1.866532	-1.372140
H	-0.121758	0.909189	-2.417340

C	1.934766	1.014462	1.554025	M06-2X/LACVP** Derived Free Energy =	-945.722282
H	2.850659	1.073271	2.121771	M06-2X/LACVP** Derived Solution Free Energy =	-945.738428
TS-2				M06-2X/LACV3P+** Derived Free Energy =	-945.957613
				M06-2X/LACV3P+** Derived Solution Free Energy =	-945.974887
				Number of Imaginary Frequencies =	0
B3LYP/6-31G** Energy =				-754.728563	
B3LYP/6-31G** Free Energy =				-754.745295	
M06-2X/LACVP** Derived Free Energy =				-754.649811	
Number of Imaginary Frequencies =				1 (-363.42)	
B3LYP/6-31G** Geometry				B3LYP/6-31G** Geometry	
C	-0.543896	2.208834	1.195469	C	-1.607931 0.532041 -0.548040
C	0.630833	1.679173	1.631359	C	-2.987291 0.184219 -0.583529
B	1.818739	0.084617	0.064644	C	-3.464841 -0.866026 0.155943
C	3.756989	-0.844207	-0.764647	C	-0.723169 -0.196100 0.245602
C	3.068319	-1.851478	0.172682	Br	-4.167817 1.197326 -1.679755
H	3.631861	-1.135924	-1.819014	H	-4.519323 -1.117020 0.112452
H	4.830210	-0.739870	-0.565741	C	-2.598785 -1.632436 0.978676
H	3.009648	-2.862092	-0.247504	C	-1.207761 -1.292923 1.033390
H	3.589566	-1.915753	1.141020	C	-0.358728 -2.066191 1.871392
O	1.760856	-1.323084	0.351547	C	-0.859777 -3.118172 2.606485
O	3.088361	0.383304	-0.512586	C	-2.232332 -3.454677 2.545556
H	-1.474685	1.872145	1.642885	C	-3.082384 -2.723056 1.748222
H	-0.546716	3.240903	0.848332	H	0.694193 -1.812446 1.930772
C	-0.513206	1.057560	-0.589662	H	-0.193748 -3.694884 3.241340
O	0.700239	0.605167	-0.781337	H	-2.611566 -4.287301 3.129839
C	-3.654025	-1.789283	0.228783	H	-4.139552 -2.968766 1.695021
C	-2.326740	-2.206560	0.141518	C	3.464841 0.866026 0.155942
C	-1.306762	-1.287794	-0.109672	C	0.723169 0.196100 0.245602
C	-1.606443	0.073475	-0.271124	C	1.607931 -0.532041 -0.548040
C	-2.948944	0.484901	-0.182060	C	2.987291 -0.184219 -0.583529
C	-3.962262	-0.436308	0.065305	H	4.519323 1.117019 0.112452
H	-4.444187	-2.509132	0.421294	Br	4.167817 -1.197326 -1.679754
H	-2.077527	-3.256397	0.265261	C	1.207761 1.292923 1.033390
H	-0.277533	-1.621039	-0.176887	C	2.598785 1.632436 0.978676
H	-3.209029	1.532584	-0.295749	C	3.082384 2.723056 1.748222
H	-4.992372	-0.098539	0.130786	C	2.232332 3.454677 2.545556
C	-0.840644	2.179120	-1.566613	C	0.859778 3.118172 2.606485
H	-1.756585	2.717512	-1.322189	C	0.358728 2.066191 1.871392
H	-0.003630	2.877817	-1.607261	H	4.139552 2.968766 1.695021
H	-0.961244	1.733507	-2.561006	H	2.611566 4.287302 3.129838
C	1.691699	0.992165	1.568303	H	0.193748 3.694884 3.241340
H	2.523390	0.860517	2.243715	H	-0.694193 1.812446 1.930772
Catalyzed Reaction Reagents				Boronate 1	
(S)-3,3'-Br₂-BINOL				B3LYP/6-31G** Energy =	
B3LYP/6-31G** Energy =				-6433.011518	
B3LYP/6-31G** Free Energy =				-6433.041212	
M06-2X/LACVP** Derived Free Energy =				-1315.664356	
Number of Imaginary Frequencies =				0	

B3LYP/6-31G** Geometry				H	-0.803603	5.051986	0.896297
				O	0.439136	3.250614	0.179597
				O	-1.334411	5.382475	0.156597
C	1.407312	-0.194765	-0.466803				
C	2.779715	-0.372535	-0.793303	B3LYP/6-31G** Energy = -6433.015880			
C	3.344843	-1.621523	-0.825903	B3LYP/6-31G** Free Energy = -6433.040369			
C	0.608736	-1.291983	-0.180303	M06-2X/LACVP** Derived Free Energy = -1315.668236			
Br	3.839282	1.162088	-1.189403	M06-2X/LACVP** Derived Solution Free Energy = -1315.686774			
H	4.394745	-1.735900	-1.072803	M06-2X/LACV3P+** Derived Free Energy = -1316.006832			
C	2.560568	-2.768340	-0.544103	M06-2X/LACV3P+** Derived Solution Free Energy = -1316.027729			
C	1.172864	-2.607470	-0.224303	Number of Imaginary Frequencies = 0			
C	0.402390	-3.775187	0.031197				
C	0.974917	-5.026275	-0.018403	B3LYP/6-31G** Geometry			
C	2.347921	-5.180345	-0.325303				
C	3.121597	-4.073128	-0.583703	C	-1.648011	0.119787	0.384769
H	-0.651112	-3.668010	0.263297	C	-3.008497	0.365360	0.047202
H	0.367037	-5.904488	0.177797	C	-3.710768	-0.507849	-0.740836
H	2.786143	-6.173135	-0.359303	C	-1.001512	-1.010041	-0.093210
H	4.175699	-4.179004	-0.825803	Br	-3.848954	1.942480	0.707782
C	-3.569180	-0.596674	0.707197	H	-4.747191	-0.303520	-0.986703
C	-0.832169	-1.073014	0.153297	C	-3.088578	-1.679198	-1.244379
C	-1.717576	-0.776334	-0.876403	C	-1.716555	-1.936477	-0.923995
C	-3.086381	-0.535164	-0.572603	C	-1.110804	-3.109791	-1.448853
H	-4.618384	-0.406797	0.905597	C	-1.826092	-3.980703	-2.240457
Br	-4.261391	-0.099889	-2.026303	C	-3.182409	-3.725878	-2.551329
C	-1.306368	-1.138325	1.501197	C	-3.798724	-2.597228	-2.062926
C	-2.694273	-0.904055	1.778697	H	-0.071549	-3.312678	-1.216553
C	-3.164771	-0.971665	3.117297	H	-1.344218	-4.871716	-2.631517
C	-2.305265	-1.255647	4.152297	H	-3.733304	-4.421525	-3.176910
C	-0.933460	-1.480416	3.885597	H	-4.839083	-2.388997	-2.297242
C	-0.446462	-1.423206	2.599297	C	3.173256	-1.714553	0.775794
H	-4.219475	-0.791289	3.307097	C	0.436228	-1.247968	0.249851
H	-2.673764	-1.305055	5.172197	C	1.418529	-0.669753	-0.542789
H	-0.256656	-1.698802	4.706397	C	2.792027	-0.907790	-0.263782
H	0.606342	-1.597683	2.409897	H	4.226691	-1.882306	0.972554
O	-1.247277	-0.725623	-2.144903	Br	4.107225	-0.051466	-1.347014
H	-1.979682	-0.495539	-2.740003	C	0.810470	-2.077948	1.353902
B	1.022462	2.050526	0.437097	C	2.199138	-2.319525	1.611273
O	0.855584	1.052623	-0.508503	C	2.572869	-3.152535	2.698933
C	1.799967	1.838043	1.769997	C	1.618722	-3.728199	3.505668
C	1.823247	2.744844	2.719297	C	0.246649	-3.490100	3.255286
C	1.835027	3.655044	3.654097	C	-0.148127	-2.686637	2.208801
H	1.078227	3.674828	4.434197	H	3.629955	-3.325828	2.881897
H	2.602310	4.424661	3.683297	H	1.914787	-4.363571	4.334775
H	2.336787	0.904955	1.944897	H	-0.502472	-3.944659	3.896799
C	-0.336669	3.496097	-1.001603	H	-1.202287	-2.508608	2.026774
H	0.218837	3.195009	-1.896903	O	1.126115	0.118192	-1.614762
H	-1.264257	2.914176	-0.954103	H	0.274310	0.569145	-1.474785
C	-0.644602	4.984590	-1.014103	B	-0.390360	2.148587	0.849108
H	0.296586	5.544210	-1.139003	O	-1.011504	0.974258	1.241989
H	-1.290107	5.220176	-1.866903	C	0.077043	3.046329	2.035962

C	0.975340	4.004264	2.013854
C	1.875721	4.950988	2.018058
H	1.604273	5.993023	1.868773
H	2.928161	4.727855	2.174234
H	-0.350684	2.797284	3.009651
C	0.231299	3.572331	-1.096590
H	-0.402295	3.747756	-1.970891
H	0.109204	4.402637	-0.395563
C	1.685819	3.473066	-1.548005
H	2.004804	4.487669	-1.820827
H	2.312986	3.152419	-0.703935
H	1.981704	1.741361	-2.385209
O	-0.246734	2.355809	-0.490889
O	1.867163	2.656255	-2.685205

Boronate 2

B3LYP/6-31G** Energy =	-6202.806265
B3LYP/6-31G** Free Energy =	-6202.830884
M06-2X/LACVP** Derived Free Energy =	-1085.480194
M06-2X/LACVP** Derived Solution Free Energy =	-1085.493865
M06-2X/LACV3P+** Derived Free Energy =	-1085.741543
M06-2X/LACV3P+** Derived Solution Free Energy =	-1085.756760
Number of Imaginary Frequencies =	0

B3LYP/6-31G** Geometry

C	-1.451681	-0.678232	-0.363729
C	-2.829512	-1.014739	-0.281767
C	-3.727904	-0.160653	0.301082
C	-0.986059	0.544435	0.098089
Br	-3.419111	-2.685949	-0.978621
H	-4.778124	-0.426640	0.349970
C	-3.282128	1.050401	0.887962
C	-1.894924	1.402932	0.814447
C	-1.472323	2.573965	1.502704
C	-2.371509	3.365060	2.182689
C	-3.746881	3.037771	2.209992
C	-4.188702	1.899707	1.577880
H	-0.421965	2.836509	1.503781
H	-2.018322	4.247049	2.708525
H	-4.445873	3.675665	2.742201
H	-5.238187	1.620137	1.609678
C	3.176092	1.642663	-0.325513
C	0.439805	0.920912	-0.126771
C	2.813481	0.411518	0.153622
H	4.223286	1.920739	-0.370434
Br	4.150422	-0.819993	0.718376
C	0.806727	2.174001	-0.735869
C	2.190479	2.539321	-0.808844
C	2.561134	3.780972	-1.392016

C	1.612045	4.622498	-1.922018
C	0.249442	4.245405	-1.897121
C	-0.142719	3.058474	-1.319022
H	3.614929	4.043788	-1.424419
H	1.905910	5.565435	-2.372868
H	-0.496587	4.895711	-2.343969
H	-1.189970	2.783724	-1.320907
B	0.459106	-2.096756	-0.168690
O	-0.617891	-1.627829	-0.900395
C	0.827798	-3.591068	-0.286040
C	1.903700	-4.104901	0.271426
C	2.972562	-4.604198	0.825088
H	2.955242	-4.987666	1.841870
H	3.918397	-4.638826	0.290975
H	0.163169	-4.249265	-0.846633
C	1.445774	0.033370	0.229403
O	1.178955	-1.246207	0.651673

Ethylene Glycol

B3LYP/6-31G** Energy =	-230.180185
B3LYP/6-31G** Free Energy =	-230.198806
M06-2X/LACVP** Derived Free Energy =	-230.169342
M06-2X/LACVP** Derived Solution Free Energy =	-230.183971
M06-2X/LACV3P+** Derived Free Energy =	-230.249832
M06-2X/LACV3P+** Derived Solution Free Energy =	-230.266439
Number of Imaginary Frequencies =	0

B3LYP/6-31G** Geometry

C	-0.684811	0.609950	-0.262699
H	-1.201034	1.516812	0.088822
H	-0.663615	0.625013	-1.361831
C	0.740418	0.572273	0.265460
H	0.714116	0.619100	1.366343
H	1.295263	1.444781	-0.094907
O	-1.318941	-0.575424	0.222290
H	-2.131032	-0.717658	-0.278245
O	1.422491	-0.582265	-0.189556
H	0.824252	-1.319873	0.001372

TSs for Reaction of Boronate 1 and Acetophenone

TS-3Si

B3LYP/6-31G** Energy =	-6817.773396
B3LYP/6-31G** Free Energy =	-6817.790178
M06-2X/LACVP** Derived Free Energy =	-1700.388182
Number of Imaginary Frequencies =	1 (-379.27)

B3LYP/6-31G** Geometry

				C	-2.816406	1.943388	-0.225422
C	2.045007	-3.706385	1.612527	C	-4.155104	1.434784	-0.227420
C	0.760608	-3.872592	1.179827	C	-5.229506	2.281577	-0.609029
B	-0.202296	-1.855404	0.049810	C	-4.999109	3.585175	-0.981838
C	-1.539788	-3.191030	-2.991481	C	-3.678211	4.091580	-0.988641
C	-0.298191	-2.595522	-2.338985	H	-6.238105	1.876876	-0.603227
H	-1.236885	-3.864036	-3.801276	H	-5.826111	4.225471	-1.273445
H	-2.140389	-2.383435	-3.436588	H	-3.499413	5.119878	-1.288548
H	0.280809	-2.015525	-3.069488	C	-0.594611	2.554614	2.470476
H	0.341211	-3.395818	-1.951177	C	-0.095815	3.286624	3.525271
O	-0.715694	-1.735014	-1.279192	C	1.184283	3.884826	3.448768
H	2.246605	-3.672977	2.680727	H	1.564581	4.459534	4.287865
H	2.839709	-4.148988	1.015332	C	1.941686	3.735619	2.309771
C	2.065902	-1.710289	1.121812	H	2.926184	4.190422	2.236669
O	1.249403	-1.554799	0.093710	H	-0.690916	3.405828	4.426069
C	6.190502	-1.080086	0.035313	H	-1.576210	2.099212	2.539878
C	5.874202	-1.554578	1.311017	C	-2.616609	3.294685	-0.621832
C	4.545801	-1.772878	1.665516	H	-1.609210	3.694088	-0.634635
C	3.512102	-1.535188	0.744913				
C	3.838502	-1.062197	-0.533990	TS-3Re			
C	5.168803	-0.828196	-0.879790	B3LYP/6-31G** Energy =			-6817.776857
H	7.226302	-0.900586	-0.237286	B3LYP/6-31G** Free Energy =			-6817.793057
H	6.662501	-1.750369	2.031719	M06-2X/LACVP** Derived Free Energy =			-1700.388909
H	4.318101	-2.141371	2.661218	M06-2X/LACVP** Derived Solution Free Energy =			-1700.409417
H	3.047203	-0.840905	-1.238493	M06-2X/LACVP3P+** Derived Free Energy =			-1700.820271
H	5.398003	-0.433203	-1.864593	M06-2X/LACVP3P+** Derived Solution Free Energy =			-1700.843124
C	1.631698	-1.107381	2.449807	Number of Imaginary Frequencies =			1 (-375.73)
H	0.630799	-1.434681	2.728809				
H	2.337598	-1.340072	3.247810	B3LYP/6-31G** Geometry			
H	1.601896	-0.020481	2.323199				
C	-0.295092	-3.541199	0.565123	C	-2.861516	-2.941288	1.162213
H	-1.192091	-4.068904	0.278526	C	-1.655816	-2.827795	0.533613
O	-0.986299	-1.048198	0.961203	B	-1.144705	-0.514699	-0.299892
O	0.072900	0.763581	-2.058810	C	-2.279900	0.590501	-3.473492
H	-0.479998	-0.001618	-1.785504	C	-1.620306	-0.575400	-2.749091
O	-2.310387	-3.962025	-2.080777	H	-2.780402	0.214803	-4.373092
H	-2.720790	-3.347421	-1.453682	H	-1.501897	1.299497	-3.796194
C	-1.730704	1.087493	0.163886	H	-0.933108	-1.096305	-3.429190
C	-1.981601	-0.230104	0.534195	H	-2.385209	-1.285096	-2.417189
C	-3.323600	-0.710409	0.502296	O	-0.873403	-0.086802	-1.634192
C	-4.377901	0.084686	0.141889	H	-2.888116	-3.108786	2.236513
Br	-3.660096	-2.540006	0.948410	H	-3.683218	-3.393485	0.610814
H	-5.385200	-0.317517	0.127991	C	-3.218606	-0.900486	1.063810
C	0.459896	1.469091	-0.973414	O	-2.590403	-0.455891	-0.007291
C	-0.333205	1.630197	0.160683	C	-7.500606	-0.858866	0.568212
C	2.224991	2.831403	0.022178	C	-6.943707	-1.333967	1.757812
C	1.740295	2.093594	-1.024517	C	-5.561408	-1.356173	1.921612
H	3.206190	3.289106	-0.044524	C	-4.711905	-0.908379	0.896310
Br	2.805498	1.863985	-2.592514	C	-5.278103	-0.431078	-0.297390
C	1.456089	2.987810	1.204276	C	-6.663904	-0.407371	-0.452890
C	0.160191	2.378707	1.277178				

H	-8.579006	-0.838161	0.441812	M06-2X/LACVP** Derived Free Energy =			-1700.384486
H	-7.586109	-1.686662	2.559213	Number of Imaginary Frequencies =			1 (-381.7)
H	-5.147309	-1.737274	2.849812				
H	-4.635303	-0.058383	-1.087891	B3LYP/6-31G** Geometry			
H	-7.088502	-0.026671	-1.376990				
C	-2.656403	-0.471687	2.409509	C	-2.693202	-3.154967	0.296201
H	-1.605504	-0.744892	2.502809	C	-1.534559	-2.698400	0.852194
H	-2.711898	0.621113	2.445607	B	-1.178315	-0.212066	0.644256
H	-3.224105	-0.884283	3.243410	C	-2.522163	2.067117	2.978994
C	-0.753613	-2.236901	-0.131188	C	-1.776844	0.744953	2.844390
H	0.164285	-2.574306	-0.591989	H	-1.790676	2.889871	3.008806
O	-0.295901	0.202198	0.634608	H	-3.075381	2.078533	3.925012
O	1.753394	-0.907016	-1.885492	H	-2.497130	-0.081575	2.840524
H	0.989396	-0.300712	-1.785692	H	-1.105165	0.612886	3.705155
O	-3.274096	1.237908	-2.695893	O	-1.003242	0.755678	1.654137
H	-2.837094	1.611907	-1.914994	H	-2.647542	-3.747675	-0.614633
C	1.793905	1.212387	0.088706	H	-3.520794	-3.400255	0.958383
C	0.416805	1.300094	0.271906	C	-3.163606	-1.273860	-0.493556
C	-0.216588	2.569797	0.122103	O	-2.611125	-0.382243	0.299848
C	0.483517	3.698893	-0.209798	C	-7.459491	-1.328463	-0.149500
Br	-2.104987	2.715007	0.390704	C	-6.820339	-2.228386	-1.005493
H	-0.033179	4.646595	-0.316800	C	-5.432632	-2.220222	-1.116826
C	2.430493	-1.062018	-0.723692	C	-4.659921	-1.316109	-0.369385
C	2.484398	-0.101116	0.280907	C	-5.308639	-0.412881	0.488931
C	3.850286	-2.560922	0.580310	C	-6.699532	-0.423091	0.591729
C	3.119687	-2.296820	-0.547190	H	-8.542281	-1.332019	-0.065587
H	4.361281	-3.511925	0.685111	H	-7.402685	-2.936555	-1.587396
Br	2.951279	-3.630722	-1.901588	H	-4.953010	-2.933053	-1.780337
C	3.919591	-1.606522	1.626708	H	-4.725091	0.309233	1.050652
C	3.215697	-0.366617	1.484207	H	-7.189033	0.287222	1.251365
C	2.550510	2.376983	-0.272497	C	-2.557074	-1.416968	-1.879563
C	1.883416	3.634886	-0.421599	H	-1.494843	-1.653668	-1.822507
C	2.629423	4.788981	-0.780101	H	-3.073831	-2.163141	-2.482983
C	3.985922	4.710574	-0.993201	H	-2.645595	-0.438944	-2.364350
C	4.649116	3.468271	-0.856599	C	-0.696934	-1.820127	1.215755
H	2.105527	5.735185	-0.886302	H	0.238526	-1.861896	1.754639
H	4.548726	5.597171	-1.269202	O	-0.325211	0.062677	-0.503927
H	5.719215	3.409265	-1.032600	O	2.453228	-0.980366	-2.144932
C	3.276102	0.561383	2.560705	H	2.004241	-0.130185	-2.276172
C	3.996001	0.281582	3.701106	O	-3.474820	2.269151	1.946690
C	4.696195	-0.940622	3.832808	H	-2.987023	2.274111	1.108538
H	5.260794	-1.147223	4.737008	C	1.788611	1.151314	-0.385949
C	4.654590	-1.864224	2.814009	C	0.415682	1.184304	-0.626160
H	5.182685	-2.810026	2.902610	C	-0.176259	2.401646	-1.078922
H	4.025005	1.006583	4.509404	C	0.562627	3.536815	-1.280692
H	2.740806	1.500186	2.475105	Br	-2.055562	2.440455	-1.428652
C	3.952910	2.333176	-0.505597	H	0.080024	4.445785	-1.623681
H	4.471705	1.386672	-0.408096	C	2.715333	-1.110960	-0.822378
				C	2.411637	-0.119698	0.103992
B3LYP/6-31G** Energy =			-6817.770646	C	3.629832	-2.531605	0.925153
B3LYP/6-31G** Free Energy =			-6817.789204	C	3.330346	-2.319751	-0.395223

H	4.102774	-3.459532	1.228597	H	7.788615	2.063441	-1.534041
Br	3.736417	-3.657833	-1.690340	H	5.370119	2.134510	-1.931593
C	3.322843	-1.549695	1.902659	H	4.715093	-0.314245	1.542226
C	2.696460	-0.327585	1.490109	H	7.157695	-0.372829	1.951975
C	2.589022	2.322671	-0.604323	C	2.844635	1.084717	-1.852941
C	1.962539	3.530582	-1.051698	H	1.788987	1.352805	-1.840980
C	2.751392	4.691813	-1.265994	H	3.402202	1.820078	-2.431802
C	4.109781	4.669055	-1.049623	H	2.923169	0.106886	-2.340354
C	4.733553	3.477463	-0.610752	C	0.896816	1.667932	1.183167
H	2.260001	5.599533	-1.605852	H	-0.049887	1.770619	1.692811
H	4.705117	5.561627	-1.216107	O	0.451847	-0.164560	-0.571294
H	5.806593	3.463639	-0.444229	O	-1.978089	1.281339	-2.213046
C	2.372069	0.632226	2.489283	H	-1.654457	0.379215	-2.364624
C	2.667981	0.400398	3.814431	O	0.202454	-2.805603	3.459593
C	3.300152	-0.800580	4.216415	H	-0.054354	-2.653686	2.537925
H	3.529113	-0.967265	5.264651	C	-1.776517	-1.010164	-0.542789
C	3.615710	-1.755543	3.277613	C	-0.408505	-1.191719	-0.748789
H	4.094505	-2.685349	3.573390	C	0.059757	-2.449309	-1.237039
H	2.411470	1.146911	4.560527	C	-0.798176	-3.484836	-1.498987
H	1.868093	1.544875	2.193795	Br	1.928276	-2.682784	-1.540846
C	3.995234	2.335141	-0.393852	H	-0.411432	-4.429423	-1.866347
H	4.482969	1.426631	-0.059038	C	-2.343813	1.378513	-0.913030
B3LYP/6-31G** Energy =			-6817.764261	C	-2.269750	0.307186	-0.028807
B3LYP/6-31G** Free Energy =			-6817.785519	C	-3.215362	2.825403	0.835127
M06-2X/LACVP** Derived Free Energy =			-1700.383019	C	-2.824552	2.639413	-0.465148
Number of Imaginary Frequencies =			1 (-379.33)	H	-3.581238	3.795423	1.154770
B3LYP/6-31G** Geometry				Br	-2.922594	4.084828	-1.703798
				C	-3.143970	1.760815	1.770776
				C	-2.659296	0.482761	1.336825
				C	-2.696477	-2.074652	-0.830810
C	2.992624	2.861384	0.291778	C	-2.194588	-3.329318	-1.304650
C	1.797370	2.484133	0.828126	C	-3.100671	-4.386615	-1.583894
B	1.272883	0.022035	0.613103	C	-4.454627	-4.217299	-1.409047
C	0.815989	-1.595733	3.875408	C	-4.955974	-2.976797	-0.949793
C	1.740945	-1.051377	2.795970	H	-2.702296	-5.332613	-1.940644
H	0.059345	-0.831843	4.112652	H	-5.139986	-5.031289	-1.624888
H	1.382495	-1.809844	4.788876	H	-6.026045	-2.845991	-0.818647
H	2.562988	-1.756978	2.611161	C	-2.576540	-0.562412	2.298482
H	2.172593	-0.090159	3.108788	C	-2.960152	-0.358027	3.605484
O	0.962504	-0.914189	1.616386	C	-3.449510	0.901715	4.026208
H	3.005454	3.429832	-0.635460	H	-3.750917	1.047961	5.059015
H	3.817931	3.074035	0.967679	C	-3.535791	1.937796	3.125054
C	3.376076	0.927136	-0.439133	H	-3.904766	2.911919	3.435424
O	2.730720	0.084511	0.339577	H	-2.879205	-1.173014	4.318471
C	7.636544	0.843941	0.237776	H	-2.196489	-1.530214	1.993827
C	7.120480	1.543542	-0.854017	C	-4.102054	-1.933373	-0.668245
C	5.745948	1.578073	-1.080003	H	-4.497239	-0.986570	-0.318264
C	4.861349	0.910912	-0.217024	B3LYP/6-31G** Energy =			-6817.751167
C	5.391340	0.211207	0.879302	B3LYP/6-31G** Free Energy =			-6817.769460
C	6.765586	0.178739	1.102617	M06-2X/LACVP** Derived Free Energy =			-1700.366988
H	8.708047	0.816170	0.411628				

Number of Imaginary Frequencies =				1 (-372.30)	Br	2.167024	-3.887084	-2.055221
					C	3.203310	-2.089904	1.586793
B3LYP/6-31G** Geometry					C	2.817005	-0.724206	1.380801
					C	2.878697	1.970610	-0.707581
C	-3.642100	1.636188	-1.584294	C	2.564392	3.348210	-0.933672	
C	-2.440497	1.033695	-1.807695	C	3.537489	4.208518	-1.507864	
B	-1.325496	-0.005814	0.156299	C	4.782291	3.733825	-1.849764	
C	-1.740991	-2.365631	2.439082	C	5.100897	2.373426	-1.626574	
C	-0.635990	-2.025720	1.442986	H	3.278484	5.251418	-1.670257	
H	-1.316389	-3.017235	3.212779	H	5.520789	4.398432	-2.287859	
H	-2.530187	-2.939832	1.925377	H	6.085299	2.001731	-1.895774	
H	-0.137386	-2.951716	1.130881	C	3.021599	0.195188	2.447008	
H	0.101806	-1.383020	1.933793	C	3.574699	-0.214017	3.639207	
O	-1.125791	-1.403714	0.254790	C	3.956104	-1.562817	3.836297	
H	-4.531398	1.260088	-2.080498	H	4.389803	-1.869721	4.783197	
H	-3.626105	2.707086	-1.386986	C	3.772409	-2.479911	2.828491	
C	-3.864699	0.698175	0.244100	H	4.058414	-3.519311	2.966385	
O	-2.667199	0.434276	0.739400	H	3.717494	0.505578	4.440012	
C	-6.379683	-2.604828	-0.966327	H	2.729695	1.229888	2.308914	
C	-6.942490	-1.357832	-0.688420	C	4.176999	1.516218	-1.071781	
C	-6.130195	-0.294531	-0.302911	H	4.435703	0.476818	-0.905587	
C	-4.737894	-0.456926	-0.181410					
C	-4.182188	-1.715822	-0.460517	B3LYP/6-31G** Energy =				-6817.754608
C	-5.000583	-2.776023	-0.850726	B3LYP/6-31G** Free Energy =				-6817.772424
H	-7.012479	-3.434728	-1.267134	M06-2X/LACVP** Derived Free Energy =				-1700.370017
H	-8.015590	-1.211836	-0.769020	Number of Imaginary Frequencies =				1 (-372.51)
H	-6.592199	0.664065	-0.094605					
H	-3.113188	-1.867018	-0.361217	B3LYP/6-31G** Geometry				
H	-4.553279	-3.743319	-1.060031					
C	-4.533905	1.830467	1.012206	C	3.758896	1.876181	-1.379809	
H	-5.371007	2.285466	0.481908	C	2.572494	1.290481	-1.713305	
H	-4.907705	1.424658	1.959703	B	1.395894	0.155693	0.141501	
H	-3.784009	2.586868	1.237612	C	0.912687	-3.458103	0.922519	
C	-1.384396	0.397797	-1.519398	C	0.917691	-1.977701	1.284012	
H	-0.488593	0.142205	-2.071799	H	0.079487	-3.667205	0.238021	
O	-0.293601	0.802286	0.798406	H	0.774887	-4.064598	1.823722	
O	1.558411	-0.871787	-2.070001	H	1.671592	-1.787599	2.063310	
H	1.485115	-1.653183	-2.643407	H	-0.059008	-1.669098	1.675512	
O	-2.268396	-1.238238	3.116289	O	1.246391	-1.261508	0.097309	
H	-2.588398	-0.619735	2.442693	H	4.671696	1.516977	-1.843908	
C	1.893500	1.105001	-0.128688	H	3.730898	2.943282	-1.163914	
C	0.630497	1.590194	0.212513	C	3.865196	0.931689	0.440195	
C	0.360391	2.977094	-0.010477	O	2.644095	0.622394	0.829499	
C	1.283189	3.825002	-0.564071	C	6.634489	-2.306719	-0.307191	
Br	-1.334213	3.701884	0.495924	C	7.048391	-0.982321	-0.478397	
H	1.036885	4.870202	-0.716963	C	6.157094	0.064582	-0.260802	
C	2.073510	-1.267592	-0.873303	C	4.828594	-0.190514	0.125300	
C	2.247205	-0.325599	0.130303	C	4.431391	-1.519813	0.302007	
C	3.003916	-3.026698	0.542486	C	5.323989	-2.570415	0.086211	
C	2.453016	-2.618493	-0.642713	H	7.332487	-3.121622	-0.475788	
H	3.287120	-4.063699	0.686179	H	8.068691	-0.764325	-0.780399	

H	6.503696	1.084181	-0.400307				
H	3.420990	-1.732709	0.611409		B3LYP/6-31G** Geometry		
H	4.976587	-3.588313	0.234516				
C	4.448298	2.059893	1.283290	C	-4.368389	-0.989425	-1.442394
H	4.691398	1.641997	2.266892	C	-3.363788	-1.073322	-2.355294
H	5.360798	2.483488	0.861587	B	-1.103292	-0.215012	-1.670196
H	3.699700	2.838394	1.419887	C	-1.198007	3.380187	-2.131400
C	1.495594	0.658984	-1.511701	C	-1.494702	2.010886	-2.729598
H	0.629092	0.417484	-2.111799	H	-1.742111	4.137284	-2.709000
O	0.271196	0.845898	0.785199	H	-0.124508	3.598392	-2.219301
O	-1.471410	-0.896213	-1.977491	H	-1.318803	2.052085	-3.815999
H	-1.329911	-1.697416	-2.508987	H	-2.556300	1.779881	-2.573298
O	2.145286	-3.858208	0.331120	O	-0.652197	1.022890	-2.164198
H	2.272787	-3.241512	-0.404983	H	-4.806485	-1.900027	-1.042993
C	-1.921605	1.131998	-0.113400	H	-5.044993	-0.138828	-1.488895
C	-0.662304	1.634796	0.218296	C	-3.013489	-0.590419	0.117205
C	-0.425901	3.030895	0.006089	O	-1.931992	-0.010914	-0.390896
C	-1.364500	3.858294	-0.553414	C	-5.521400	2.094273	2.379004
Br	1.230702	3.812995	0.551384	C	-5.649593	0.714573	2.547905
H	-1.141298	4.909793	-0.698620	C	-4.846391	-0.159125	1.818305
C	-2.027410	-1.264005	-0.792789	C	-3.893792	0.333479	0.907504
C	-2.257607	-0.296201	0.173907	C	-3.775399	1.723379	0.742104
C	-2.985511	-2.994797	0.643820	C	-4.582403	2.591376	1.473903
C	-2.397112	-2.612304	-0.532182	H	-6.147203	2.774071	2.949703
H	-3.254913	-4.032495	0.808025	H	-6.373892	0.314670	3.251205
Br	-2.019115	-3.924111	-1.879476	H	-4.968186	-1.224824	1.973106
C	-3.235709	-2.031192	1.651815	H	-3.050301	2.135281	0.049703
C	-2.863907	-0.666194	1.416009	H	-4.466207	3.661776	1.333801
C	-2.921803	1.974596	-0.698804	C	-2.834683	-2.009717	0.618607
C	-2.631901	3.355595	-0.934111	H	-2.140683	-1.985413	1.465705
C	-3.616599	4.192794	-1.522815	H	-3.768781	-2.457621	0.955507
C	-4.849001	3.691494	-1.871111	H	-2.406782	-2.645316	-0.154094
C	-5.143504	2.326896	-1.639204	C	-2.184890	-0.951518	-2.808195
H	-3.376098	5.239093	-1.692319	H	-1.757389	-1.166317	-3.777695
H	-5.596200	4.337894	-2.321713	O	0.042112	-1.096307	-1.526797
H	-6.117804	1.933897	-1.914901	O	0.123202	1.620596	0.917801
C	-3.121904	0.282212	2.445204	H	-0.390695	0.810593	0.757001
C	-3.711504	-0.098981	3.629006	O	-1.628708	3.506286	-0.785000
C	-4.077706	-1.447680	3.855414	H	-0.990405	3.037690	-0.222400
H	-4.541706	-1.732074	4.794915	C	1.329912	-1.046200	0.492703
C	-3.842809	-2.392384	2.884617	C	0.504015	-1.702304	-0.421296
H	-4.117411	-3.431683	3.044622	C	0.240421	-3.094205	-0.227795
H	-3.896602	0.643023	4.400103	C	0.647324	-3.767702	0.892706
H	-2.842902	1.317110	2.284299	Br	-0.675276	-4.042010	-1.612093
C	-4.208605	1.492397	-1.068801	H	0.421529	-4.822603	1.007107
H	-4.447806	0.448998	-0.897795	C	1.384202	1.487900	0.417300
				C	1.975807	0.263803	0.144802
B3LYP/6-31G** Energy =		-6817.757034		C	3.373997	2.678908	-0.330402
B3LYP/6-31G** Free Energy =		-6817.774213		C	2.110497	2.692703	0.194299
M06-2X/LACVP** Derived Free Energy =		-1700.370866		H	3.900692	3.612710	-0.494403
Number of Imaginary Frequencies =		1 (-372.20)		Br	1.297390	4.362700	0.625298

C	3.994902	1.452211	-0.671801	H	-3.260891	-1.632508	0.544916
C	3.292507	0.227908	-0.431399	H	-4.797583	-3.273310	1.497827
C	1.739916	-1.720096	1.694404	C	-4.398910	1.903172	-1.258011
C	1.372322	-3.088699	1.905405	H	-4.817205	1.326063	-2.090207
C	1.771725	-3.748395	3.097905	H	-5.198914	2.502370	-0.822216
C	2.508223	-3.088691	4.054404	H	-3.618713	2.553573	-1.648915
C	2.879318	-1.739191	3.849103	C	-1.258106	0.746510	1.454101
H	1.484530	-4.787097	3.239006	H	-0.385906	0.503519	2.045004
H	2.807326	-3.600190	4.964205	O	-0.263203	0.761298	-0.944698
H	3.460215	-1.221187	4.606402	O	1.616807	-0.816001	-2.184684
C	3.943812	-0.987690	-0.779998	H	0.903803	-0.159904	-2.043990
C	5.205912	-0.987385	-1.331899	O	-2.015979	-3.817901	0.590535
C	5.894206	0.225517	-1.564601	H	-1.706684	-3.131794	1.200429
H	6.888806	0.210521	-2.000001	C	1.939993	1.114416	-0.072798
C	5.296001	1.420515	-1.239201	C	0.715291	1.607807	-0.526303
H	5.809097	2.362617	-1.413202	C	0.539084	3.017304	-0.654114
H	5.676415	-1.930583	-1.593698	C	1.540578	3.904012	-0.360819
H	3.431316	-1.927792	-0.614797	Br	-1.131720	3.711890	-1.265621
C	2.511313	-1.074993	2.700102	H	1.370472	4.970310	-0.462427
H	2.800509	-0.040492	2.554501	C	2.035308	-1.222289	-0.962080
B3LYP/6-31G** Energy =				C	2.142302	-0.354681	0.123313
B3LYP/6-31G** Free Energy =				C	2.763517	-3.104175	0.406535
M06-2X/LACVP** Derived Free Energy =				C	2.377015	-2.594386	-0.804570
Number of Imaginary Frequencies =				H	3.016122	-4.155073	0.497943
				Br	2.241024	-3.750398	-2.313061
B3LYP/6-31G** Geometry				C	2.788011	-2.273167	1.555128
				C	2.463203	-0.883870	1.419517
				C	3.028488	2.024825	0.170997
C	-3.406614	2.150897	1.271788	C	2.813780	3.434522	0.044085
C	-2.247710	1.516105	1.624194	C	3.880275	4.338831	0.295480
B	-1.326100	0.077198	-0.144493	C	5.129277	3.876440	0.636085
C	-1.238679	-3.627006	-0.587066	C	5.359184	2.483842	0.727696
C	-1.357786	-2.201610	-1.117577	H	3.690068	5.404629	0.201172
H	-0.182778	-3.862598	-0.400863	H	5.940673	4.573746	0.821481
H	-1.609674	-4.331813	-1.337961	H	6.352086	2.118449	0.972400
H	-2.364587	-2.025018	-1.517979	C	2.453798	-0.089360	2.601512
H	-0.627986	-2.047612	-1.922577	C	2.756199	-0.632650	3.831416
O	-1.111893	-1.319400	-0.019483	C	3.095506	-1.999847	3.953627
H	-4.302314	1.975196	1.859689	H	3.337008	-2.414638	4.927530
H	-3.300519	3.156994	0.867381	C	3.110112	-2.799455	2.834233
C	-3.776705	0.918283	-0.275303	H	3.359118	-3.854453	2.911941
O	-2.626402	0.449786	-0.741998	H	2.735394	-0.002842	4.716112
C	-6.498991	-1.935720	1.499515	H	2.207491	0.963737	2.526704
C	-6.945798	-0.652524	1.171906	C	4.340690	1.584635	0.503402
C	-6.070003	0.273576	0.611699	H	4.540196	0.522437	0.566910
C	-4.725201	-0.064118	0.371503	B3LYP/6-31G** Energy =			
C	-4.288294	-1.348913	0.715514	B3LYP/6-31G** Free Energy =			
C	-5.168289	-2.279514	1.267220	M06-2X/LACVP** Derived Free Energy =			
H	-7.186687	-2.658820	1.928120	Number of Imaginary Frequencies =			
H	-7.980799	-0.373829	1.346802				
H	-6.444108	1.261372	0.362792				

B3LYP/6-31G** Geometry				C	-2.997401	0.046097	1.326491
				C	-2.242489	2.684807	-0.483890
C	3.569398	0.464874	2.382111	C	-1.440285	3.845206	-0.723181
C	2.207497	0.511376	2.462108	C	-2.062581	5.111409	-0.885575
B	1.036899	-0.666209	0.622797	C	-3.430981	5.234912	-0.823478
C	0.937293	-3.949903	-0.279323	C	-4.230585	4.089612	-0.598487
C	-0.040804	-2.811802	-0.023118	H	-1.435078	5.980508	-1.064268
H	0.446993	-4.692397	-0.922329	H	-3.899678	6.205914	-0.951073
H	1.163690	-4.440810	0.680574	H	-5.311284	4.189015	-0.559589
H	-0.976707	-3.238401	0.356076	C	-2.785001	0.986291	2.373997
H	-0.267200	-2.290096	-0.960416	C	-3.340205	0.800784	3.621795
O	0.455496	-1.906010	0.962288	C	-4.143208	-0.330815	3.894186
H	4.134095	-0.042533	3.159610	H	-4.576611	-0.463820	4.880584
H	4.069601	1.315875	1.923418	C	-4.369908	-1.259609	2.904480
C	3.532297	-1.008418	0.966502	H	-4.981811	-2.136308	3.099572
O	2.487600	-0.771310	0.185600	H	-3.163205	1.534380	4.403000
C	7.285505	-0.230216	-1.015183	H	-2.185298	1.868190	2.176505
C	7.278700	-0.715223	0.294213	C	-3.654588	2.849710	-0.431393
C	6.071198	-0.962124	0.942509	H	-4.279591	1.980411	-0.264601
C	4.848600	-0.723717	0.293807				
C	4.865005	-0.236409	-1.022389	B3LYP/6-31G** Energy =			-6817.757238
C	6.075908	0.006892	-1.668785	B3LYP/6-31G** Free Energy =			-6817.775761
H	8.227307	-0.042015	-1.521780	M06-2X/LACVP** Derived Free Energy =			-1700.371222
H	8.214599	-0.904329	0.811315	Number of Imaginary Frequencies =			1 (-348.32)
H	6.088794	-1.332730	1.962307				
H	3.924707	-0.054203	-1.526691	B3LYP/6-31G** Geometry			
H	6.072111	0.375899	-2.690083	C	-3.818885	2.763404	1.155122
C	3.455192	-2.257723	1.831394	C	-2.533684	2.747296	1.589819
H	3.447692	-3.110819	1.143489	B	-1.038793	0.906795	0.752006
H	4.307690	-2.355729	2.503796	C	-1.443400	-2.116413	2.606292
H	2.524790	-2.282824	2.397591	C	-1.414194	-0.591413	2.692700
C	1.024098	0.302482	2.061404	H	-2.198799	-2.509613	3.295993
H	0.052998	0.591883	2.439403	H	-0.466901	-2.523717	2.904188
O	0.355404	0.065500	-0.443500	H	-1.003789	-0.288319	3.666900
O	-2.117193	-0.707683	-2.189812	H	-2.433293	-0.193409	2.615504
H	-1.538691	0.069116	-2.234405	O	-0.588595	-0.092512	1.652600
O	2.140096	-3.551503	-0.929217	H	-4.601184	2.380204	1.805023
H	2.267799	-2.606004	-0.768711	H	-4.133083	3.544308	0.466727
C	-1.607193	1.407204	-0.316897	C	-3.411296	1.169809	-0.295887
C	-0.218593	1.283701	-0.448594	O	-2.326097	0.537903	0.088508
C	0.553812	2.468700	-0.671685	C	-6.998703	-1.197378	0.005713
C	-0.032885	3.700803	-0.798478	C	-7.058400	0.089725	-0.534680
Br	2.454311	2.355896	-0.797180	C	-5.903998	0.861420	-0.626780
H	0.584218	4.576502	-0.968771	C	-4.669698	0.362814	-0.173686
C	-2.649296	-0.770989	-0.946313	C	-4.615702	-0.934389	0.362108
C	-2.429597	0.202604	0.020494	C	-5.776304	-1.703585	0.447707
C	-4.016604	-2.066395	0.592775	H	-7.898806	-1.801275	0.074412
C	-3.446400	-1.909089	-0.642622	H	-8.004099	0.491529	-0.886176
H	-4.618307	-2.944396	0.801468	H	-5.970495	1.860822	-1.044876
Br	-3.671600	-3.253980	-1.971431	H	-3.667302	-1.353095	0.683603
C	-3.806604	-1.101402	1.610881				

H	-5.717607	-2.709187	0.853503				
C	-3.207196	2.018314	-1.544683	C	-3.255037	-3.191978	0.477744
H	-4.081994	2.605419	-1.825378	C	-1.946340	-3.582190	0.502332
H	-2.341292	2.670210	-1.411682	B	-0.320227	-1.843091	-0.220940
H	-2.978300	1.327717	-2.364487	C	-1.260643	-2.411025	-3.318348
C	-1.335085	2.347792	1.685114	C	0.047357	-2.735750	-2.590558
H	-0.501482	2.708286	2.271213	H	-1.149548	-2.707407	-4.373353
O	-0.091895	1.176896	-0.312596	H	-1.443032	-1.333923	-3.287027
O	1.307392	-0.712200	-2.366909	H	0.875056	-2.609846	-3.298959
H	0.950687	-1.261995	-3.083410	H	0.039948	-3.795356	-2.290678
O	-1.798205	-2.554905	1.302592	O	0.370568	-1.917675	-1.479744
H	-1.241305	-2.033204	0.703193	H	-3.794934	-3.136990	1.417847
C	2.226304	0.567886	-0.101605	H	-3.848342	-3.496856	-0.382160
C	1.208906	1.516490	-0.222098	C	-2.825820	-1.236976	0.171579
C	1.572411	2.890490	-0.378593	O	-1.612721	-1.136478	-0.350523
C	2.875014	3.312684	-0.344594	C	-3.443292	0.481056	4.091213
Br	0.205016	4.190096	-0.706182	C	-4.514800	-0.094821	3.402806
H	3.109917	4.365184	-0.460690	C	-4.313908	-0.661399	2.148094
C	1.432892	-1.476505	-1.256813	C	-3.036810	-0.671800	1.557190
C	1.889398	-0.888213	-0.081711	C	-1.969903	-0.094323	2.257598
C	1.288886	-3.659910	-0.164622	C	-2.175493	0.479655	3.513609
C	1.126987	-2.866704	-1.268918	H	-3.600985	0.929540	5.067822
H	1.046582	-4.715809	-0.207727	H	-5.508098	-0.098520	3.841909
Br	0.476479	-3.627194	-2.908920	H	-5.160614	-1.103381	1.631489
C	1.772392	-3.094818	1.041579	H	-0.983804	-0.087724	1.813894
C	2.058098	-1.691119	1.089085	H	-1.336887	0.937038	4.029315
C	3.600804	0.981780	-0.095907	C	-3.889120	-0.902246	-0.866411
C	3.923910	2.374179	-0.189002	H	-3.748828	-1.527632	-1.747523
C	5.282712	2.787875	-0.166604	H	-4.904420	-1.013144	-0.483810
C	6.298708	1.866170	-0.073112	H	-3.735811	0.142358	-1.160392
C	5.989103	0.487271	-0.007417	C	-0.697640	-3.444599	0.356531
H	5.502415	3.850274	-0.233299	H	0.158954	-4.084210	0.507916
H	7.334810	2.191066	-0.058312	O	0.566183	-1.216818	0.750868
H	6.792701	-0.241233	0.050878	O	0.243490	0.647043	-2.347996
C	2.493703	-1.143826	2.328586	H	0.566882	-0.225367	-2.027813
C	2.664203	-1.940533	3.437682	O	-2.413646	-3.037025	-2.754456
C	2.403797	-3.331531	3.377976	H	-2.291555	-3.992425	-2.828174
H	2.548098	-3.948536	4.259673	C	1.945296	0.588183	-0.016702
C	1.961092	-3.892424	2.202975	C	1.789286	-0.723824	0.426074
H	1.744288	-4.955722	2.143670	C	2.950278	-1.534137	0.597955
H	2.998808	-1.497738	4.371383	C	4.209482	-1.070944	0.322560
H	2.684908	-0.078927	2.388690	Br	2.758264	-3.318748	1.259322
C	4.681102	0.057175	-0.020515	H	5.069777	-1.715655	0.466545
H	4.464098	-1.003124	0.025081	C	-0.019599	1.458426	-1.299580
				C	0.753604	1.487998	-0.142781
B3LYP/6-31G** Energy =			-6817.758762	C	-1.457081	3.230823	-0.430742
B3LYP/6-31G** Free Energy =			-6817.775570	C	-1.139492	2.331338	-1.412859
M06-2X/LACVP** Derived Free Energy =			-1700.377060	H	-2.317775	3.880833	-0.546527
Number of Imaginary Frequencies =			1 (-385.61)	Br	-2.257798	2.181377	-2.953558
				C	-0.681376	3.296894	0.754957
B3LYP/6-31G** Geometry				C	0.428617	2.403780	0.910137

C	3.252100	1.093977	-0.324597	C	-1.619816	-1.544276	-2.658792
C	4.396193	0.250663	-0.153817	H	-0.540218	-1.695191	-2.646291
C	5.690096	0.750857	-0.458611	H	-2.111727	-2.395770	-3.130393
C	5.856606	2.035864	-0.920287	H	-1.847504	-0.653474	-3.258793
C	4.729014	2.872278	-1.095768	C	-0.524420	-1.683290	1.368509
H	6.546691	0.096247	-0.320826	H	0.080280	-1.653897	2.264109
H	6.849410	2.409660	-1.152084	O	-0.249786	0.875907	1.046907
H	4.864222	3.884783	-1.464849	O	1.598490	-1.063718	-1.757891
C	1.175820	2.472950	2.119436	H	1.203602	-0.183113	-1.868591
C	0.846632	3.374235	3.108454	O	-4.835389	0.720068	2.752805
C	-0.247760	4.256648	2.947274	H	-4.692595	0.211766	1.940805
H	-0.495451	4.962736	3.734188	C	1.691521	1.313480	-0.263792
C	-0.994664	4.213977	1.792476	C	0.382925	1.613098	0.119308
H	-1.840958	4.882287	1.656191	C	-0.244560	2.775706	-0.428493
H	1.435435	3.409813	4.020652	C	0.409552	3.607698	-1.298893
H	2.017715	1.803240	2.254820	Br	-2.037254	3.185829	0.081306
C	3.462611	2.415884	-0.805773	H	-0.095336	4.483304	-1.693094
H	2.605516	3.064095	-0.947758	C	2.219889	-1.081227	-0.549591
B3LYP/6-31G** Energy =			-6817.759307	C	2.324704	0.054572	0.242909
B3LYP/6-31G** Free Energy =			-6817.777986	C	3.416470	-2.407342	1.094410
M06-2X/LACVP** Derived Free Energy =			-1700.372735	C	2.759873	-2.316034	-0.104790
Number of Imaginary Frequencies =			1 (-316.01)	H	3.821258	-3.360147	1.418612
B3LYP/6-31G** Geometry				Br	2.509053	-3.869330	-1.184389
				C	3.558885	-1.265544	1.925910
				C	2.997702	-0.016836	1.500410
				C	2.400432	2.176371	-1.165891
C	-1.481540	-3.264278	-0.423992	C	1.746249	3.338179	-1.688493
C	-0.904833	-2.642785	0.631108	C	2.443960	4.192869	-2.582592
B	-1.237200	-0.174680	0.854607	C	3.740357	3.917352	-2.951791
C	-3.700492	0.456253	3.561206	C	4.391041	2.771044	-2.437491
C	-2.402089	0.756836	2.826507	H	1.932673	5.070676	-2.968793
H	-3.779685	1.095155	4.447805	H	4.266366	4.576845	-3.635292
H	-3.689607	-0.592246	3.901606	H	5.415339	2.559330	-2.729690
H	-1.544092	0.495325	3.463307	C	3.136117	1.110462	2.355009
H	-2.331375	1.823735	2.586406	C	3.796115	1.007754	3.559209
O	-2.411198	-0.004464	1.624406	C	4.351698	-0.225553	3.975911
H	-0.833345	-3.631487	-1.216791	H	4.869396	-0.291060	4.928111
H	-2.417547	-3.796666	-0.281192	C	4.233484	-1.337252	3.173911
C	-2.140414	-1.294369	-1.256592	H	4.654571	-2.290057	3.483811
O	-1.460301	-0.377678	-0.613693	H	3.891126	1.881453	4.197309
C	-6.435213	-1.252112	-0.941796	H	2.711329	2.058468	2.043109
C	-5.789628	-2.400921	-1.404794	C	3.740329	1.922253	-1.569591
C	-4.400328	-2.438339	-1.482894	H	4.248618	1.048146	-1.177690
C	-3.628314	-1.336049	-1.081194	B3LYP/6-31G** Energy =			-6817.758288
C	-4.287198	-0.172441	-0.647094	B3LYP/6-31G** Free Energy =			-6817.775829
C	-5.680699	-0.137222	-0.576395	M06-2X/LACVP** Derived Free Energy =			-1700.374215
H	-7.518813	-1.222997	-0.878696	Number of Imaginary Frequencies =			1 (-370.01)
H	-6.368640	-3.269113	-1.704995	B3LYP/6-31G** Geometry			
H	-3.915540	-3.337745	-1.848993				
H	-3.706387	0.706752	-0.399995				
H	-6.174187	0.768685	-0.237296				

C	-1.712764	3.887982	-1.572595	C	-2.994065	-2.749037	1.051504
C	-1.487254	2.916686	-2.497396	C	-3.730051	-3.613548	1.905506
B	-0.207324	0.899902	-1.709103	C	-3.113738	-4.270740	2.943903
C	3.393468	1.287552	-2.569715	C	-1.727639	-4.092222	3.160498
C	1.963561	1.808333	-2.509810	H	-4.789749	-3.755162	1.710910
H	3.688476	0.914655	-1.577816	H	-3.682427	-4.935748	3.586905
H	4.066956	2.110062	-2.837316	H	-1.235930	-4.631016	3.964997
H	1.676353	2.183730	-3.502609	C	0.063908	-0.218298	2.868396
H	1.891452	2.641731	-1.794708	C	0.482803	0.377107	4.037894
O	1.123577	0.730921	-2.136608	C	1.859802	0.489226	4.338090
H	-2.732365	4.104769	-1.264591	H	2.178100	0.957430	5.264589
H	-1.029275	4.733192	-1.523896	C	2.789906	0.008839	3.445686
C	-1.177641	2.569689	0.002102	H	3.853106	0.093653	3.655383
O	-0.288231	1.720800	-0.464402	H	-0.253200	0.765697	4.735597
C	0.522531	5.409809	2.761398	H	-0.996092	-0.299511	2.659099
C	-0.837371	5.475091	2.449004	C	-0.991554	-3.248111	2.359197
C	-1.394162	4.563384	1.556405	H	0.070445	-3.133397	2.535093
C	-0.598750	3.573795	0.955201				
C	0.765951	3.513514	1.278196	B3LYP/6-31G** Energy =			-6817.757596
C	1.318942	4.425220	2.175595	B3LYP/6-31G** Free Energy =			-6817.775364
H	0.955524	6.119214	3.460098	M06-2X/LACVP** Derived Free Energy =			-1700.375106
H	-1.465180	6.236982	2.900807	Number of Imaginary Frequencies =			1 (-380.76)
H	-2.450063	4.638570	1.317808				
H	1.374560	2.732922	0.838593	B3LYP/6-31G** Geometry			
H	2.374044	4.359434	2.422891				
C	-2.557032	2.013670	0.299007	C	3.620208	-0.235476	-2.281500
H	-2.449419	1.285470	1.110006	C	2.257608	-0.177683	-2.390301
H	-3.258241	2.781660	0.625810	B	1.081909	-0.772598	-0.288204
H	-2.965728	1.499065	-0.570793	C	0.876224	-3.476505	1.619885
C	-1.079541	1.796392	-2.930098	C	-0.121281	-2.539309	0.951988
H	-1.089538	1.345593	-3.912299	H	0.422326	-3.942312	2.502883
O	-0.789605	-0.443605	-1.641802	H	1.751521	-2.900102	1.956988
O	1.275418	-2.205178	-1.468611	H	-0.398586	-1.721713	1.625092
H	0.498411	-1.712388	-1.804608	H	-1.028278	-3.096512	0.689986
O	3.551077	0.280254	-3.552116	O	0.426217	-2.039901	-0.271409
H	3.077989	-0.495851	-3.217116	H	4.175012	-0.939270	-2.896704
C	-0.856082	-1.645708	0.427498	H	4.136203	0.699527	-2.071096
C	-1.494594	-1.094815	-0.683000	C	3.549513	-1.258683	-0.531505
C	-2.879491	-1.341734	-0.904695	O	2.513010	-0.799991	0.143996
C	-3.618077	-2.119845	-0.055093	C	7.292105	-0.029169	1.235102
Br	-3.721807	-0.551944	-2.424692	C	7.294810	-0.880964	0.129099
H	-4.674076	-2.281859	-0.241690	C	6.092313	-1.280769	-0.449803
C	1.564016	-1.721474	-0.240711	C	4.865910	-0.832978	0.066198
C	0.590115	-1.361389	0.692893	C	4.872504	0.023318	1.178701
C	3.347713	-1.068552	1.293083	C	6.077601	0.420523	1.755303
C	2.942416	-1.591656	0.095484	H	8.229603	0.280135	1.687504
H	4.405113	-0.975738	1.516279	H	8.234112	-1.236757	-0.283702
Br	4.241019	-2.108238	-1.199321	H	6.119416	-1.937065	-1.313406
C	2.388510	-0.601666	2.227587	H	3.927302	0.370612	1.576101
C	0.994411	-0.735384	1.923791	H	6.066098	1.079219	2.618605
C	-1.597067	-2.532418	1.288000	C	3.449021	-2.684181	-1.058210

H	3.347324	-3.360285	-0.203113	C	2.921643	2.172341	2.090892
H	4.329123	-2.979874	-1.629610	B	1.080313	0.714877	1.255498
H	2.562022	-2.796484	-1.682811	C	1.569133	-2.831627	2.374420
C	1.071707	-0.254991	-1.957802	C	0.956663	-1.439213	2.448811
H	0.087308	-0.043395	-2.352702	H	1.382526	-3.257629	1.385122
O	0.429204	0.249796	0.523000	H	1.061618	-3.469612	3.118523
O	-2.214892	-0.348709	-1.988305	H	1.212372	-0.987813	3.425508
H	-2.488687	-1.078309	-2.569307	H	-0.138639	-1.519390	2.412309
O	1.267731	-4.519801	0.732581	O	1.442383	-0.643830	1.390507
H	1.246828	-4.112497	-0.145717	H	4.790544	2.122494	1.109195
C	-1.537503	1.484287	-0.001097	H	3.804278	3.657814	0.887485
C	-0.150702	1.397694	0.117904	C	2.737737	1.694131	-0.463405
C	0.625891	2.573700	-0.130192	O	1.558328	1.320059	-0.009505
C	0.047985	3.761098	-0.498588	C	5.477973	-1.307239	-1.881083
Br	2.524591	2.516209	0.071909	C	5.882903	0.029953	-1.810691
H	0.669880	4.631302	-0.679684	C	5.009124	0.997975	-1.328797
C	-2.686091	-0.600517	-0.736605	C	3.716515	0.646706	-0.894098
C	-2.377197	0.281181	0.289098	C	3.316285	-0.695886	-0.978390
C	-4.000184	-1.989430	0.783888	C	4.195165	-1.661208	-1.469783
C	-3.496685	-1.736922	-0.464310	H	6.160157	-2.062356	-2.260677
H	-4.616279	-2.864934	0.958185	H	6.879510	0.316529	-2.133290
Br	-3.862177	-2.947018	-1.908515	H	5.341146	2.030768	-1.278703
C	-3.709690	-1.106032	1.853392	H	2.319579	-0.983362	-0.678489
C	-2.883996	0.039573	1.604697	H	3.855543	-2.690101	-1.531777
C	-2.165509	2.713484	-0.381392	C	2.610066	2.935327	-1.331913
C	-1.357416	3.866390	-0.639288	H	1.960181	3.657245	-0.834018
C	-1.975523	5.087088	-1.019984	H	3.571376	3.388605	-1.574514
C	-3.342523	5.175181	-1.144284	H	2.134561	2.634032	-2.273512
C	-4.146717	4.038776	-0.889989	C	1.877531	1.606767	2.530994
H	-1.345228	5.951693	-1.210779	H	1.440827	1.548482	3.517594
H	-3.806628	6.112580	-1.435780	O	-0.356981	0.971510	1.388894
H	-5.225917	4.112371	-0.988889	O	-0.013619	-0.922816	-1.617095
C	-2.597201	0.905571	2.696701	H	-0.123597	0.037387	-1.526200
C	-3.099900	0.652663	3.952799	O	2.978832	-2.850257	2.543422
C	-3.917494	-0.477942	4.191994	H	3.179141	-2.408057	3.379120
H	-4.306394	-0.663649	5.188593	C	-1.992487	0.637435	-0.310007
C	-4.214389	-1.338040	3.160991	C	-1.172669	1.480622	0.446189
H	-4.838585	-2.211344	3.330487	C	-1.278638	2.892723	0.242181
H	-2.866104	1.327461	4.771002	C	-2.151924	3.432837	-0.665124
H	-1.970806	1.773475	2.525003	Br	-0.188613	4.071205	1.272876
C	-3.575710	2.841977	-0.519092	H	-2.205000	4.509337	-0.788230
H	-4.202905	1.978774	-0.326596	C	-0.895733	-1.533492	-0.788092
				C	-1.897020	-0.844166	-0.116298
B3LYP/6-31G** Energy =			-6817.754597	C	-1.633782	-3.642970	0.169620
B3LYP/6-31G** Free Energy =			-6817.772650	C	-0.761165	-2.936894	-0.616183
M06-2X/LACVP** Derived Free Energy =			-1700.366938	H	-1.513205	-4.714972	0.283926
Number of Imaginary Frequencies =			1 (-344.59)	Br	0.702917	-3.827031	-1.452376
				C	-2.682668	-2.977342	0.855814
B3LYP/6-31G** Geometry				C	-2.809037	-1.555140	0.724705
				C	-2.911472	1.180350	-1.269911
C	3.820755	2.607715	1.172091	C	-2.989741	2.598550	-1.447020

C	-3.896728	3.139065	-2.396625	H	3.746992	-0.474642	1.351790
C	-4.698744	2.314678	-3.151421	H	3.322771	-2.083335	1.919294
C	-4.622176	0.911977	-2.983812	C	0.340140	-3.563294	-0.491393
H	-3.943604	4.218265	-2.515931	H	-0.579268	-4.097182	-0.679389
H	-5.389034	2.736389	-3.875825	O	-0.679928	-1.203080	-0.794390
H	-5.255089	0.264588	-3.583511	O	-0.091190	0.550414	2.227306
C	-3.849124	-0.904713	1.443900	H	-0.586402	-0.239179	1.913408
C	-4.717140	-1.621290	2.237402	O	1.490685	-1.557608	3.621401
C	-4.594071	-3.025891	2.358411	H	1.347596	-0.704706	3.181301
H	-5.286384	-3.577672	2.987013	C	-1.871097	0.726938	-0.037487
C	-3.595285	-3.686617	1.681016	C	-1.850917	-0.594863	-0.475086
H	-3.486909	-4.764519	1.768723	C	-3.088928	-1.281545	-0.649081
H	-5.504030	-1.103269	2.777897	C	-4.292218	-0.691127	-0.366476
H	-3.949999	0.171788	1.360193	Br	-3.084957	-3.068546	-1.327479
C	-3.753489	0.358663	-2.069308	H	-5.215027	-1.243114	-0.509572
H	-3.702013	-0.717537	-1.949602	C	0.211417	1.373209	1.191104
B3LYP/6-31G** Energy =				C	-0.592185	1.500219	0.064508
B3LYP/6-31G** Free Energy =				C	1.782438	3.018986	0.312596
M06-2X/LACVP** Derived Free Energy =				C	1.406229	2.139691	1.292298
Number of Imaginary Frequencies =				H	2.700646	3.586873	0.416292
				Br	2.532331	1.882977	2.812894
B3LYP/6-31G** Geometry				C	0.990535	3.170196	-0.853800
C	2.911739	-3.603232	-0.550103	C	-0.205177	2.392413	-0.988195
C	1.567935	-3.836212	-0.619798	C	-3.116586	1.363856	0.281118
B	0.109666	-1.957791	0.165407	C	-4.340898	0.640473	0.116624
C	0.234177	-2.197690	3.733606	C	-5.575287	1.267791	0.432528
C	-0.206739	-2.918985	2.463609	C	-5.607566	2.560892	0.900327
H	0.328769	-2.953790	4.523507	C	-4.400156	3.278474	1.070421
H	-0.550212	-1.494778	4.051809	H	-6.494596	0.703703	0.299732
H	-1.077747	-3.547072	2.698113	H	-6.555659	3.032006	1.141631
H	0.604651	-3.576697	2.133906	H	-4.429640	4.297475	1.444821
O	-0.587230	-2.026779	1.415210	C	-0.967680	2.540723	-2.180192
H	3.474936	-3.536840	-1.476306	C	-0.572171	3.410516	-3.172794
H	3.458736	-4.042938	0.282894	C	0.605640	4.181900	-3.031100
C	2.701869	-1.631228	-0.089504	H	0.903847	4.865295	-3.820501
O	1.471874	-1.401010	0.338101	C	1.369343	4.060489	-1.893103
C	3.809781	0.237754	-3.822510	H	2.279352	4.642177	-1.772707
C	4.777974	-0.415060	-3.054814	H	-1.171774	3.506525	-4.073392
C	4.422971	-1.027054	-1.856212	H	-1.871389	1.954336	-2.301088
C	3.091473	-1.001135	-1.404106	C	-3.188365	2.697857	0.768417
C	2.127579	-0.344921	-2.181603	H	-2.269356	3.255644	0.907013
C	2.487983	0.270673	-3.380905	B3LYP/6-31G** Energy =			
H	4.088284	0.719249	-4.755312	B3LYP/6-31G** Free Energy =			
H	5.811172	-0.444275	-3.388218	M06-2X/LACVP** Derived Free Energy =			
H	5.189466	-1.530764	-1.275514	Number of Imaginary Frequencies =			
H	1.101382	-0.308106	-1.839299				
H	1.729488	0.787283	-3.960901	B3LYP/6-31G** Geometry			
C	3.698675	-1.529741	1.057392	C	-2.008686	-1.561098	-2.032509
H	4.701270	-1.866556	0.791388	C	-1.758296	-0.217096	-2.100504

B	-1.533206	0.879798	0.118900	C	5.693586	2.184155	-1.819786
C	-3.502228	3.455177	1.956806	C	5.622095	0.867853	-1.306290
C	-2.393420	2.414486	1.859504	H	4.628374	4.016449	-2.146681
H	-3.392933	4.032475	2.881208	H	6.619385	2.545263	-2.257084
H	-4.481524	2.948571	1.993403	H	6.496900	0.226059	-1.352091
H	-2.505116	1.655982	2.648401	C	2.625097	-0.018882	2.734302
H	-1.415624	2.893092	1.970507	C	2.929397	-0.378784	4.027901
O	-2.501614	1.823589	0.565502	C	2.926006	-1.738785	4.420097
H	-2.937583	-1.932804	-2.454711	H	3.167707	-2.006687	5.444197
H	-1.151082	-2.225992	-2.137109	C	2.616714	-2.716085	3.502894
C	-2.490189	-1.524709	-0.089009	H	2.611121	-3.763985	3.791290
O	-1.840298	-0.526506	0.495694	H	3.172891	0.388515	4.756905
C	-6.818690	-1.403139	-0.250714	H	2.627690	1.025719	2.442805
C	-6.130481	-2.557732	-0.631418	C	4.456898	0.390842	-0.747894
C	-4.739681	-2.588123	-0.589216	H	4.418404	-0.618859	-0.355597
C	-4.003189	-1.465619	-0.165712				
C	-4.704399	-0.313425	0.213292	B3LYP/6-31G** Energy =			-6817.761617
C	-6.099598	-0.285835	0.168690	B3LYP/6-31G** Free Energy =			-6817.779067
H	-7.903990	-1.378546	-0.282416	M06-2X/LACVP** Derived Free Energy =			-1700.376466
H	-6.676975	-3.436536	-0.960722	Number of Imaginary Frequencies =			1 (-378.30)
H	-4.229874	-3.496118	-0.894218				
H	-4.151605	0.561077	0.532195	B3LYP/6-31G** Geometry			
H	-6.623205	0.617960	0.466793				
C	-1.915580	-2.865306	0.351287	C	-3.771603	-0.304618	-2.137602
H	-2.241074	-3.701506	-0.267317	C	-2.419304	-0.200410	-2.325605
H	-0.829381	-2.820698	0.346989	B	-1.130199	-0.709701	-0.276205
H	-2.250980	-3.046412	1.378685	C	0.322423	-3.977891	0.706395
C	-1.538004	0.936603	-1.630900	C	-0.141686	-2.555894	0.976695
H	-1.314711	1.903706	-2.056996	H	0.547927	-4.486989	1.649495
O	-0.173310	1.159106	0.591203	H	1.241821	-3.949686	0.102394
O	1.357312	-1.406476	-1.795103	H	0.646111	-1.976989	1.475293
H	1.355606	-0.442075	-1.909600	H	-1.022385	-2.573299	1.635396
O	-3.446332	4.370681	0.873709	O	-0.477691	-1.975896	-0.283106
H	-3.331927	3.810785	0.090507	H	-4.333300	-1.043122	-2.704201
C	2.059395	0.742324	-0.100396	H	-4.308209	0.618879	-1.927503
C	0.940489	1.580716	-0.027595	C	-3.578996	-1.262715	-0.367302
C	1.065680	2.913818	-0.545689	O	-2.527698	-0.740009	0.236397
C	2.229878	3.368028	-1.109387	C	-7.264900	-0.088537	1.549202
Br	-0.408229	4.119507	-0.433687	C	-7.292396	-1.014538	0.505102
H	2.279870	4.382830	-1.489683	C	-6.108695	-1.398632	-0.121899
C	1.673812	-1.666978	-0.498505	C	-4.877097	-0.861723	0.284899
C	1.985804	-0.663579	0.408799	C	-4.859001	0.070977	1.334499
C	1.979022	-3.375781	1.203391	C	-6.045004	0.451870	1.959100
C	1.672321	-3.025479	-0.086208	H	-8.187502	0.208457	2.039002
H	1.969729	-4.419782	1.497387	H	-8.235994	-1.440844	0.178103
Br	1.185633	-4.365478	-1.355614	H	-6.155991	-2.114332	-0.935898
C	2.298714	-2.378482	2.160394	H	-3.910104	0.489883	1.644797
C	2.300105	-1.001880	1.760499	H	-6.014107	1.170071	2.773099
C	3.294092	1.207534	-0.670192	C	-3.445688	-2.701815	-0.849802
C	3.374384	2.538337	-1.188488	H	-2.608787	-2.792911	-1.541402
C	4.589081	3.001647	-1.759785	H	-3.232383	-3.337913	0.015099

H	-4.352986	-3.064122	-1.333200	C	0.612094	5.162990	-1.724037
C	-1.210703	-0.219502	-1.955006	C	0.500894	3.654591	-1.578826
H	-0.255706	0.014904	-2.403406	H	0.522591	5.448382	-2.777639
O	-0.438404	0.322704	0.490193	H	1.603695	5.486692	-1.369043
O	2.063398	-0.532482	-1.905309	H	1.347692	3.157187	-2.069325
H	2.218703	-1.363281	-2.384608	H	-0.427507	3.298987	-2.051020
O	-0.689274	-4.734798	0.052697	O	0.491799	3.370300	-0.183724
H	-0.924978	-4.201900	-0.719903	H	-2.278788	2.266326	3.362194
C	1.525288	1.527116	-0.096410	H	-2.020190	0.496323	2.953105
C	0.138988	1.451307	0.036192	C	-2.114698	2.110408	0.861494
C	-0.634819	2.619902	-0.252708	O	-1.158300	1.598203	0.113994
C	-0.056627	3.783406	-0.690809	C	-5.917699	0.163704	0.304722
Br	-2.528619	2.590191	0.004594	C	-5.774695	1.135112	1.299514
H	-0.675732	4.648902	-0.901609	C	-4.545495	1.759113	1.496605
C	2.584301	-0.659878	-0.656010	C	-3.436798	1.416607	0.706004
C	2.357195	0.341821	0.276290	C	-3.589002	0.438301	-0.285088
C	3.931611	-1.917069	0.950090	C	-4.821502	-0.181201	-0.485980
C	3.369908	-1.788173	-0.292009	H	-6.878900	-0.316896	0.147929
H	4.526216	-2.790965	1.193289	H	-6.622194	1.407816	1.921215
Br	3.606515	-3.176672	-1.594509	H	-4.450492	2.505619	2.279600
C	3.729304	-0.906370	1.922589	H	-2.739604	0.179296	-0.901790
C	2.926197	0.232726	1.584790	H	-4.910005	-0.930307	-1.267674
C	2.153280	2.729020	-0.554111	C	-2.164596	3.627409	1.017684
C	1.346672	3.870514	-0.863911	H	-1.234095	4.014912	1.431678
C	1.965064	5.063118	-1.324913	H	-2.298500	4.073703	0.026881
C	3.329964	5.134026	-1.479514	H	-3.000395	3.933714	1.646485
C	4.132271	4.008332	-1.175915	C	0.675907	1.928015	1.907786
H	1.336559	5.919814	-1.553912	H	1.726908	2.012816	2.144682
H	3.793957	6.049729	-1.833615	O	1.032797	1.035098	-0.542709
H	5.209571	4.068038	-1.300915	O	0.324691	-1.435116	-2.431589
C	2.722192	1.224525	2.584589	H	-0.307913	-1.534421	-3.160986
C	3.285695	1.098729	3.833989	O	-0.426303	5.825794	-1.015838
C	4.083802	-0.024266	4.159388	H	-0.385800	5.443801	-0.127035
H	4.521903	-0.108363	5.149288	C	1.830399	-1.171299	-0.098197
C	4.297907	-1.005965	3.220989	C	2.041399	0.200200	-0.247407
H	4.904813	-1.875862	3.457789	C	3.383699	0.690401	-0.165315
H	3.114690	1.868929	4.580288	C	4.458699	-0.140898	0.007887
H	2.109887	2.087121	2.348089	Br	3.691799	2.571599	-0.266730
C	3.561479	2.839328	-0.725113	H	5.459700	0.272901	0.064580
H	4.185884	1.982732	-0.497113	C	-0.261105	-1.844907	-1.283384
				C	0.441399	-1.721699	-0.090488
B3LYP/6-31G** Energy =			-6817.755809	C	-2.150701	-2.871399	-0.113070
B3LYP/6-31G** Free Energy =			-6817.774046	C	-1.567205	-2.409107	-1.262276
M06-2X/LACVP** Derived Free Energy =			-1700.370661	H	-3.146601	-3.298899	-0.137963
Number of Imaginary Frequencies =			1 (-359.52)	Br	-2.554812	-2.458719	-2.908772
				C	-1.462596	-2.757790	1.118426
B3LYP/6-31G** Geometry				C	-0.158197	-2.162590	1.132117
				C	2.941599	-2.065898	0.052506
C	-1.694591	1.527022	2.818697	C	4.272500	-1.540997	0.104597
C	-0.362791	1.743721	2.611491	C	5.374400	-2.424697	0.253999
B	0.274900	2.019703	0.205887	C	5.180800	-3.783396	0.342710

C	3.869100	-4.310496	0.283119	C	-0.206286	-2.011101	1.190392
H	6.375800	-2.004097	0.292593	H	-1.263487	-2.184902	1.047393
H	6.029200	-4.451995	0.453612	O	-0.008191	-0.860491	-1.130103
H	3.719000	-5.384396	0.345926	O	-2.892794	0.089907	-1.568896
C	0.496207	-2.030581	2.390614	H	-3.632393	-0.511493	-1.761896
C	-0.099688	-2.466873	3.552319	O	-2.147989	-2.700892	-1.455408
C	-1.384888	-3.061873	3.529428	H	-1.688890	-1.867291	-1.648705
H	-1.840785	-3.403666	4.453732	C	-0.632294	1.395006	-0.630093
C	-2.049993	-3.201282	2.334132	C	0.201507	0.469509	-1.254398
H	-3.040192	-3.647981	2.299938	C	1.222405	0.942515	-2.131298
H	0.422215	-2.355066	4.498217	C	1.414103	2.277116	-2.373892
H	1.478908	-1.575381	2.423308	Br	2.351506	-0.326380	-2.997404
C	2.781499	-3.477598	0.144016	H	2.202202	2.599019	-3.046091
H	1.783600	-3.896998	0.094023	C	-2.812191	0.264101	-0.226294
B3LYP/6-31G** Energy =			-6817.765837	C	-1.704092	0.919301	0.297207
B3LYP/6-31G** Free Energy =			-6817.784104	C	-3.770988	-0.009709	2.001406
M06-2X/LACVP** Derived Free Energy =			-1700.381708	C	-3.834290	-0.202004	0.647105
Number of Imaginary Frequencies =			1 (-350.83)	H	-4.567486	-0.372713	2.641805
B3LYP/6-31G** Geometry				Br	-5.324790	-1.123602	-0.124597
C	1.704815	-1.749006	2.891391	C	-2.658988	0.659790	2.570406
C	0.547915	-1.944704	2.207591	C	-1.607290	1.120595	1.711807
B	0.688111	-1.843694	-0.306308	C	-0.475096	2.796407	-0.894787
C	-1.367489	-3.765490	-1.983513	C	0.570102	3.240013	-1.767887
C	0.114111	-3.430087	-2.133314	C	0.731900	4.628014	-2.023581
H	-1.482487	-4.620293	-1.305917	C	-0.109600	5.552910	-1.451277
H	-1.744690	-4.074785	-2.973715	C	-1.154699	5.120305	-0.601377
H	0.242008	-2.603184	-2.844011	H	1.532799	4.943717	-2.686981
H	0.623011	-4.307785	-2.553118	H	0.020697	6.611711	-1.654372
O	0.744812	-3.127491	-0.901914	H	-1.825399	5.851802	-0.160173
H	2.182318	-2.585907	3.395187	C	-0.483190	1.750093	2.317608
H	1.890315	-0.771607	3.331994	C	-0.418188	1.930088	3.681209
C	2.818713	-1.782496	1.019889	C	-1.469087	1.489983	4.521509
O	2.008311	-1.294794	0.117092	H	-1.405585	1.642778	5.594609
C	6.091011	0.862305	1.934595	C	-2.563786	0.864684	3.973108
C	5.841314	-0.239100	2.757391	H	-3.374485	0.512380	4.605408
C	4.780215	-1.094600	2.475989	H	0.449212	2.417087	4.117510
C	3.943612	-0.856696	1.373691	H	0.331509	2.086498	1.687208
C	4.208310	0.244008	0.543996	C	-1.333097	3.782104	-0.330982
C	5.277009	1.094407	0.825998	H	-2.141795	3.465700	0.317218
H	6.920310	1.528505	2.153197	B3LYP/6-31G** Energy =			-6817.758032
H	6.473215	-0.430302	3.619589	B3LYP/6-31G** Free Energy =			-6817.776657
H	4.591317	-1.940302	3.129785	M06-2X/LACVP** Derived Free Energy =			-1700.375810
H	3.606709	0.388010	-0.344903	Number of Imaginary Frequencies =			1 (-380.07)
H	5.476706	1.936811	0.170501	B3LYP/6-31G** Geometry			
C	3.123315	-3.268495	0.974782	C	3.113379	-3.295493	-1.159833
H	3.715716	-3.587699	1.832780	C	1.780979	-3.580192	-1.217023
H	2.210016	-3.856897	0.897082	B	0.231989	-1.932694	-0.107605
H	3.711614	-3.449491	0.067780	C	0.813516	-2.405303	3.260489

C	0.213206	-3.136099	2.062092	H	-6.551706	0.365311	0.312256
H	0.015421	-1.912505	3.834597	H	-6.750395	2.593108	1.376064
H	1.506014	-1.621403	2.930486	H	-4.699790	3.924804	1.858550
H	-0.547691	-3.839200	2.419296	C	-1.104321	2.795812	-1.840482
H	1.002202	-3.727199	1.583684	C	-0.737428	3.799314	-2.710482
O	-0.403301	-2.254896	1.127899	C	0.403874	4.596113	-2.455089
H	3.630673	-3.046391	-2.081536	H	0.680970	5.384214	-3.148790
H	3.719085	-3.825495	-0.426138	C	1.160784	4.364208	-1.329696
C	2.795787	-1.408095	-0.382425	H	2.045786	4.961408	-1.126201
O	1.578192	-1.330795	0.119185	H	-1.332335	3.983017	-3.600677
C	3.637761	1.022814	-3.852225	H	-1.980024	2.190913	-2.047876
C	4.675665	0.345611	-3.206635	C	-3.364198	2.470206	1.047436
C	4.408174	-0.441892	-2.090935	H	-2.477796	3.054805	1.265030
C	3.095978	-0.571192	-1.599625				
C	2.061573	0.110111	-2.256515	B3LYP/6-31G** Energy =			-6817.754658
C	2.334564	0.901913	-3.372615	B3LYP/6-31G** Free Energy =			-6817.770585
H	3.847654	1.642316	-4.719226	M06-2X/LACVP** Derived Free Energy =			-1700.370590
H	5.695263	0.433711	-3.570244	Number of Imaginary Frequencies =			1 (-355.60)
H	5.229678	-0.964794	-1.611544				
H	1.047176	0.027211	-1.888007	B3LYP/6-31G** Geometry			
H	1.522361	1.439016	-3.852407				
C	3.835796	-1.432798	0.730466	C	-1.784066	-2.383225	-3.352799
H	4.856494	-1.558498	0.369158	C	-0.702961	-2.859812	-2.683497
H	3.761401	-0.476800	1.261470	B	-0.319676	-1.818207	-0.486197
H	3.601102	-2.226700	1.441866	C	-0.510963	-3.254308	2.586803
C	0.544781	-3.387591	-1.031512	C	-1.440172	-2.435119	1.694502
H	-0.348322	-3.932190	-1.298005	H	-0.505051	-4.298908	2.239204
O	-0.627817	-1.081491	-0.908596	H	-0.927065	-3.244312	3.601103
O	-0.170089	0.308900	2.293504	H	-1.394885	-1.387418	2.010502
H	-0.645593	-0.447098	1.895506	H	-2.466568	-2.786732	1.862101
O	1.466722	-3.413206	4.031481	O	-1.189268	-2.593216	0.301402
H	1.738529	-3.010808	4.865480	H	-2.728360	-2.910936	-3.245500
C	-1.932908	0.670308	0.057820	H	-1.634170	-1.892323	-4.311299
C	-1.832613	-0.597292	-0.513885	C	-1.937889	-0.661726	-2.074400
C	-3.028616	-1.336689	-0.757277	O	-0.908689	-0.665514	-1.257699
C	-4.265312	-0.842289	-0.435465	C	-5.891589	-0.780873	-0.358305
Br	-2.932523	-3.051588	-1.595083	C	-5.720084	-1.090572	-1.710305
H	-5.153915	-1.428988	-0.642460	C	-4.445983	-1.096957	-2.272603
C	0.102203	1.256203	1.368905	C	-3.315387	-0.818542	-1.487501
C	-0.701305	1.496906	0.260312	C	-3.502793	-0.493644	-0.136902
C	1.607000	3.064403	0.727497	C	-4.778994	-0.472560	0.423197
C	1.268406	2.045401	1.576497	H	-6.886990	-0.769185	0.075694
H	2.499302	3.652802	0.912591	H	-6.581380	-1.322282	-2.329806
Br	2.419417	1.608996	3.037487	H	-4.335778	-1.326755	-3.328002
C	0.811591	3.336007	-0.415196	H	-2.649397	-0.217934	0.465699
C	-0.348612	2.531608	-0.664289	H	-4.887798	-0.194660	1.467196
C	-3.214604	1.200008	0.424831	C	-1.808500	0.396375	-3.156899
C	-4.394806	0.432509	0.169039	H	-0.825698	0.341687	-3.628198
C	-5.666203	0.960309	0.518950	H	-2.593097	0.310066	-3.910401
C	-5.774698	2.197007	1.111255	H	-1.901012	1.378174	-2.680300
C	-4.609795	2.953406	1.381148	C	0.172838	-2.903901	-1.770296

H	1.026545	-3.536691	-1.583294	H	-3.203387	1.004871	-2.798537
O	0.823816	-1.342692	0.290005	H	-2.898477	1.034547	-4.550235
O	0.287892	0.425202	2.459204	H	-0.474180	0.570151	-4.057416
H	0.715502	-0.381993	2.124504	H	-1.558484	-0.778942	-3.659803
O	0.808530	-2.739392	2.702405	O	-0.730892	0.297379	-2.068313
H	1.238133	-2.843887	1.841406	H	-2.965910	-3.840484	0.388132
C	1.957292	0.760321	0.093105	H	-3.312501	-3.887809	-1.415370
C	1.943808	-0.632379	0.015606	C	-3.582803	-1.457195	-0.468904
C	3.175917	-1.332264	-0.151792	O	-2.717999	-0.599703	-0.960212
C	4.369210	-0.679750	-0.303591	C	-4.592925	-1.266136	3.720187
Br	3.187640	-3.242864	-0.030092	C	-5.170222	-2.242547	2.903497
H	5.286617	-1.243639	-0.432389	C	-4.830514	-2.313965	1.557101
C	-0.071517	1.268297	1.463702	C	-3.902211	-1.415374	0.997393
C	0.677183	1.499006	0.309404	C	-3.335113	-0.433964	1.823883
C	-1.741535	2.910877	0.762600	C	-3.681521	-0.364944	3.173879
C	-1.296126	1.974083	1.655101	H	-4.858230	-1.208321	4.771585
H	-2.676742	3.430466	0.940698	H	-5.884825	-2.948239	3.316304
Br	-2.382122	1.519270	3.156399	H	-5.283212	-3.085874	0.942808
C	-1.007737	3.168485	-0.422500	H	-2.648910	0.287829	1.405476
C	0.196873	2.433400	-0.671398	H	-3.235123	0.403764	3.797272
C	3.209783	1.463436	0.012007	C	-4.749397	-1.675507	-1.420808
C	4.418792	0.734250	-0.229391	H	-4.380793	-1.836122	-2.435403
C	5.654784	1.427465	-0.330290	H	-5.389800	-2.507602	-1.129200
C	5.711368	2.791666	-0.169590	H	-5.358097	-0.763407	-1.416624
C	4.527959	3.513652	0.111308	C	-0.623100	-2.067308	-1.074680
H	6.557392	0.853676	-0.522289	H	0.424301	-2.174513	-1.318273
H	6.660861	3.313277	-0.242389	O	-0.699505	0.155811	0.266388
H	4.577945	4.587653	0.264307	O	2.155707	-0.219323	-1.938390
C	0.863171	2.661307	-1.908797	H	1.275108	0.210377	-1.979502
C	0.388762	3.579501	-2.819798	O	-2.042881	2.567960	-3.529452
C	-0.787348	4.319687	-2.555499	H	-1.935086	2.796273	-2.595655
H	-1.149355	5.042783	-3.280100	C	1.422796	1.235011	0.433585
C	-1.472146	4.109580	-1.380700	C	0.043397	1.295510	0.270577
H	-2.385254	4.658569	-1.166502	C	-0.572801	2.577009	0.160055
H	0.920861	3.731607	-3.754397	C	0.139100	3.743410	0.253043
H	1.758278	2.095818	-2.136795	Br	-2.450599	2.685107	-0.172056
C	3.313666	2.870437	0.199806	H	-0.369598	4.697209	0.163427
H	2.419759	3.438427	0.425206	C	2.426899	-0.729306	-0.713683
B3LYP/6-31G** Energy =			-6817.762057	C	2.104094	-0.094389	0.481107
B3LYP/6-31G** Free Energy =			-6817.780681	C	3.461690	-2.572090	0.513449
M06-2X/LACVP** Derived Free Energy =			-1700.371742	C	3.105898	-1.983007	-0.671161
Number of Imaginary Frequencies =			1 (-340.11)	H	3.975589	-3.527291	0.509665
B3LYP/6-31G** Geometry				Br	3.464206	-2.880130	-2.316347
				C	3.137185	-1.953173	1.747238
				C	2.436486	-0.703973	1.732817
				C	2.196797	2.439111	0.530472
C	-2.749505	-3.441199	-0.598273	C	1.541300	3.709211	0.453951
C	-1.517002	-2.938804	-0.853173	C	2.303500	4.902811	0.559938
B	-1.236198	-0.430205	-0.953706	C	3.667499	4.851812	0.728647
C	-2.447382	1.207660	-3.565836	C	4.322797	3.599512	0.793767
C	-1.276885	0.247261	-3.384816	H	1.787301	5.857311	0.501023

H	4.243599	5.768813	0.807937	O	0.389510	0.789000	1.034196
H	5.400796	3.564212	0.919974	O	-1.819025	-1.123513	-1.913969
C	2.103480	-0.109055	2.980908	H	-2.059135	-1.964816	-2.336058
C	2.447773	-0.713238	4.169518	O	0.404435	1.433331	3.939089
C	3.141872	-1.946339	4.178739	H	0.093526	1.111424	3.078595
H	3.406466	-2.411626	5.123446	C	-1.447496	1.197099	-0.438096
C	3.477777	-2.551156	2.989449	C	-0.163591	1.496793	0.017092
H	4.009776	-3.498857	2.981465	C	0.513915	2.628882	-0.533825
H	2.182169	-0.240125	5.110410	C	-0.056586	3.406576	-1.508529
H	1.568382	0.833946	2.984692	Br	2.245623	3.124075	0.097659
C	3.609396	2.425611	0.696380	H	0.485818	4.258767	-1.903942
H	4.122295	1.472212	0.745396	C	-2.349217	-1.108896	-0.662866
B3LYP/6-31G** Energy =				C	-2.184402	0.024311	0.125522
B3LYP/6-31G** Free Energy =				C	-3.575915	-2.237767	1.123154
M06-2X/LACVP** Derived Free Energy =				C	-3.050323	-2.230484	-0.141249
Number of Imaginary Frequencies =				H	-4.102419	-3.111059	1.492667
				Br	-3.231043	-3.777595	-1.267430
B3LYP/6-31G** Geometry				C	-3.429900	-1.098259	1.953042
C	1.717767	-2.254040	-1.725380	C	-2.731593	0.048730	1.448125
C	1.008774	-2.242722	-0.559876	C	-2.072696	2.013494	-1.438000
B	1.397601	-0.268309	0.939000	C	-1.358991	3.125282	-1.987017
C	1.624631	0.779124	4.226488	C	-1.971292	3.935876	-2.980122
C	2.510321	0.546804	3.007584	C	-3.247897	3.670182	-3.416111
H	2.166741	1.417027	4.936877	C	-3.964801	2.580694	-2.867294
H	1.461126	-0.196169	4.717400	H	-1.410787	4.775068	-3.383735
H	3.510321	0.240299	3.343981	H	-3.709797	4.296178	-4.173714
H	2.604725	1.476996	2.437774	H	-4.977206	2.379598	-3.205385
O	1.997807	-0.513201	2.192999	C	-2.608678	1.180238	2.300712
H	2.485660	-3.008648	-1.870978	C	-3.123370	1.168456	3.576915
H	1.196363	-1.946346	-2.630480	C	-3.808376	0.032566	4.070332
C	2.875883	-0.632444	-1.191305	H	-4.208970	0.038681	5.079335
O	2.285495	0.021571	-0.214109	C	-3.961190	-1.075041	3.270645
C	6.568373	-2.654363	-0.226408	H	-4.486995	-1.953833	3.634758
C	5.663683	-2.312146	0.779493	H	-2.992059	2.036961	4.214005
C	4.471986	-1.658539	0.468895	H	-2.089974	2.059130	1.935999
C	4.164679	-1.341451	-0.864006	C	-3.394402	1.775699	-1.907089
C	5.079570	-1.693969	-1.871109	H	-3.959806	0.950908	-1.489277
C	6.272067	-2.341075	-1.553910	B3LYP/6-31G** Energy =			
H	7.497471	-3.159469	0.020791	B3LYP/6-31G** Free Energy =			
H	5.886688	-2.550836	1.815195	M06-2X/LACVP** Derived Free Energy =			
H	3.773793	-1.393125	1.255397	Number of Imaginary Frequencies =			
H	4.870465	-1.463878	-2.910110				
H	6.969959	-2.598790	-2.345111	B3LYP/6-31G** Geometry			
C	2.794581	0.158743	-2.488714	C	3.603698	0.416609	2.274112
H	1.765983	0.487950	-2.643110	C	2.242098	0.443811	2.419809
H	3.415689	1.053738	-2.369427	B	1.061600	-0.685493	0.553510
H	3.133071	-0.396970	-3.363310	C	1.025300	-3.789596	-0.626381
C	0.606385	-1.782607	0.547322	C	-0.015800	-2.731195	-0.284886
H	-0.115712	-2.115993	1.276730	H	1.921700	-3.301898	-1.039781

H	0.632600	-4.471398	-1.390380	H	-5.258894	4.284709	-0.219714
H	-0.944401	-3.220793	0.029714	C	-2.637902	0.835515	2.456200
H	-0.233398	-2.106497	-1.157887	C	-3.114304	0.544219	3.715400
O	0.441198	-1.941892	0.817413	C	-3.881705	-0.621880	3.947402
H	4.206796	-0.072189	3.035113	H	-4.251207	-0.838376	4.945003
H	4.064199	1.287308	1.810510	C	-4.157205	-1.474782	2.904504
C	3.545499	-1.020994	0.874515	H	-4.745205	-2.374281	3.066606
O	2.489301	-0.779396	0.118213	H	-2.903805	1.220321	4.538999
C	7.241204	-0.254704	-1.223281	H	-2.068101	1.742815	2.289199
C	7.274701	-0.730900	0.088721	C	-3.613095	2.925609	-0.215607
C	6.087200	-0.976597	0.774219	H	-4.241997	2.054910	-0.069305
C	4.845501	-0.747098	0.160516				
C	4.821103	-0.268901	-1.158884	B3LYP/6-31G** Energy =			-6817.760026
C	6.011704	-0.025304	-1.841984	B3LYP/6-31G** Free Energy =			-6817.778403
H	8.167105	-0.065405	-1.758380	M06-2X/LACVP** Derived Free Energy =			-1700.379711
H	8.226100	-0.912699	0.579623	Number of Imaginary Frequencies =			1 (-396.31)
H	6.136397	-1.339194	1.795920				
H	3.864404	-0.091102	-1.632987	B3LYP/6-31G** Geometry			
H	5.976707	0.339293	-2.864384				
C	3.491597	-2.265592	1.752618	C	1.573426	-4.460797	-0.633678
H	3.398897	-3.142494	1.104222	C	0.396425	-4.080605	-1.209480
H	4.388496	-2.381191	2.361720	B	-0.691183	-2.040004	-0.219393
H	2.616996	-2.237189	2.403617	C	-1.992677	-3.144490	2.854115
C	1.052399	0.197112	2.068408	C	-2.094077	-3.384099	1.354117
H	0.078198	0.445913	2.464306	H	-2.331774	-4.039788	3.387921
O	0.369002	0.109905	-0.446892	H	-2.665081	-2.316590	3.129611
O	-2.236495	-0.352298	-2.241996	H	-3.117676	-3.696405	1.102620
H	-2.519495	-1.058699	-2.845594	H	-1.415574	-4.199498	1.073422
O	1.355297	-4.566694	0.520122	O	-1.803783	-2.197403	0.636009
H	1.278997	-3.948592	1.262120	H	2.481026	-4.439897	-1.229180
C	-1.580697	1.462107	-0.239200	H	1.539129	-5.249293	0.117426
C	-0.199897	1.327806	-0.403698	C	1.788120	-2.691691	0.382311
C	0.576205	2.512904	-0.602900	O	0.607517	-2.111594	0.529308
C	0.003606	3.757005	-0.662003	C	4.661710	-0.711595	-2.160503
Br	2.471905	2.381402	-0.797796	C	3.319809	-0.334500	-2.188505
H	0.626307	4.631904	-0.814905	C	2.388611	-0.977399	-1.372200
C	-2.699797	-0.630295	-1.000396	C	2.789916	-2.009992	-0.512594
C	-2.407998	0.247808	0.035602	C	4.146018	-2.383886	-0.493793
C	-3.945501	-2.086390	0.518706	C	5.072114	-1.741288	-1.310597
C	-3.464298	-1.799493	-0.730394	H	5.385308	-0.203996	-2.791307
H	-4.521302	-2.989388	0.689808	H	2.994606	0.482095	-2.824010
Br	-3.770597	-3.020197	-2.178991	H	1.352511	-0.665303	-1.389402
C	-3.678002	-1.204587	1.594904	H	4.487022	-3.180581	0.159112
C	-2.897801	-0.026388	1.351802	H	6.115716	-2.040584	-1.278596
C	-2.204896	2.748607	-0.324204	C	2.291022	-3.247180	1.709214
C	-1.398094	3.912106	-0.534206	H	1.465325	-3.726480	2.237317
C	-2.012793	5.190106	-0.614711	H	3.123625	-3.943077	1.601218
C	-3.376693	5.324208	-0.499714	H	2.630419	-2.399975	2.316908
C	-4.181294	4.176909	-0.301711	C	-0.624479	-3.354011	-1.378784
H	-1.382192	6.061105	-0.773112	H	-1.486079	-3.401118	-2.027183
H	-3.838392	6.304908	-0.564617	O	-0.819088	-0.805809	-0.983700

O	0.580699	2.389492	-1.738021	H	-0.985832	2.873463	-2.459088
H	-0.337301	2.114687	-1.893419	H	-1.562967	1.922339	-3.846398
O	-0.663378	-2.893881	3.282013	O	-0.827024	0.800671	-2.278795
H	-0.335082	-2.149084	2.754809	H	1.829770	4.517108	-1.486650
C	-1.428597	1.304094	-0.057613	H	3.374713	3.629188	-1.064137
C	-1.765092	0.129188	-0.731505	C	1.482565	2.421982	0.037237
C	-3.100892	-0.023319	-1.216104	O	0.535210	1.676735	-0.503576
C	-4.059296	0.933878	-1.011010	C	-0.072132	5.645489	2.443634
Br	-3.584786	-1.577628	-2.215094	C	1.295083	5.362662	2.458948
H	-5.063796	0.783071	-1.391808	C	1.803046	4.323692	1.683249
C	0.888500	2.094901	-0.449519	C	0.951596	3.547350	0.877736
C	-0.026198	1.520203	0.424985	C	-0.422819	3.840178	0.866123
C	2.605600	2.104418	1.268780	C	-0.924283	4.880748	1.646022
C	2.206499	2.392509	-0.009622	H	-0.468281	6.454466	3.050334
H	3.617300	2.336224	1.583478	H	1.968145	5.950295	3.076258
Br	3.426695	3.198507	-1.231228	H	2.869856	4.128849	1.707159
C	1.707404	1.499221	2.184684	H	-1.101881	3.251844	0.259112
C	0.370705	1.204613	1.760587	H	-1.990194	5.086591	1.630611
C	-2.415701	2.325191	0.162381	C	2.716699	1.678746	0.516047
C	-3.750499	2.128483	-0.313817	H	2.403526	0.996925	1.313241
C	-4.730904	3.131881	-0.094123	H	3.153539	1.085273	-0.287951
C	-4.412008	4.291686	0.573470	H	3.481359	2.343684	0.916058
C	-3.093708	4.491994	1.045768	C	1.554141	1.586999	-2.886366
H	-5.738804	2.964874	-0.464422	H	1.593576	1.110906	-3.855068
H	-5.167611	5.053684	0.738365	O	0.897240	-0.561041	-1.596183
H	-2.845912	5.408998	1.571962	O	-1.280070	-2.242656	-1.670614
C	-0.514592	0.600215	2.695391	H	-0.473093	-1.764313	-1.948303
C	-0.097191	0.298825	3.974192	O	-2.908410	2.114553	-0.752512
C	1.224608	0.590733	4.389090	H	-2.428473	1.349577	-0.403810
H	1.539210	0.347740	5.399491	C	0.596081	-1.756667	0.460708
C	2.104605	1.179830	3.510686	C	1.409267	-1.281319	-0.567381
H	3.121305	1.410637	3.818484	C	2.777089	-1.675346	-0.628767
H	-0.782889	-0.179574	4.666096	C	3.334123	-2.504020	0.306934
H	-1.525192	0.364609	2.379693	Br	3.860769	-1.014382	-2.055553
C	-2.121105	3.537297	0.845574	H	4.382038	-2.775665	0.241344
H	-1.114805	3.701603	1.213372	C	-1.706312	-1.683684	-0.516817
				C	-0.845040	-1.359643	0.534294
B3LYP/6-31G** Energy =			-6817.760308	C	-3.628169	-0.858092	0.741666
B3LYP/6-31G** Free Energy =			-6817.777122	C	-3.103626	-1.438959	-0.382330
M06-2X/LACVP** Derived Free Energy =			-1700.378304	H	-4.694580	-0.673748	0.811056
Number of Imaginary Frequencies =			1 (-377.36)	Br	-4.254187	-1.883813	-1.835145
				C	-2.775003	-0.445951	1.797677
B3LYP/6-31G** Geometry				C	-1.364889	-0.680276	1.690092
				C	1.144520	-2.687842	1.413710
C	2.365920	3.570636	-1.465049	C	2.532340	-3.039268	1.345824
C	2.083380	2.639025	-2.418255	C	3.080178	-3.943743	2.294725
B	0.472268	0.834937	-1.727382	C	2.288997	-4.513290	3.264014
C	-2.914988	1.966760	-2.167513	C	0.909580	-4.205363	3.310701
C	-1.507480	1.952237	-2.747797	H	4.137491	-4.186187	2.229036
H	-3.438835	1.045533	-2.459123	H	2.715026	-5.207670	3.981816
H	-3.468229	2.822232	-2.570315	H	0.278797	-4.676800	4.058491

C	-0.535526	-0.202937	2.744003	H	-0.171893	1.633414	-2.129396
C	-1.067971	0.443230	3.837400	O	-3.081628	-1.377642	3.090052
C	-2.462684	0.651656	3.945986	H	-2.985120	-1.035736	2.188056
H	-2.869720	1.161030	4.814184	C	-1.401911	1.165291	-0.257213
C	-3.295050	0.216916	2.941675	C	-1.657793	-0.086407	-0.820923
H	-4.367459	0.381760	3.000664	C	-2.945085	-0.330115	-1.393540
H	-0.408699	0.801262	4.622709	C	-3.944193	0.606376	-1.358745
H	0.535384	-0.355479	2.680414	Br	-3.295360	-1.984013	-2.282053
C	0.353743	-3.320188	2.414099	H	-4.910886	0.382270	-1.796858
H	-0.706469	-3.106745	2.459788	C	0.930587	1.924814	-0.614682
B3LYP/6-31G** Energy =			-6817.756327	C	-0.044220	1.503100	0.282705
B3LYP/6-31G** Free Energy =			-6817.775508	C	2.491162	2.354816	1.197439
M06-2X/LACVP** Derived Free Energy =			-1700.375197	C	2.197677	2.360422	-0.140364
Number of Imaginary Frequencies =			1 (-380.34)	H	3.464355	2.692324	1.537553
B3LYP/6-31G** Geometry				Br	3.491887	2.978441	-1.395945
C	1.767936	-4.559082	-0.017109	C	1.529354	1.918403	2.144325
C	0.577541	-4.281989	-0.619221	C	0.240564	1.491294	1.684208
B	-0.551786	-2.119303	0.048777	C	-2.431020	2.170783	-0.228619
C	-2.023022	-2.313134	3.238560	C	-3.722211	1.875975	-0.770036
C	-1.819200	-3.105024	1.953357	C	-4.744220	2.861165	-0.732742
H	-1.083029	-1.806928	3.503874	C	-4.505837	4.100165	-0.185132
H	-2.291325	-2.988842	4.059553	C	-3.228746	4.401272	0.343085
H	-2.694493	-3.738531	1.757943	H	-5.718213	2.616460	-1.147754
H	-0.939396	-3.754617	2.043263	H	-5.292444	4.848058	-0.159537
O	-1.690096	-2.179718	0.885064	H	-3.042459	5.382072	0.770393
H	2.670443	-4.587671	-0.620399	C	-0.711744	1.077880	2.654395
H	1.765832	-5.240687	0.832987	C	-0.407060	1.079175	3.997498
C	1.920110	-2.622885	0.777404	C	0.867231	1.498884	4.447316
O	0.722404	-2.073996	0.823894	H	1.094419	1.497080	5.509219
C	4.801327	-0.938344	-1.957253	C	1.813138	1.910098	3.536129
C	5.216023	-1.839447	-0.973953	H	2.794531	2.239703	3.867343
C	4.288218	-2.387160	-0.092567	H	-1.152265	0.739665	4.710388
C	2.926016	-2.045272	-0.179281	H	-1.690338	0.746674	2.329581
C	2.520820	-1.142669	-1.173181	C	-2.218537	3.465182	0.321791
C	3.453625	-0.594456	-2.053267	H	-1.245145	3.709887	0.730104
H	5.526132	-0.504635	-2.639742	B3LYP/6-31G** Energy =			-6817.756209
H	6.263725	-2.112638	-0.889243	B3LYP/6-31G** Free Energy =			-6817.776060
H	4.633615	-3.087261	0.661033	M06-2X/LACVP** Derived Free Energy =			-1700.369333
H	1.479618	-0.858077	-1.248391	Number of Imaginary Frequencies =			1 (-337.54)
H	3.122527	0.123245	-2.795666	B3LYP/6-31G** Geometry			
C	2.403097	-2.996590	2.172607	C	1.843775	-2.260880	2.475150
H	2.650383	-2.069491	2.702015	C	1.069175	-2.425945	1.375045
H	1.597795	-3.493100	2.716294	B	1.260193	-0.707302	-0.451812
H	3.284302	-3.638082	2.171014	C	3.328193	-0.987048	-3.479017
C	-0.458463	-3.605997	-0.882129	C	1.986090	-1.199651	-2.790624
H	-1.324354	-3.769101	-1.505240	H	3.636703	0.059745	-3.322992
O	-0.681485	-1.023499	-0.901418	H	3.225592	-1.146920	-4.558422
O	0.729202	1.950720	-1.957283	H	1.578880	-2.185940	-3.058849

H	1.272898	-0.428237	-3.098106	C	-1.921107	-0.416378	3.942092
O	2.224089	-1.148589	-1.390322	C	-2.626920	-1.627476	4.144462
H	2.753769	-2.845792	2.572736	H	-2.705725	-2.048900	5.142052
H	1.369777	-1.968298	3.409657	C	-3.213326	-2.261544	3.074845
C	2.594695	-0.328568	1.720298	H	-3.759236	-3.190942	3.214022
O	1.818200	0.020664	0.727306	H	-1.467403	0.087496	4.791105
C	6.746188	-1.141091	0.897681	H	-1.275591	1.065550	2.542529
C	6.207583	-1.480016	2.142173	C	-3.417774	2.731612	0.897269
C	4.863586	-1.240109	2.410778	H	-4.007583	1.839814	1.076546
C	4.028492	-0.664076	1.437390				
C	4.588696	-0.290752	0.205401	B3LYP/6-31G** Energy =			-6817.764743
C	5.935394	-0.539759	-0.063904	B3LYP/6-31G** Free Energy =			-6817.782019
H	7.792786	-1.337596	0.685277	M06-2X/LACVP** Derived Free Energy =			-1700.375445
H	6.834778	-1.936740	2.901962	Number of Imaginary Frequencies =			1 (-357.32)
H	4.461182	-1.517728	3.380270				
H	3.967302	0.213673	-0.521287	B3LYP/6-31G** Geometry			
H	6.343698	-0.263939	-1.031097				
C	2.312902	0.476203	2.976018	C	2.946017	-3.334093	-0.432907
H	1.240303	0.501909	3.173917	C	1.697318	-2.909306	-0.761224
H	2.845498	0.092576	3.846909	B	1.315508	-0.418611	-0.918784
H	2.655113	1.502404	2.793844	C	2.598617	0.895828	-3.741007
C	0.547078	-2.149112	0.254351	C	1.418218	-0.005968	-3.386293
H	-0.189627	-2.654290	-0.353362	H	3.457014	0.644147	-3.101997
O	0.184801	0.064823	-1.036194	H	2.886723	0.700905	-4.781202
O	-2.835499	-0.048121	-2.062599	H	1.712123	-1.061968	-3.466866
H	-3.288505	-0.630300	-2.694114	H	0.600221	0.174612	-4.092001
O	4.312183	-1.891870	-3.005340	O	0.912610	0.286660	-2.085902
H	4.185782	-1.923292	-2.044940	H	3.568723	-3.758709	-1.218394
C	-1.561187	1.325816	-0.022965	H	3.119014	-3.739469	0.559603
C	-0.305287	1.249218	-0.619066	C	3.663308	-1.361686	-0.249450
C	0.413025	2.457717	-0.867135	O	2.802407	-0.533402	-0.802973
C	-0.091363	3.684814	-0.525406	C	4.374885	-1.117484	4.002848
Br	2.112325	2.364621	-1.738636	C	5.050693	-2.067399	3.231774
H	0.480747	4.583713	-0.728982	C	4.807200	-2.156332	1.865375
C	-2.919805	-0.594750	-0.828113	C	3.880601	-1.301250	1.239050
C	-2.313700	0.061217	0.237904	C	3.213692	-0.347435	2.020625
C	-3.721025	-2.365079	0.656943	C	3.462385	-0.260602	3.391324
C	-3.616918	-1.812749	-0.592444	H	4.564380	-1.046358	5.069748
H	-4.262134	-3.293977	0.801219	H	5.766794	-2.738985	3.695693
Br	-4.431826	-2.684804	-2.097265	H	5.336007	-2.907942	1.287395
C	-3.122419	-1.717013	1.765359	H	2.525192	0.339751	1.551305
C	-2.408507	-0.491415	1.552990	H	2.938778	0.487110	3.979404
C	-2.123875	2.597213	0.320666	C	4.910513	-1.505501	-1.112540
C	-1.369962	3.790411	0.077196	H	5.452609	-0.553598	-1.072959
C	-1.920849	5.052309	0.425927	H	4.626919	-1.692626	-2.149737
C	-3.172349	5.144007	0.989528	H	5.583214	-2.291790	-0.770018
C	-3.926262	3.969409	1.222398	C	0.779115	-2.086816	-1.048347
H	-1.333641	5.946508	0.233650	H	-0.239883	-2.232529	-1.376849
H	-3.585340	6.113505	1.251252	O	0.671199	0.172713	0.243100
H	-4.917660	4.045908	1.659400	O	-1.876187	-0.502249	-1.964698
C	-1.812401	0.134752	2.684906	H	-1.137190	0.133555	-1.904609

O	2.275411	2.270529	-3.652441	O	1.599993	-0.388209	-1.494498
H	2.127105	2.452051	-2.712446	H	2.814097	-4.369397	0.131329
C	-1.467806	1.235705	0.294564	H	1.119498	-4.915393	0.587138
C	-0.081906	1.302808	0.180269	C	1.440600	-2.354089	1.130518
C	0.529189	2.587509	0.062443	O	0.670498	-1.576694	0.409014
C	-0.197315	3.747405	0.060111	C	5.495303	-1.125385	1.931396
Br	2.425191	2.705212	-0.118250	C	5.051704	-2.383181	2.348807
H	0.308282	4.702205	-0.035408	C	3.750703	-2.790783	2.072214
C	-2.328491	-0.857623	-0.736692	C	2.867601	-1.954288	1.365110
C	-2.142600	-0.093195	0.409391	C	3.316800	-0.685191	0.966700
C	-3.520091	-2.558697	0.542441	C	4.623501	-0.281489	1.245293
C	-3.022986	-2.097923	-0.647667	H	6.511203	-0.806984	2.145291
H	-4.042087	-3.508799	0.579161	H	5.720405	-3.047177	2.888210
Br	-3.204774	-3.153960	-2.225943	H	3.428104	-3.775080	2.397522
C	-3.336000	-1.811069	1.733225	H	2.640798	-0.022494	0.443497
C	-2.629105	-0.566468	1.669999	H	4.954800	0.702808	0.928184
C	-2.256811	2.435902	0.284332	C	0.687704	-2.952380	2.305825
C	-1.609215	3.707002	0.172106	H	1.254105	-3.725577	2.825029
C	-2.385620	4.895799	0.163674	H	0.490906	-2.138775	3.013619
C	-3.756821	4.839495	0.255968	H	-0.269798	-3.353783	1.969531
C	-4.403916	3.585795	0.357194	C	0.716891	-2.790011	-1.847777
H	-1.874324	5.850799	0.077954	H	0.377488	-2.813719	-2.872776
H	-4.344024	5.752792	0.246643	O	-0.758807	-0.733507	-1.340887
H	-5.487216	3.544891	0.422189	O	-1.372808	2.206290	-1.747207
C	-2.439214	0.156461	2.879984	H	-1.035710	2.842784	-2.398813
C	-2.925218	-0.321713	4.076492	O	3.924288	-0.113421	-2.962506
C	-3.627613	-1.548714	4.133018	H	3.771391	-0.479214	-2.078004
H	-4.005717	-1.913094	5.083324	C	-2.014801	0.462405	0.306707
C	-3.825905	-2.276242	2.982333	C	-1.851905	-0.615301	-0.565085
H	-4.360500	-3.222043	3.011053	C	-2.919205	-1.550603	-0.709375
H	-2.766226	0.247909	4.987580	C	-4.094803	-1.425797	-0.016072
H	-1.899118	1.096163	2.850065	Br	-2.711709	-3.008711	-1.924765
C	-3.676311	2.416398	0.370925	H	-4.885104	-2.156697	-0.149765
H	-4.185307	1.462697	0.445345	C	-0.613205	2.287098	-0.630510
				C	-0.904301	1.453406	0.444696
B3LYP/6-31G** Energy =			-6817.753090	C	1.234900	3.314407	0.598077
B3LYP/6-31G** Free Energy =			-6817.772451	C	0.475396	3.196999	-0.534320
M06-2X/LACVP** Derived Free Energy =			-1700.367012	H	2.056500	4.021207	0.635668
Number of Imaginary Frequencies =			1 (-341.70)	Br	0.891392	4.255587	-2.080129
				C	0.946003	2.503815	1.723284
B3LYP/6-31G** Geometry				C	-0.125098	1.552915	1.641394
				C	-3.246599	0.633611	1.018710
C	1.743197	-4.216597	0.032830	C	-4.292400	-0.333690	0.864220
C	1.252093	-3.665206	-1.104571	C	-5.511898	-0.170484	1.574523
B	0.559894	-1.241906	-1.031588	C	-5.708395	0.911422	2.400315
C	2.681086	-0.246725	-3.629302	C	-4.687295	1.880922	2.541805
C	1.534189	0.260782	-2.761402	H	-6.291098	-0.917185	1.445830
H	2.741183	0.341668	-4.552207	H	-6.645093	1.028526	2.936918
H	2.492585	-1.295627	-3.913893	H	-4.849492	2.741828	3.183899
H	0.564787	0.095678	-3.246498	C	-0.371694	0.735623	2.781800
H	1.648790	1.339682	-2.600310	C	0.379810	0.866131	3.928197

C	1.430310	1.812532	4.004087	H	-3.465828	-0.980159	1.947878
H	2.014013	1.903439	4.914985	C	-1.348382	1.208826	-0.250592
C	1.706407	2.610124	2.919480	C	-1.634199	-0.012064	-0.863805
H	2.511907	3.338724	2.958872	C	-2.917300	-0.195237	-1.465312
H	0.161911	0.238438	4.787703	C	-3.879484	0.779779	-1.435208
H	-1.172994	0.007823	2.737908	Br	-3.307223	-1.830922	-2.371628
C	-3.492096	1.746818	1.871403	H	-4.843385	0.604598	-1.901014
H	-2.721897	2.500818	1.985195	C	1.007931	1.927989	-0.504375
				C	0.005620	1.465798	0.340415
B3LYP/6-31G** Energy =			-6817.758773	C	2.550127	2.151246	1.359134
B3LYP/6-31G** Free Energy =			-6817.778186	C	2.280734	2.277563	0.021833
M06-2X/LACVP** Derived Free Energy =			-1700.378000	H	3.528629	2.423627	1.739940
Number of Imaginary Frequencies =			1 (-379.19)	Br	3.619051	2.936452	-1.164554
				C	1.559414	1.666855	2.251625
B3LYP/6-31G** Geometry				C	0.266811	1.318981	1.738616
				C	-2.339965	2.249642	-0.214187
C	1.690622	-4.527926	-0.070131	C	-3.623266	2.024168	-0.806696
C	0.462229	-4.249402	-0.588833	C	-4.605849	3.048885	-0.768890
B	-0.560437	-2.031190	0.055382	C	-4.337932	4.257275	-0.169178
C	-3.061160	-2.683072	2.726065	C	-3.070630	4.486848	0.415929
C	-1.640858	-2.707891	2.176171	H	-5.573950	2.858605	-1.224397
H	-3.080772	-3.117982	3.731060	H	-5.094719	5.035287	-0.143775
H	-3.711767	-3.293656	2.080156	H	-2.862717	5.442541	0.887739
H	-1.312275	-3.749195	2.034762	C	-0.709401	0.834789	2.651007
H	-0.953953	-2.220309	2.879579	C	-0.424510	0.705172	3.992307
O	-1.654241	-1.998180	0.950277	C	0.850794	1.054646	4.497016
H	1.747407	-5.193036	0.790263	H	1.060887	0.951634	5.557616
H	2.545624	-4.572834	-0.738228	C	1.821106	1.523138	3.640625
C	1.922351	-2.597337	0.698788	H	2.804909	1.795218	4.014632
O	0.749860	-2.000718	0.759487	H	-1.190619	0.325779	4.661800
C	4.804290	-0.994859	-2.081585	H	-1.682104	0.536309	2.282100
C	5.202869	-1.937175	-1.130491	C	-2.097547	3.512232	0.394225
C	4.274657	-2.463568	-0.236800	H	-1.130945	3.699912	0.846831
C	2.927564	-2.059945	-0.280703				
C	2.536783	-1.120630	-1.245996	B3LYP/6-31G** Energy =			-6817.755591
C	3.471097	-0.590037	-2.135287	B3LYP/6-31G** Free Energy =			-6817.773634
H	5.530900	-0.576265	-2.771478	M06-2X/LACVP** Derived Free Energy =			-1700.369859
H	6.239164	-2.258093	-1.079990	Number of Imaginary Frequencies =			1 (-377.44)
H	4.606741	-3.194980	0.492695				
H	1.505889	-0.794712	-1.288497	B3LYP/6-31G** Geometry			
H	3.153512	0.157775	-2.853682				
C	2.416538	-2.976258	2.088387	C	2.176184	-1.090815	2.759200
H	2.683251	-2.051067	2.611796	C	1.069389	-1.569114	2.117591
H	1.609628	-3.457949	2.642779	B	1.048896	-1.194894	-0.365006
H	3.287928	-3.630972	2.077285	C	2.976509	-2.210065	-2.792307
C	-0.578758	-3.564182	-0.803133	C	1.466408	-2.275973	-2.559714
H	-1.484259	-3.722662	-1.368738	H	3.339204	-1.203865	-2.538798
O	-0.700116	-0.989378	-0.953409	H	3.207113	-2.397255	-3.848008
O	0.829039	2.066505	-1.843675	H	1.056214	-3.188272	-3.008522
H	-0.076364	1.785421	-2.052081	H	0.969106	-1.406672	-3.003608
O	-3.555338	-1.356465	2.835674	O	1.216104	-2.360186	-1.157615

H	2.062178	-0.279621	3.474406	H	-2.920429	-0.403761	5.587487
H	2.967287	-1.797513	3.001896	C	-3.412418	-1.152048	3.644779
C	2.836485	-0.056197	1.123610	H	-4.019116	-1.972954	4.017970
O	2.379192	-0.647191	0.036704	H	-1.536935	1.470552	4.697907
C	7.089686	-0.610582	1.628920	H	-1.258527	1.779574	2.278710
C	6.389793	-1.329078	0.658613	C	-3.208626	3.046881	0.264714
C	5.016793	-1.151183	0.497509	H	-3.844924	2.281475	0.693606
C	4.319785	-0.242993	1.311614				
C	5.032078	0.474303	2.287023	B3LYP/6-31G** Energy =			-6817.751472
C	6.404579	0.292608	2.443226	B3LYP/6-31G** Free Energy =			-6817.770271
H	8.159886	-0.750979	1.749523	M06-2X/LACVP** Derived Free Energy =			-1700.367444
H	6.911798	-2.031270	0.015609	Number of Imaginary Frequencies =			1 (-370.90)
H	4.491598	-1.710579	-0.268198				
H	4.522373	1.177996	2.936527	B3LYP/6-31G** Geometry			
H	6.937973	0.858604	3.201233				
C	2.249978	1.312497	1.426219	C	-3.071472	-2.670038	-1.435787
H	1.161178	1.259392	1.471115	C	-1.976072	-2.465823	-0.650191
H	2.621473	1.740091	2.357324	B	-1.393303	-0.065914	-0.180398
H	2.526278	1.973805	0.599326	C	-1.336324	2.288492	2.647297
C	0.335493	-1.814709	1.116787	C	-2.069321	1.710080	1.444702
H	-0.586804	-2.358613	0.983279	H	-1.864235	3.175086	3.015998
O	0.121595	-0.288593	-1.009201	H	-0.327830	2.604606	2.336293
O	-2.825302	-0.486499	-1.889914	H	-2.021533	2.402779	0.597500
H	-3.280897	-1.210597	-2.349321	H	-3.126618	1.547666	1.693105
O	3.644511	-3.195768	-2.011713	O	-1.459905	0.451288	1.142202
H	3.088909	-3.277277	-1.218515	H	-2.908973	-2.856039	-2.496887
C	-1.481816	1.316594	-0.285293	H	-3.944564	-3.160849	-1.015083
C	-0.261412	0.991105	-0.882592	C	-3.675299	-0.690146	-1.283388
C	0.506085	2.038113	-1.480581	O	-2.635707	0.059368	-0.990593
C	0.092479	3.344211	-1.465171	C	-6.750381	-1.181182	1.714824
Br	2.156290	1.610528	-2.339378	C	-7.084586	-1.187489	0.360725
H	0.704177	4.111217	-1.927963	C	-6.092491	-1.034778	-0.607179
C	-2.954306	-0.664411	-0.556616	C	-4.748392	-0.861759	-0.237384
C	-2.317613	0.225886	0.303394	C	-4.422987	-0.854352	1.129615
C	-3.884907	-1.900431	1.336470	C	-5.416682	-1.015164	2.093019
C	-3.729203	-1.727618	-0.013527	H	-7.522376	-1.301692	2.469027
H	-4.483705	-2.720936	1.717061	H	-8.118985	-1.309304	0.053330
Br	-4.573693	-2.938912	-1.239340	H	-6.378595	-1.040684	-1.652777
C	-3.266114	-1.000435	2.239381	H	-3.392788	-0.720238	1.437312
C	-2.471917	0.074373	1.717693	H	-5.145678	-1.004458	3.144418
C	-1.950122	2.671192	-0.283984	C	-4.107907	-0.476055	-2.727187
C	-1.142225	3.699301	-0.868372	H	-4.789598	-1.244465	-3.094183
C	-1.599331	5.043998	-0.861664	H	-4.607520	0.497038	-2.799087
C	-2.816034	5.371888	-0.310565	H	-3.218809	-0.443344	-3.357890
C	-3.627832	4.358580	0.251724	C	-1.110679	-1.793210	-0.018996
H	-0.969433	5.808905	-1.308255	H	-0.223773	-2.059296	0.536102
H	-3.158640	6.402286	-0.312058	O	-0.297512	0.398400	-1.012603
H	-4.593935	4.617972	0.674722	O	2.651600	-0.782062	-2.054611
C	-1.854025	0.954268	2.651901	H	2.924408	-1.505360	-2.642311
C	-2.015229	0.781256	4.007900	O	-1.277708	1.354596	3.714199
C	-2.801525	-0.281052	4.515388	H	-0.994198	0.523798	3.302299

C	1.841683	1.025330	-0.131111	H	-2.743440	-3.545321	2.592473
C	0.620476	1.342613	-0.722008	C	-3.334523	-1.727754	0.763934
C	0.382857	2.694509	-1.116509	O	-2.838013	-0.545953	1.017009
C	1.298544	3.690421	-0.900614	C	-3.360430	-3.158239	-3.301737
Br	-1.263652	3.116785	-1.987404	C	-3.710638	-4.020014	-2.258518
H	1.078929	4.706818	-1.209415	C	-3.679537	-3.569286	-0.943228
C	2.549811	-1.260161	-0.793310	C	-3.286926	-2.252583	-0.641255
C	2.145204	-0.396765	0.219890	C	-2.954617	-1.389509	-1.696673
C	2.768342	-3.102655	0.800992	C	-2.990819	-1.845736	-3.014963
C	2.853730	-2.613857	-0.476208	H	-3.384932	-3.508660	-4.329429
H	3.009957	-4.139652	1.007494	H	-4.007747	-5.042816	-2.470698
Br	3.403841	-3.768852	-1.909009	H	-3.950543	-4.253367	-0.144814
C	2.363934	-2.248259	1.857192	H	-2.703208	-0.359406	-1.485794
C	2.048615	-0.879664	1.562391	H	-2.734112	-1.163855	-3.819978
C	2.824870	2.043644	0.091983	C	-4.610326	-1.988226	1.548838
C	2.540750	3.395939	-0.285819	H	-4.467724	-1.722605	2.597832
C	3.510037	4.408353	-0.055624	H	-5.391519	-1.338628	1.135523
C	4.721843	4.106570	0.520572	H	-4.954234	-3.019925	1.470059
C	5.012863	2.770975	0.885974	C	-0.576519	-1.145950	2.070425
H	3.274723	5.428549	-0.347625	H	0.354283	-0.780349	2.477918
H	5.456333	4.887580	0.692468	O	-0.775606	0.145906	-0.141103
H	5.973068	2.534489	1.335270	O	2.351397	0.675220	1.800690
C	1.629507	-0.047067	2.638291	H	2.863694	0.433531	2.589896
C	1.530619	-0.536067	3.921393	O	-3.285682	3.440217	4.121325
C	1.850838	-1.886262	4.206694	H	-2.856385	3.191530	4.950331
H	1.770047	-2.257861	5.223595	C	1.278404	1.187776	-0.717122
C	2.259345	-2.721658	3.194094	C	-0.102695	1.244391	-0.555725
H	2.506561	-3.760254	3.398094	C	-0.787284	2.440888	-0.930351
H	1.188912	0.121430	4.714692	C	-0.116875	3.547874	-1.379574
H	1.384993	0.987029	2.430990	Br	-2.693484	2.489607	-0.867354
C	4.092376	1.768263	0.677379	H	-0.669266	4.441073	-1.651193
H	4.329990	0.749167	0.960680	C	2.535290	-0.284002	0.854311
B3LYP/6-31G** Energy =				C	2.001493	-0.086124	-0.410895
B3LYP/6-31G** Free Energy =				C	3.409972	-2.471124	0.205357
M06-2X/LACVP** Derived Free Energy =				C	3.230779	-1.490102	1.143037
Number of Imaginary Frequencies =				H	3.947664	-3.378822	0.456876
				Br	3.913175	-1.720170	2.924342
B3LYP/6-31G** Geometry				C	2.882375	-2.299946	-1.098747
				C	2.166985	-1.096646	-1.409473
				C	2.003414	2.326960	-1.192446
C	-2.087937	-3.210243	1.791266	C	1.294126	3.528859	-1.511671
C	-1.137829	-2.281245	2.061948	C	2.010836	4.664643	-1.973295
B	-1.463507	0.047838	1.132898	C	3.378235	4.623928	-2.118892
C	-2.419085	3.058487	3.059734	C	4.083825	3.437129	-1.809366
C	-2.318897	1.540583	2.916666	H	1.455743	5.568543	-2.210215
H	-2.840779	3.463571	2.136126	H	3.917543	5.498016	-2.471509
H	-1.410980	3.483681	3.174927	H	5.163224	3.408117	-1.927264
H	-3.322400	1.124389	2.766473	C	1.645988	-0.951470	-2.725276
H	-1.912601	1.097499	3.843276	C	1.824381	-1.934791	-3.671456
O	-1.474298	1.270352	1.821672	C	2.531970	-3.120491	-3.359430
H	-1.900142	-3.938960	1.007882	H	2.664665	-3.887108	-4.117014

C	3.049068	-3.296368	-2.097626	C	0.354092	1.136801	-0.823101
H	3.594360	-4.201568	-1.843806	C	-0.245813	2.361598	-1.256400
H	1.417983	-1.800608	-4.669659	C	0.420782	3.557501	-1.179099
H	1.101896	-0.047270	-2.973197	Br	-2.004514	2.329791	-1.992599
C	3.415815	2.319743	-1.360144	H	-0.064022	4.468899	-1.512598
H	3.966807	1.415444	-1.126724	C	2.793000	-0.998290	-0.792403
				C	2.294297	-0.104493	0.149998
B3LYP/6-31G** Energy =			-6817.755241	C	3.615606	-2.465088	0.963995
B3LYP/6-31G** Free Energy =			-6817.774858	C	3.457905	-2.181888	-0.367205
M06-2X/LACVP** Derived Free Energy =			-1700.374183	H	4.131910	-3.370287	1.264894
Number of Imaginary Frequencies =			1 (-366.58)	Br	4.139809	-3.382984	-1.680206
				C	3.103803	-1.588491	1.955496
B3LYP/6-31G** Geometry				C	2.423298	-0.393693	1.546497
				C	2.386087	2.401607	-0.267801
C	-2.802190	-3.466813	0.258397	C	1.749681	3.613206	-0.687500
C	-1.675693	-2.832109	0.684697	C	2.461077	4.840308	-0.621999
B	-1.385902	-0.479107	-0.117701	C	3.757877	4.877313	-0.165000
C	-2.085610	1.829488	2.740500	C	4.394582	3.681816	0.242699
C	-1.958805	0.412589	2.195199	H	1.960473	5.749707	-0.943099
H	-2.119510	1.804787	3.834900	H	4.295074	5.819715	-0.118699
H	-3.029912	2.272184	2.384600	H	5.420382	3.714319	0.597599
H	-2.851502	-0.173415	2.458499	C	1.887295	0.454204	2.557998
H	-1.083502	-0.073708	2.643098	C	2.040097	0.142904	3.892097
O	-1.809706	0.525790	0.789899	C	2.731702	-1.024994	4.291896
H	-2.693087	-4.255612	-0.483404	H	2.847303	-1.252094	5.347496
H	-3.617289	-3.610017	0.962197	C	3.246805	-1.874091	3.339596
C	-3.428497	-1.833614	-0.913002	H	3.771508	-2.780290	3.631095
O	-2.409300	-1.021011	-1.060702	H	1.620495	0.804401	4.644299
C	-6.961902	-0.355731	1.080400	H	1.329292	1.341001	2.278199
C	-6.853997	-1.714830	0.774500	C	3.728786	2.477013	0.193999
C	-5.705095	-2.202125	0.158699	H	4.228190	1.567614	0.507498
C	-4.635299	-1.344720	-0.152801				
C	-4.761104	0.022479	0.139200	B3LYP/6-31G** Energy =			
C	-5.916506	0.506874	0.755500	B3LYP/6-31G** Free Energy =			
H	-7.858404	0.025766	1.560001	M06-2X/LACVP** Derived Free Energy =			
H	-7.665994	-2.394933	1.013999	Number of Imaginary Frequencies =			
H	-5.642091	-3.260624	-0.075402	1 (-378.95)			
H	-3.961206	0.699782	-0.131100	B3LYP/6-31G** Geometry			
H	-5.998510	1.567774	0.972801				
C	-3.723095	-2.588714	-2.202503	C	-1.990588	-0.493205	-3.166811
H	-2.800293	-3.002411	-2.613103	C	-1.417281	-1.579802	-2.568313
H	-4.461691	-3.380518	-2.069802	B	-1.200991	-1.445708	-0.073911
H	-4.124097	-1.866816	-2.923301	C	-2.328100	-1.539528	3.025384
C	-0.821196	-1.901205	0.748197	C	-1.905688	-2.622421	2.037482
H	0.140304	-1.809602	1.232897	H	-2.216901	-1.927830	4.044583
O	-0.292204	-0.037702	-0.968802	H	-1.668708	-0.662622	2.933489
O	2.688599	-0.794189	-2.125603	H	-2.532882	-3.508327	2.187477
H	2.146095	-0.002992	-2.268803	H	-0.861587	-2.905513	2.203185
O	-0.976613	2.632792	2.370701	O	-2.112487	-2.207819	0.689983
H	-0.910513	2.550294	1.407100	H	-2.976285	-0.602612	-3.610415
C	1.657792	1.165005	-0.325602	H	-1.330692	0.193602	-3.695507

C	-2.436002	0.430385	-1.415010	H	1.047658	5.367016	-1.671082
O	-1.701301	-0.091012	-0.440809	H	2.481292	2.277436	-4.294787
C	-6.731198	-0.143350	-1.308427	H	2.350800	0.640029	-2.475092
C	-6.176103	0.903356	-2.045521	C	4.451492	0.720939	-0.321685
C	-4.794505	1.080068	-2.083716	H	4.061383	1.716436	-0.154083
C	-3.935100	0.216973	-1.379916				
C	-4.504894	-0.837434	-0.648421	B3LYP/6-31G** Energy =			-6817.755609
C	-5.888693	-1.011146	-0.614227	B3LYP/6-31G** Free Energy =			-6817.773212
H	-7.808096	-0.278560	-1.275031	M06-2X/LACVP** Derived Free Energy =			-1700.375232
H	-6.818307	1.589053	-2.590321	Number of Imaginary Frequencies =			1 (-403.72)
H	-4.395310	1.903773	-2.664212				
H	-3.863990	-1.524031	-0.107021	B3LYP/6-31G** Geometry			
H	-6.305687	-1.829252	-0.034530				
C	-1.950112	1.833891	-1.749904	C	1.487291	-4.399304	-0.739279
H	-2.225421	2.497985	-0.923102	C	0.264988	-4.031602	-1.225070
H	-0.865012	1.827800	-1.831999	B	-0.754296	-1.981193	-0.169474
H	-2.376413	2.231290	-2.671004	C	-1.320681	-4.008076	2.201844
C	-0.964478	-2.267402	-1.610213	C	-2.335586	-3.253077	1.345548
H	-0.494371	-3.236897	-1.534615	H	-1.839979	-4.799570	2.754854
O	0.095106	-1.302200	0.612993	H	-0.580288	-4.499182	1.551240
O	0.752683	0.671800	2.339002	H	-3.170779	-2.929771	1.976453
H	0.517492	-0.201800	1.966198	H	-2.738596	-3.932882	0.579456
O	-3.691903	-1.173839	2.878480	O	-1.817188	-2.076683	0.754836
H	-3.780204	-0.787036	1.996682	H	2.347186	-4.361710	-1.401487
C	2.151199	-0.256180	-0.015996	H	1.517096	-5.201098	-0.001974
C	1.379608	-1.403288	0.174197	C	1.758306	-2.647397	0.283908
C	1.991719	-2.688882	0.070196	O	0.582410	-2.091093	0.522815
C	3.312322	-2.835970	-0.257800	C	4.458289	-0.624624	-2.420229
Br	0.970731	-4.264192	0.432987	C	4.930793	-1.636919	-1.582227
H	3.743330	-3.827266	-0.345302	C	4.058699	-2.291011	-0.716215
C	0.955479	1.512106	1.300705	C	2.695401	-1.946306	-0.669305
C	1.548987	1.109014	0.102707	C	2.230396	-0.930911	-1.517507
C	0.732563	3.798506	0.482312	C	3.108590	-0.277719	-2.382920
C	0.572167	2.873201	1.478708	H	5.138585	-0.110430	-3.092638
H	0.441754	4.830504	0.647514	H	5.980392	-1.915523	-1.599334
Br	-0.183843	3.399990	3.145808	H	4.449502	-3.074409	-0.075613
C	1.242871	3.407414	-0.781987	H	1.187797	-0.640607	-1.490500
C	1.634983	2.043718	-0.986291	H	2.731087	0.514278	-3.021622
C	3.565801	-0.392268	-0.264091	C	2.366716	-3.200391	1.568605
C	4.135612	-1.696262	-0.424493	H	2.762324	-2.352588	2.140197
C	5.523014	-1.837549	-0.695589	H	1.589020	-3.670985	2.171516
C	6.340306	-0.735343	-0.774383	H	3.180712	-3.905195	1.395903
C	5.795895	0.553353	-0.568781	C	-0.776510	-3.320500	-1.308765
H	5.926924	-2.838146	-0.823791	H	-1.678915	-3.361901	-1.900057
H	7.400907	-0.851533	-0.975679	O	-0.867099	-0.760697	-0.944281
H	6.446287	1.422358	-0.599276	O	0.523606	2.517794	-1.581015
C	2.074591	1.671227	-2.288690	H	1.259704	2.988089	-2.005524
C	2.146086	2.592830	-3.310887	O	-0.687770	-3.175472	3.157533
C	1.788074	3.943627	-3.092684	H	-0.381772	-2.393076	2.671725
H	1.856571	4.661730	-3.904181	C	-1.413984	1.354911	0.011511
C	1.342067	4.336519	-1.851784	C	-1.784993	0.204707	-0.676880

C	-3.123298	0.097508	-1.157566	O	1.673894	-0.248614	-0.599487
C	-4.051793	1.083313	-0.949365	C	6.514082	-1.650557	-0.928481
Br	-3.661911	-1.445196	-2.152452	C	5.801575	-2.463655	-1.814377
H	-5.061197	0.967414	-1.329155	C	4.428176	-2.296844	-1.966476
C	0.917616	2.132301	-0.340915	C	3.738885	-1.318435	-1.229882
C	-0.006279	1.516009	0.493496	C	4.468192	-0.486437	-0.365487
C	2.657230	1.947906	1.364770	C	5.844591	-0.659447	-0.211486
C	2.247820	2.336600	0.117671	H	7.584581	-1.785365	-0.806282
H	3.679734	2.118306	1.683661	H	6.316568	-3.231263	-2.384473
Br	3.487112	3.174688	-1.085645	H	3.888770	-2.943444	-2.652273
C	1.740736	1.312615	2.238883	H	3.955299	0.307971	0.159710
C	0.393932	1.091916	1.798096	H	6.386396	-0.013048	0.472410
C	-2.362578	2.403315	0.241213	C	1.771487	-0.896627	-2.847284
C	-3.701883	2.259616	-0.241975	H	2.128296	0.074568	-3.211489
C	-4.646978	3.294520	-0.011573	H	2.144180	-1.668733	-3.521579
C	-4.291068	4.433324	0.672716	H	0.679988	-0.879317	-2.849282
C	-2.968564	4.580623	1.153803	C	0.391581	-1.857196	0.920523
H	-5.658881	3.167621	-0.387264	H	-0.276420	-1.966985	1.762223
H	-5.020664	5.218928	0.845317	O	0.319704	0.763407	1.084409
H	-2.691356	5.481026	1.694496	O	-1.975712	-0.918690	-1.791481
C	-0.505363	0.444525	2.692008	H	-2.219619	-1.747190	-2.235976
C	-0.093054	0.038532	3.941907	O	4.717897	-0.105721	3.014612
C	1.237551	0.262330	4.373594	H	4.497692	-0.667222	2.256815
H	1.546260	-0.062664	5.362493	C	-1.576193	1.346516	-0.243893
C	2.132846	0.887522	3.537581	C	-0.256291	1.549706	0.148005
H	3.156450	1.066721	3.856571	C	0.458819	2.660498	-0.394601
H	-0.790949	-0.473362	4.597016	C	-0.117475	3.528098	-1.284506
H	-1.519466	0.251426	2.362319	Br	2.269822	2.957685	0.138296
C	-2.030368	3.594919	0.943501	H	0.454232	4.361691	-1.678210
H	-1.020565	3.719018	1.318392	C	-2.482712	-0.947378	-0.530981
				C	-2.318802	0.163524	0.287413
B3LYP/6-31G** Energy =			-6817.758275	C	-3.678621	-2.137459	1.236627
B3LYP/6-31G** Free Energy =			-6817.778149	C	-3.163821	-2.090971	-0.031174
M06-2X/LACVP** Derived Free Energy =			-1700.370930	H	-4.192228	-3.026053	1.587532
Number of Imaginary Frequencies =			1 (-344.54)	Br	-3.323834	-3.614275	-1.191666
				C	-3.536811	-1.018156	2.094921
B3LYP/6-31G** Geometry				C	-2.847401	0.144836	1.616213
				C	-2.208385	2.247816	-1.160598
C	1.455770	-3.069114	-1.084771	C	-1.464177	3.350307	-1.689504
C	0.782874	-2.656103	0.018427	C	-2.086669	4.245907	-2.599108
B	1.243794	-0.319603	0.831014	C	-3.397771	4.069316	-2.975906
C	3.518998	-0.023007	3.770712	C	-4.140280	2.985425	-2.450801
C	2.350802	0.454499	2.920309	H	-1.505463	5.076800	-2.990313
H	3.268491	-0.997602	4.220417	H	-3.865566	4.759917	-3.671110
H	3.698405	0.685997	4.586307	H	-5.177281	2.852533	-2.745399
H	2.516010	1.481696	2.576904	C	-2.719491	1.254339	2.497408
H	1.423502	0.442710	3.509810	C	-3.241891	1.213151	3.769909
O	2.264094	-0.428407	1.804915	C	-3.920401	0.061759	4.238015
H	2.346965	-3.678422	-0.960369	H	-4.326200	0.044768	5.245015
H	0.903268	-3.235515	-2.006970	C	-4.063611	-1.029845	3.414821
C	2.274587	-1.063323	-1.424682	H	-4.583418	-1.919738	3.759925

	-3.132584	2.073253	4.423704	C	-0.164953	-3.310814	-1.887177
H	-2.201684	2.140233	2.148503	Br	2.481232	-2.421673	-1.408072
C	-3.562286	2.099525	-1.568996	H	0.329261	-4.141010	-2.379870
H	-4.143693	1.276632	-1.168292	C	-2.153024	1.248668	-0.639621
				C	-2.054909	0.050274	0.057489
B3LYP/6-31G** Energy =			-6817.762627	C	-3.327247	2.294964	1.232867
B3LYP/6-31G** Free Energy =			-6817.782133	C	-2.792042	2.362163	-0.025731
M06-2X/LACVP** Derived Free Energy =			-1700.368806	H	-3.812860	3.161461	1.668258
Number of Imaginary Frequencies =			1 (-363.33)	Br	-2.896861	3.999154	-1.025444
				C	-3.244133	1.087871	1.970376
B3LYP/6-31G** Geometry				C	-2.593014	-0.045624	1.378387
				C	-2.212673	-2.128838	-1.231296
C	2.417343	2.732153	2.220088	C	-1.580054	-3.244634	-1.868284
C	1.387654	1.863940	2.391690	C	-2.376338	-4.249150	-2.479681
B	1.483091	-0.326268	1.133307	C	-3.748938	-4.161769	-2.471987
C	2.334729	-3.498243	2.825435	C	-4.379757	-3.057673	-1.851297
C	2.138508	-1.989646	2.844322	H	-1.877523	-5.088746	-2.956572
H	1.344636	-3.981158	2.777134	H	-4.349526	-4.934482	-2.942383
H	2.815630	-3.817930	3.757039	H	-5.463758	-2.988989	-1.851703
H	3.116100	-1.492831	2.880623	C	-2.498300	-1.238817	2.150497
H	1.566699	-1.694547	3.738818	C	-3.026105	-1.305414	3.420595
O	1.438807	-1.630164	1.664817	C	-3.679823	-0.187920	3.994083
H	2.274134	3.591747	1.571581	H	-4.094026	-0.257718	4.995282
H	3.118538	2.882070	3.038890	C	-3.782436	0.983774	3.281374
C	3.473169	1.351859	0.939703	H	-4.275051	1.851870	3.711265
O	2.890284	0.182051	1.025210	H	-2.939394	-2.226509	3.989302
C	3.458356	3.402830	-2.854513	H	-1.988586	-2.096312	1.726605
C	3.945642	4.049746	-1.715115	C	-3.634074	-2.069158	-1.248802
C	3.931046	3.399755	-0.485610	H	-4.129988	-1.227362	-0.778911
C	3.419663	2.094349	-0.366403				
C	2.949177	1.447233	-1.518300	B3LYP/6-31G** Energy =			-6817.751554
C	2.968974	2.102325	-2.750505	B3LYP/6-31G** Free Energy =			-6817.772237
H	3.470553	3.908923	-3.815316	M06-2X/LACVP** Derived Free Energy =			-1700.364329
H	4.337527	5.060051	-1.785622	Number of Imaginary Frequencies =			1 (-369.79)
H	4.311334	3.918967	0.389087				
H	2.603092	0.425529	-1.452994	B3LYP/6-31G** Geometry			
H	2.603685	1.584613	-3.632303				
C	4.802165	1.373584	1.679208	C	-2.362007	-0.364147	2.945202
H	5.235950	2.371891	1.741203	C	-1.396706	-1.075960	2.300117
H	4.683067	0.958189	2.681611	B	-1.331698	-0.883902	-0.218586
H	5.499176	0.733589	1.125416	C	-0.327793	-2.981345	-2.601048
C	0.727071	0.791930	2.263496	C	-1.612994	-2.209838	-2.296165
H	-0.216926	0.457519	2.668894	H	-0.358297	-3.955236	-2.102331
O	0.745095	-0.225587	-0.109497	H	0.536506	-2.425439	-2.213754
O	-1.647220	1.316665	-1.893019	H	-2.467093	-2.783143	-2.675657
H	-1.775330	2.217361	-2.232526	H	-1.595791	-1.242446	-2.813281
O	3.170439	-3.915739	1.762941	O	-1.799297	-2.035913	-0.895169
H	2.811738	-3.516250	0.954837	H	-3.209410	-0.891539	3.374608
C	-1.406890	-1.121921	-0.607199	H	-2.060408	0.533962	3.481788
C	-0.018789	-1.213803	-0.630692	C	-3.186801	0.365323	1.156886
C	0.579030	-2.323699	-1.298182	O	-2.352598	0.129405	0.171994

C	-6.940404	-1.766972	1.150011	H	1.044498	1.967736	2.236873
C	-6.767005	-0.661358	1.985293	C	3.172406	3.024199	0.251361
C	-5.553804	0.022042	1.997385	H	3.758803	2.257806	0.744576
C	-4.491702	-0.383774	1.169695				
C	-4.674901	-1.496688	0.333914	B3LYP/6-31G** Energy =			-6817.751715
C	-5.890201	-2.180587	0.330322	B3LYP/6-31G** Free Energy =			-6817.771096
H	-7.886704	-2.299771	1.139717	M06-2X/LACVP** Derived Free Energy =			-1700.365921
H	-7.577206	-0.329446	2.627784	Number of Imaginary Frequencies =			1 (-389.96)
H	-5.439905	0.873052	2.660271				
H	-3.859699	-1.823800	-0.301878	B3LYP/6-31G** Geometry			
H	-6.015800	-3.039698	-0.322064				
C	-3.207299	1.849429	1.493961	C	2.711164	-3.617224	-1.295276
H	-3.767902	2.090545	2.396955	C	1.378662	-3.641917	-1.576866
H	-2.182000	2.208830	1.595559	B	-0.098017	-2.004192	-0.319774
H	-3.661196	2.371915	0.643851	C	-0.229002	-2.891959	2.996837
C	-0.712903	-1.483878	1.316826	C	-0.510316	-3.490570	1.616344
H	0.145795	-2.132179	1.232839	H	-1.094096	-2.305249	3.316237
O	-0.258795	-0.237916	-0.946094	H	0.630803	-2.209866	2.931424
O	2.695506	-0.650333	-1.685977	H	-1.315721	-4.228663	1.715157
H	3.186707	-1.397241	-2.066463	H	0.382378	-4.024681	1.255344
O	-0.201690	-3.246969	-3.995742	O	-0.918314	-2.489476	0.710937
H	-0.084087	-2.395376	-4.437456	H	3.410162	-3.307237	-2.066283
C	1.387305	1.341793	-0.266416	H	3.103363	-4.348620	-0.589571
C	0.178807	1.035184	-0.893314	C	2.533685	-1.804712	-0.236692
C	-0.516790	2.074973	-1.584733	O	1.291389	-1.663599	0.169714
C	-0.046488	3.362072	-1.619855	C	4.023885	0.837745	-3.309229
Br	-2.118988	1.670559	-2.540832	C	4.915484	0.087046	-2.539428
H	-0.601885	4.125363	-2.154169	C	4.436885	-0.763240	-1.546716
C	2.773703	-0.722010	-0.335976	C	3.055885	-0.878727	-1.300705
C	2.144901	0.255904	0.427905	C	2.169786	-0.117028	-2.077207
C	3.591595	-1.841577	1.677546	C	2.654086	0.731958	-3.072418
C	3.484299	-1.769700	0.313844	H	4.396885	1.501935	-4.083337
H	4.145392	-2.650770	2.141161	H	5.985184	0.163537	-2.711035
Br	4.312001	-3.106720	-0.786630	H	5.149684	-1.340840	-0.968215
C	2.975694	-0.853963	2.485627	H	1.104787	-0.175817	-1.892499
C	2.237997	0.202328	1.855206	H	1.952087	1.323658	-3.651420
C	1.918207	2.671991	-0.322637	C	3.448390	-2.138107	0.933405
C	1.177611	3.698581	-0.992157	H	3.001588	-2.941398	1.521716
C	1.693812	5.021079	-1.041778	H	4.456486	-2.429718	0.639801
C	2.903912	5.327488	-0.464678	H	3.507002	-1.246402	1.568395
C	3.649808	4.313897	0.182240	C	0.167765	-3.284007	-1.501363
H	1.114715	5.785471	-1.553393	H	-0.750741	-3.621804	-1.957352
H	3.292013	6.340586	-0.510095	O	-0.729613	-0.904495	-1.019880
H	4.611306	4.555404	0.625840	O	-0.256681	0.386234	2.272504
C	1.611195	1.165943	2.695688	H	0.381822	0.209137	2.981601
C	1.720191	1.094066	4.065890	O	-0.030204	-3.904550	3.978645
C	2.457588	0.053476	4.681310	H	0.858493	-4.262158	3.857743
H	2.536284	0.011294	5.763311	C	-1.773192	0.968124	0.025208
C	3.068989	-0.900438	3.903128	C	-1.855505	-0.280982	-0.585279
H	3.634886	-1.707931	4.360144	C	-3.145312	-0.838374	-0.829364
H	1.237190	1.845778	4.683675	C	-4.295704	-0.197762	-0.449163

Br	-3.309931	-2.503282	-1.753447	C	5.782998	-1.921511	-0.861113
H	-5.259909	-0.652956	-0.648252	C	4.581497	-2.629311	-0.826505
C	0.295919	1.242621	1.382392	C	3.355598	-1.950011	-0.760605
C	-0.430585	1.588916	0.250494	C	3.362098	-0.546811	-0.734315
C	2.134326	2.709000	0.710465	C	4.561898	0.157289	-0.777322
C	1.588625	1.802214	1.578778	H	6.713697	0.022989	-0.872129
H	3.122731	3.116494	0.892354	H	6.722797	-2.464111	-0.903413
Br	2.589031	1.223921	3.115977	H	4.613098	-3.712511	-0.841098
C	1.403022	3.111795	-0.434434	H	2.417098	-0.021110	-0.671715
C	0.112416	2.533602	-0.674520	H	4.537598	1.241489	-0.768330
C	-2.958883	1.660637	0.429709	C	2.056399	-4.157908	-0.357887
C	-4.237690	1.062145	0.195124	H	1.080398	-4.605909	-0.535681
C	-5.416681	1.744058	0.598425	H	2.823097	-4.713312	-0.898186
C	-5.344369	2.972164	1.213412	H	2.261503	-4.229001	0.716413
C	-4.082562	3.568056	1.449397	C	-0.716807	-2.405419	-2.018789
H	-6.378687	1.274163	0.411435	H	-1.750108	-2.363721	-2.327886
H	-6.251062	3.485473	1.519413	O	-1.082099	-1.083704	0.270603
H	-4.029551	4.537061	1.937288	O	0.289294	2.268084	-1.663822
C	-0.587389	2.930795	-1.849120	H	1.019693	2.737881	-2.098128
C	-0.047188	3.849583	-2.720632	O	0.784509	-3.150588	2.777210
C	1.223219	4.424275	-2.472646	H	0.951006	-2.689893	1.942508
H	1.633619	5.151065	-3.167156	C	-1.705100	1.172494	-0.059309
C	1.931723	4.058081	-1.352347	C	-1.991201	-0.191907	-0.159199
H	2.909828	4.487075	-1.151358	C	-3.295802	-0.575309	-0.609592
H	-0.602391	4.139078	-3.608232	C	-4.222903	0.345788	-1.024095
H	-1.561494	2.498502	-2.048108	Br	-3.828602	-2.413109	-0.600779
C	-2.922669	2.931343	1.068797	H	-5.195004	0.011186	-1.369789
H	-1.961565	3.396638	1.257585	C	0.541299	2.214892	-0.330623
				C	-0.398098	1.626498	0.508484
B3LYP/6-31G** Energy =			-6817.755910	C	2.013006	2.688504	1.564770
B3LYP/6-31G** Free Energy =			-6817.774826	C	1.732701	2.756896	0.226570
M06-2X/LACVP** Derived Free Energy =			-1700.366052	H	2.932807	3.110307	1.954964
Number of Imaginary Frequencies =			1 (-381.51)	Br	2.965498	3.629988	-0.964140
				C	1.091409	2.068010	2.443177
B3LYP/6-31G** Geometry				C	-0.133693	1.543307	1.913283
				C	-2.674901	2.153591	-0.450111
C	1.726891	-2.804723	-2.717294	C	-3.940103	1.730289	-0.967404
C	0.369592	-2.659523	-2.611791	C	-4.899004	2.695886	-1.375308
B	-0.419901	-2.241907	-0.289591	C	-4.632504	4.040186	-1.267718
C	-0.255591	-4.094389	2.560920	C	-3.392302	4.467589	-0.736724
C	-1.326095	-3.603896	1.594821	H	-5.851006	2.348683	-1.768103
H	0.148507	-5.048692	2.184825	H	-5.370605	4.772884	-1.579720
H	-0.711988	-4.293283	3.538523	H	-3.188402	5.529990	-0.639331
H	-1.729293	-2.645693	1.939116	C	-1.058190	0.967312	2.828191
H	-2.149195	-4.329096	1.560828	C	-0.777286	0.897822	4.173290
O	-0.786798	-3.484204	0.283918	C	0.440915	1.402725	4.687483
H	2.133391	-3.789024	-2.938689	H	0.649519	1.334931	5.750782
H	2.286590	-1.981826	-3.157101	C	1.353213	1.979419	3.836977
C	2.038298	-2.681710	-0.732396	H	2.290215	2.378221	4.216370
O	1.061700	-1.947907	-0.202298	H	-1.497883	0.447926	4.849696
C	5.777897	-0.527211	-0.840223	H	-1.997192	0.580711	2.450596

C	-2.443001	3.553592	-0.338822	H	4.119553	-3.278850	-1.177834
H	-1.503800	3.900595	0.074973	C	1.170324	2.155583	-0.196103
				C	1.464514	1.073176	0.623392
B3LYP/6-31G** Energy =			-6817.756169	C	0.154846	3.365189	1.669505
B3LYP/6-31G** Free Energy =			-6817.774340	C	0.517240	3.293189	0.351504
M06-2X/LACVP** Derived Free Energy =			-1700.365492	H	-0.345941	4.246994	2.053911
Number of Imaginary Frequencies =			1 (-368.46)	Br	0.128152	4.758497	-0.829990
				C	0.440137	2.280383	2.534400
B3LYP/6-31G** Geometry				C	1.106621	1.123776	2.009695
				C	3.569597	0.001354	-0.305221
C	-2.444923	-0.565463	-3.253697	C	4.265880	-1.148053	-0.799228
C	-1.595633	-1.537875	-2.826103	C	5.631280	-1.040368	-1.175532
B	-1.003221	-1.470390	-0.396805	C	6.301895	0.154123	-1.057831
C	-2.929541	-3.812574	1.770295	C	5.628111	1.288030	-0.546225
C	-1.724831	-2.931688	1.479593	H	6.137468	-1.925273	-1.552337
H	-2.806942	-4.297578	2.744993	H	7.345995	0.228011	-1.346636
H	-2.992853	-4.603771	1.005793	H	6.163224	2.227222	-0.439524
H	-0.815038	-3.537898	1.399787	C	1.400712	0.063670	2.912190
H	-1.580118	-2.210692	2.296394	C	1.046919	0.140369	4.239791
O	-1.989528	-2.247380	0.257696	C	0.378734	1.280076	4.748397
H	-3.499526	-0.807950	-3.353092	H	0.103939	1.323977	5.797799
H	-2.074916	0.173235	-3.961696	C	0.085343	2.328382	3.909602
C	-2.347802	0.486330	-1.415893	H	-0.421844	3.213387	4.284807
O	-1.395805	-0.041884	-0.679299	H	1.284211	-0.683435	4.906587
C	-6.404297	0.339175	0.061223	H	1.915299	-0.813835	2.540284
C	-6.152497	0.784975	-1.238876	C	4.303112	1.213845	-0.179720
C	-4.850299	0.808361	-1.730181	H	3.806025	2.090050	0.218885
C	-3.772101	0.381445	-0.935488				
C	-4.034400	-0.037955	0.377012	B3LYP/6-31G** Energy =			-6817.760254
C	-5.341499	-0.067941	0.866618	B3LYP/6-31G** Free Energy =			-6817.779692
H	-7.420796	0.314285	0.442328	M06-2X/LACVP** Derived Free Energy =			-1700.374848
H	-6.972096	1.110987	-1.872471	Number of Imaginary Frequencies =			1 (-380.01)
H	-4.677099	1.151062	-2.745981				
H	-3.211601	-0.340368	1.008808	B3LYP/6-31G** Geometry			
H	-5.518699	-0.419343	1.878317				
C	-1.940188	1.836426	-1.985090	C	-1.693507	-2.887581	-0.935550
H	-1.907275	2.558423	-1.162589	C	-0.819002	-2.629703	0.074552
H	-0.940290	1.768316	-2.415596	B	-1.137695	-0.432527	1.302998
H	-2.646686	2.208538	-2.728187	C	-3.686686	-0.498973	3.792305
C	-0.847736	-2.153987	-2.014009	C	-2.599490	-1.315161	3.101885
H	-0.253647	-3.053294	-2.082214	H	-3.257482	0.001508	4.674314
O	0.245082	-1.483707	0.329689	H	-4.494285	-1.155079	4.135296
O	1.510417	2.097583	-1.511204	H	-3.040794	-1.890345	2.278776
H	1.326626	2.962386	-1.913401	H	-2.152987	-2.024776	3.814769
O	-4.133431	-3.061259	1.826703	O	-1.614790	-0.413253	2.634599
H	-4.170029	-2.575656	0.989705	H	-1.332911	-2.909761	-1.960852
C	2.184398	-0.107630	0.055486	H	-2.543807	-3.535584	-0.735260
C	1.523082	-1.329922	-0.065316	C	-2.461605	-0.910882	-0.882608
C	2.274566	-2.474830	-0.477222	O	-2.267200	-0.438106	0.326501
C	3.586666	-2.389745	-0.858629	C	-6.615608	-1.695160	-1.735708
Br	1.451445	-4.203719	-0.424625	C	-5.641512	-1.986742	-2.693917

C	-4.298711	-1.742948	-2.420717	H	3.914495	1.378326	-1.605286
C	-3.903706	-1.209274	-1.181708				
C	-4.888502	-0.917492	-0.223699	B3LYP/6-31G** Energy =			-6817.750472
C	-6.233003	-1.160285	-0.505798	B3LYP/6-31G** Free Energy =			-6817.770453
H	-7.663809	-1.881555	-1.950307	M06-2X/LACVP** Derived Free Energy =			-1700.362538
H	-5.927917	-2.403322	-3.655124	Number of Imaginary Frequencies =			1 (-346.46)
H	-3.556314	-1.986035	-3.174425				
H	-4.607098	-0.484911	0.730609	B3LYP/6-31G** Geometry			
H	-6.982800	-0.921098	0.242409				
C	-1.622408	-0.308861	-1.993199	C	-4.200274	1.961334	1.287915
H	-1.883707	0.753341	-2.048576	C	-3.206273	1.698728	2.174412
H	-0.555307	-0.388666	-1.781505	B	-1.171086	0.530907	1.278910
H	-1.831112	-0.761741	-2.962706	C	-1.004501	-2.056887	3.580918
C	-0.314098	-1.968922	1.031663	C	-0.490103	-1.704096	2.184615
H	0.486104	-2.175638	1.727256	H	-1.994306	-2.517078	3.510923
O	-0.158095	0.622974	1.204514	H	-1.111791	-1.142184	4.187415
O	1.860992	-1.002768	-1.827126	H	-0.380812	-2.629099	1.607117
H	2.082590	-1.849759	-2.248344	H	0.499902	-1.238604	2.267611
O	-4.263088	0.447945	2.904127	O	-1.387397	-0.856390	1.495515
H	-3.513089	0.926052	2.515133	H	-5.074379	1.316141	1.254020
C	1.495900	1.321103	-0.341078	H	-4.374265	2.994834	0.995612
C	0.222102	1.443694	0.215430	C	-3.003584	1.285318	-0.392587
C	-0.606998	2.530803	-0.205145	O	-1.790885	1.045409	0.037611
C	-0.198300	3.422621	-1.162730	C	-5.329818	-2.022667	-1.884468
Br	-2.327195	2.778489	0.591166	C	-5.868607	-0.733062	-1.886671
H	-0.852400	4.235928	-1.458810	C	-5.131696	0.334033	-1.381277
C	2.534797	-0.921492	-0.648426	C	-3.843196	0.132124	-0.854780
C	2.388901	0.217793	0.131397	C	-3.312607	-1.167381	-0.854078
C	4.060502	-1.910627	0.982348	C	-4.051718	-2.232476	-1.368072
C	3.374896	-1.977702	-0.200851	H	-5.903026	-2.853363	-2.285265
H	4.694202	-2.733033	1.295929	H	-6.863306	-0.558155	-2.285969
Br	3.519491	-3.539680	-1.311183	H	-5.569987	1.327137	-1.388279
C	3.941006	-0.759242	1.800571	H	-2.325707	-1.333388	-0.444780
C	3.095605	0.317067	1.371996	H	-3.612927	-3.225880	-1.367070
C	1.949297	2.246622	-1.334261	C	-3.049476	2.570115	-1.204591
C	1.082298	3.304532	-1.758237	H	-2.534281	2.381108	-2.153992
C	1.525594	4.223051	-2.746520	H	-4.061973	2.906924	-1.427489
C	2.779892	4.111060	-3.299827	H	-2.500267	3.346213	-0.668695
C	3.643992	3.072352	-2.878951	C	-2.043575	1.375619	2.559210
H	0.853594	5.019758	-3.054701	H	-1.540971	1.441617	3.512708
H	3.110690	4.818476	-4.054214	O	0.221718	0.937695	1.334305
H	4.636091	2.990859	-3.313556	O	0.049793	-0.825913	-1.755289
C	2.996011	1.461050	2.211020	H	-0.535115	-1.509509	-2.120886
C	3.689315	1.532725	3.397418	O	-0.157607	-3.006992	4.217018
C	4.521515	0.466916	3.816394	H	0.739696	-2.646800	4.204114
H	5.061219	0.538697	4.755693	C	1.802211	0.868876	-0.447801
C	4.643110	-0.655068	3.031471	C	0.922220	1.576986	0.369900
H	5.279111	-1.480775	3.339351	C	0.851833	2.995486	0.220695
H	3.595418	2.416414	4.021636	C	1.611436	3.670076	-0.700109
H	2.360509	2.282457	1.901438	Br	-0.315355	4.007300	1.342696
C	3.241295	2.166433	-1.923567	H	1.531144	4.748777	-0.780513

C	0.975690	-1.417418	-0.961891	C	4.216795	-0.557438	1.227705
C	1.898699	-0.616425	-0.302396	C	4.694099	-0.387721	-0.081091
C	1.982576	-3.436125	-0.019587	C	6.022500	-0.683320	-0.388892
C	1.020679	-2.827018	-0.780286	H	7.924095	-1.376037	0.354004
H	1.987267	-4.514125	0.098616	H	7.102687	-1.646367	2.687197
Br	-0.371633	-3.873609	-1.588178	H	4.765187	-1.126468	3.243998
C	2.961985	-2.649530	0.636907	H	4.027303	0.001592	-0.837888
C	2.910597	-1.221630	0.506003	H	6.377403	-0.546207	-1.405889
C	2.606615	1.548165	-1.417105	C	2.633995	0.828346	2.710020
C	2.507926	2.970467	-1.543610	H	2.977399	1.812750	2.369335
C	3.308429	3.648057	-2.501714	H	1.576995	0.904946	2.971017
C	4.176221	2.953346	-3.311515	H	3.217792	0.552032	3.588618
C	4.274708	1.546245	-3.194311	C	0.553493	-2.020217	0.539773
H	3.221339	4.728556	-2.581317	H	-0.268408	-2.550508	0.080263
H	4.785023	3.479538	-4.040618	O	0.257103	0.000607	-1.085999
H	4.959402	1.001138	-3.837611	O	-2.743294	-0.256772	-1.907711
C	3.881906	-0.451837	1.205797	H	-3.230296	-0.925763	-2.416423
C	4.850002	-1.059743	1.972697	O	1.176296	-3.811277	-2.421750
C	4.902091	-2.469842	2.090201	H	1.592394	-3.571790	-1.579246
H	5.673289	-2.934248	2.697300	C	-1.404195	1.434599	-0.158984
C	3.973882	-3.245637	1.436306	C	-0.183293	1.242404	-0.799983
H	3.998773	-4.328837	1.521709	C	0.550712	2.384909	-1.239665
H	5.582610	-0.451147	2.494792	C	0.090015	3.660908	-1.049748
H	3.848915	0.628663	1.124294	Br	2.211214	2.130116	-2.150163
C	3.511705	0.862355	-2.274506	H	0.673218	4.506811	-1.397134
H	3.594896	-0.215745	-2.195003	C	-2.802699	-0.578890	-0.594817
B3LYP/6-31G** Energy =			-6817.755010	C	-2.160799	0.241095	0.327197
B3LYP/6-31G** Free Energy =			-6817.775366	C	-3.580509	-2.057213	1.190960
M06-2X/LACVP** Derived Free Energy =			-1700.368972	C	-3.504505	-1.729394	-0.136935
Number of Imaginary Frequencies =			1 (-341.94)	H	-4.127013	-2.939516	1.505846
B3LYP/6-31G** Geometry				Br	-4.362304	-2.836673	-1.449453
				C	-2.941309	-1.240829	2.156374
				C	-2.217905	-0.082324	1.719592
				C	-1.924091	2.756899	0.025733
C	2.084186	-1.932351	2.606779	C	-1.158387	3.883602	-0.417049
C	1.181489	-2.186734	1.627673	C	-1.667283	5.196301	-0.229431
B	1.301599	-0.755905	-0.438007	C	-2.890484	5.399896	0.365668
C	0.826101	-2.573567	-3.023434	C	-3.657088	4.290493	0.794150
C	1.881804	-1.508474	-2.744716	H	-1.070979	6.038204	-0.571117
H	0.741304	-2.741252	-4.103836	H	-3.271982	6.407296	0.502581
H	-0.151699	-2.214469	-2.665132	H	-4.626990	4.453989	1.254950
H	1.568708	-0.534268	-3.132503	C	-1.568605	0.707959	2.710905
H	2.826504	-1.794670	-3.221618	C	-1.641310	0.376240	4.045200
O	2.153200	-1.439995	-1.345314	C	-2.363215	-0.765564	4.470282
H	1.734485	-1.504263	3.543684	H	-2.414619	-1.012578	5.526278
H	2.972685	-2.553554	2.677973	C	-2.997615	-1.555648	3.541069
C	2.814495	-0.143938	1.557406	H	-3.553619	-2.436551	3.851155
O	1.980800	0.101578	0.579508	H	-1.144911	1.001229	4.782311
C	6.891695	-1.143937	0.598305	H	-1.016202	1.586061	2.397619
C	6.430891	-1.295954	1.909301	C	-3.188292	3.006094	0.629533
C	5.108291	-0.999455	2.221701	H	-3.787995	2.164591	0.957219

B3LYP/6-31G** Energy = -6817.755460
 B3LYP/6-31G** Free Energy = -6817.772493
 M06-2X/LACVP** Derived Free Energy = -1700.373896
 Number of Imaginary Frequencies = 1 (-386.53)

B3LYP/6-31G** Geometry

C	-1.172929	-4.233991	-0.484000
C	-0.264930	-3.889895	-1.444803
B	0.086983	-1.417297	-1.708902
C	-2.311009	0.616718	-2.766692
C	-0.866212	0.357910	-3.204897
H	-2.684305	1.541121	-3.224189
H	-2.360904	0.741517	-1.676591
H	-0.173806	1.057705	-2.727699
H	-0.784216	0.473910	-4.292197
O	-0.533119	-0.995393	-2.912799
H	-0.852529	-4.837293	0.361699
H	-2.204331	-4.399785	-0.790196
C	-1.095216	-2.371392	0.372901
O	-0.894313	-1.483192	-0.583298
C	-5.125508	-2.156170	1.910016
C	-4.117909	-2.732377	2.683612
C	-2.815111	-2.814184	2.192007
C	-2.498313	-2.315484	0.918307
C	-3.521312	-1.739078	0.143711
C	-4.820511	-1.661971	0.639515
H	-6.139507	-2.092465	2.293720
H	-4.341708	-3.117476	3.674112
H	-2.048712	-3.261189	2.814704
H	-3.302914	-1.354178	-0.846390
H	-5.595809	-1.211266	0.027519
C	0.053587	-2.599600	1.340997
H	0.207094	-1.672901	1.900498
H	-0.144115	-3.411400	2.041497
H	0.969784	-2.829404	0.796394
C	0.442772	-3.094099	-2.129205
H	1.099968	-3.217801	-2.975107
O	1.284089	-0.642304	-1.427306
O	-0.843393	0.595805	1.662903
H	-1.787692	0.591111	1.892707
O	-3.152916	-0.454277	-3.179390
H	-2.565521	-1.228480	-3.162092
C	1.705103	0.688292	0.521894
C	1.972894	-0.416209	-0.289108
C	3.084191	-1.248616	0.054887
C	3.846596	-1.030622	1.172985
Br	3.545478	-2.719818	-1.070815
H	4.675992	-1.692227	1.398381
C	-0.623591	1.560105	0.734204

C	0.629608	1.657398	0.146099
C	-1.416184	3.506410	-0.512792
C	-1.643387	2.481911	0.366208
H	-2.215781	4.191715	-0.772188
Br	-3.392886	2.208120	1.098013
C	-0.133186	3.665203	-1.094396
C	0.899210	2.723597	-0.770901
C	2.489409	0.939685	1.695692
C	3.566705	0.059679	2.031287
C	4.341311	0.304474	3.196585
C	4.070720	1.381975	4.006887
C	3.012024	2.261181	3.676791
H	5.154708	-0.376731	3.432681
H	4.667623	1.562471	4.895785
H	2.803731	3.113782	4.316593
C	2.172609	2.894391	-1.382205
C	2.407712	3.933990	-2.253405
C	1.385716	4.861596	-2.567101
H	1.586718	5.675995	-3.256401
C	0.141117	4.726303	-1.998197
H	-0.653779	5.429708	-2.231693
H	3.388511	4.043585	-2.706509
H	2.962706	2.189686	-1.150209
C	2.244318	2.047886	2.553994
H	1.438621	2.730991	2.311597

B3LYP/6-31G** Energy = -6817.755739
 B3LYP/6-31G** Free Energy = -6817.773986
 M06-2X/LACVP** Derived Free Energy = -1700.369324
 Number of Imaginary Frequencies = 1 (-358.86)

B3LYP/6-31G** Geometry

C	3.002690	-2.977206	-2.022303
C	1.687589	-3.292701	-1.890103
B	0.265695	-1.634196	-0.652104
C	-0.266413	-2.989495	2.789996
C	-0.543412	-2.956194	1.295795
H	-0.867016	-3.777192	3.258195
H	-0.567610	-2.025794	3.231096
H	-1.612511	-2.794489	1.103495
H	-0.263915	-3.924194	0.856696
O	0.253793	-1.919396	0.736496
H	3.380992	-2.728008	-3.011102
H	3.722788	-3.448509	-1.358601
C	2.717797	-1.012105	-1.198302
O	1.431498	-0.800101	-1.061703
C	5.189294	-1.151515	2.336699
C	5.739894	-1.453017	1.088499
C	4.941395	-1.431113	-0.051401
C	3.573496	-1.117309	0.032999

C	3.034796	-0.795707	1.288698	B3LYP/6-31G** Energy =			-6817.765418
C	3.838295	-0.818810	2.430298	B3LYP/6-31G** Free Energy =			-6817.784586
H	5.811694	-1.170317	3.226300	M06-2X/LACVP** Derived Free Energy =			-1700.382754
H	6.792093	-1.707721	1.003000	Number of Imaginary Frequencies =			1 (-387.83)
H	5.386795	-1.675416	-1.011001				
H	1.991498	-0.521203	1.363097	B3LYP/6-31G** Geometry			
H	3.401496	-0.563109	3.390598				
C	3.280801	-0.216408	-2.367502	C	2.327864	-3.541538	-1.716976
H	2.701801	-0.423505	-3.269602	C	1.074561	-3.816624	-1.252174
H	3.162805	0.848993	-2.141002	B	-0.045418	-1.882107	-0.106881
H	4.336801	-0.417711	-2.550701	C	-0.551123	-2.565085	3.528222
C	0.473490	-3.122297	-1.579604	C	0.298477	-2.481500	2.268621
H	-0.431512	-3.689493	-1.739804	H	-1.495128	-3.079177	3.290725
O	-0.915903	-1.023992	-1.220505	H	-0.799612	-1.548481	3.868718
O	-0.802791	1.936908	-2.186104	H	0.580867	-3.493504	1.954125
H	-0.255589	2.331806	-2.883804	H	1.216783	-1.921108	2.476218
O	1.092887	-3.282000	3.066797	O	-0.469417	-1.834796	1.256018
H	1.611889	-2.692701	2.499897	H	2.494763	-3.497745	-2.790476
C	-2.003797	0.736112	0.009295	H	3.178660	-3.897444	-1.139175
C	-2.002502	-0.510588	-0.616505	C	2.150384	-1.525234	-1.286985
C	-3.233804	-1.229183	-0.706706	O	1.361586	-1.426522	-0.233985
C	-4.412803	-0.733179	-0.219007	C	6.232196	-0.464171	-0.393493
Br	-3.227610	-2.962583	-1.516806	C	5.910889	-0.991574	-1.646990
H	-5.325104	-1.313975	-0.301507	C	4.597085	-1.346662	-1.939788
C	-0.166791	2.076205	-1.001704	C	3.584187	-1.194348	-0.978488
C	-0.727294	1.503107	0.134996	C	3.915894	-0.665045	0.277210
C	1.681611	2.992299	0.315498	C	5.229898	-0.295757	0.561507
C	1.050212	2.803401	-0.884303	H	7.255898	-0.179381	-0.168995
H	2.604413	3.559895	0.366298	H	6.683687	-1.122786	-2.398391
Br	1.828415	3.519898	-2.488503	H	4.365680	-1.755764	-2.918486
C	1.128509	2.435500	1.494497	H	3.137996	-0.505134	1.012410
C	-0.079894	1.668405	1.401197	H	5.459803	0.137645	1.529805
C	-3.230595	1.293917	0.501994	C	1.595888	-1.022835	-2.610787
C	-4.446798	0.545122	0.391093	H	1.440800	0.056567	-2.511692
C	-5.660696	1.094126	0.883093	H	2.289986	-1.195146	-3.433986
C	-5.688392	2.344026	1.456293	H	0.630183	-1.475927	-2.832584
C	-4.494589	3.096821	1.553394	C	-0.007236	-3.564110	-0.644673
H	-6.570298	0.506329	0.792392	H	-0.900541	-4.131600	-0.431371
H	-6.621591	2.756430	1.827792	O	-0.961712	-1.178402	-0.974984
H	-4.519886	4.088821	1.995194	O	-0.028290	0.736703	2.048406
C	-0.589697	1.088207	2.597796	H	-0.491699	-0.088594	1.782710
C	0.046103	1.270904	3.804996	O	0.215471	-3.273089	4.494025
C	1.230805	2.042100	3.891697	H	-0.267728	-3.256079	5.328825
H	1.717205	2.182498	4.852298	C	-1.927091	0.837412	-0.114692
C	1.759708	2.608698	2.755897	C	-2.038105	-0.488489	-0.521587
H	2.672211	3.197094	2.803698	C	-3.321711	-1.109977	-0.522083
H	-0.365199	0.817806	4.702196	C	-4.449104	-0.445263	-0.118885
H	-1.494100	0.494410	2.545695	Br	-3.476730	-2.916477	-1.125074
C	-3.301491	2.588117	1.090794	H	-5.410609	-0.947254	-0.130981
H	-2.397789	3.181413	1.167195	C	0.244016	1.475595	0.949703
				C	-0.602684	1.538499	-0.153497

C	1.813231	3.011874	-0.115905	C	5.188202	1.888184	0.578419
C	1.451924	2.231382	0.949698	H	6.679802	2.795475	1.843225
H	2.742136	3.571265	-0.088809	H	6.241790	1.256473	3.748120
Br	2.601724	2.114978	2.469498	H	4.520384	-0.491619	3.556911
C	0.986130	3.078477	-1.266805	H	3.669000	0.766493	-0.465188
C	-0.236277	2.329690	-1.289801	H	5.383907	2.544885	-0.263879
C	-3.092284	1.554425	0.319805	C	3.460982	-2.476311	1.505504
C	-4.366090	0.900639	0.318810	H	4.049978	-2.587015	2.417205
C	-5.519682	1.608951	0.748506	H	2.644078	-3.196407	1.496301
C	-5.427369	2.915653	1.168100	H	4.113183	-2.683711	0.648706
C	-4.170863	3.565640	1.174197	C	-0.044716	-1.681696	1.589797
H	-6.477988	1.096462	0.739510	H	-1.084116	-1.961692	1.510494
H	-6.314564	3.449263	1.495699	O	0.043095	-0.876591	-0.895302
H	-4.101452	4.596341	1.509391	O	-2.932001	-0.527977	-1.779309
C	-1.048377	2.413193	-2.455301	H	-3.611304	-1.170274	-2.042112
C	-0.672471	3.189083	-3.529505	O	3.096080	-4.661803	-1.206101
C	0.534837	3.926371	-3.501510	H	2.763778	-4.439204	-0.325602
H	0.818242	4.534664	-4.355212	C	-1.087897	1.219213	-0.690600
C	1.345037	3.868969	-2.390909	C	-0.020099	0.447510	-1.147799
H	2.275444	4.429859	-2.355112	C	0.946106	1.061407	-2.000495
H	-1.309470	3.235586	-4.408005	C	0.881312	2.384408	-2.348192
H	-1.975283	1.851501	-2.488597	Br	2.365704	0.005103	-2.716193
C	-3.035070	2.904927	0.761999	H	1.639515	2.813506	-2.994389
H	-2.077464	3.412417	0.774196	C	-3.045904	-0.289879	-0.453209
B3LYP/6-31G** Energy =				C	-2.148202	0.585416	0.150896
B3LYP/6-31G** Free Energy =				C	-4.204711	-0.640080	1.671587
M06-2X/LACVP** Derived Free Energy =				C	-4.063908	-0.898677	0.333487
Number of Imaginary Frequencies =				H	-4.996115	-1.116077	2.240384
				Br	-5.272511	-2.106769	-0.542019
B3LYP/6-31G** Geometry				C	-3.314909	0.256116	2.314192
C	1.835283	-0.955308	3.184503	C	-2.270305	0.870713	1.547296
C	0.701182	-1.395901	2.574299	C	-1.197990	2.599414	-1.065297
B	0.842089	-1.602997	0.063999	C	-0.187386	3.191812	-1.889293
C	2.520686	-3.688699	-2.068301	C	-0.286579	4.561613	-2.251891
C	1.081787	-3.374794	-1.679704	C	-1.348878	5.326816	-1.831392
H	3.101490	-2.753701	-2.053597	C	-2.360681	4.743619	-1.032596
H	2.558987	-4.088497	-3.088601	H	0.493125	4.991311	-2.875287
H	0.472183	-4.283992	-1.755608	H	-1.417472	6.372618	-2.115089
H	0.663591	-2.611490	-2.341703	H	-3.204981	5.346522	-0.710996
O	1.050084	-2.954697	-0.313703	C	-1.376703	1.748307	2.224800
H	2.401078	-1.640611	3.811204	C	-1.520206	2.009905	3.568301
H	1.890886	0.091691	3.476005	C	-2.560410	1.408308	4.317696
C	2.935488	-1.058308	1.363106	H	-2.662011	1.626906	5.376397
O	2.056292	-0.804702	0.425104	C	-3.435712	0.546813	3.700292
C	5.919299	2.025078	1.757221	H	-4.236015	0.073115	4.262690
C	5.674992	1.159278	2.826918	H	-0.827904	2.686902	4.060705
C	4.701889	0.171081	2.716014	H	-0.573100	2.210105	1.663104
C	3.948592	0.037787	1.537912	C	-2.288889	3.419518	-0.661199
C	4.205099	0.904089	0.465414	H	-3.075191	2.987220	-0.053602
				B3LYP/6-31G** Energy =			
				-6817.768695			

B3LYP/6-31G** Free Energy =				C	-3.751402	-0.758910	0.246916
M06-2X/LACVP** Derived Free Energy =				H	-4.732799	-1.342218	2.050114
Number of Imaginary Frequencies =				Br	-4.729905	-1.988104	-0.839388
				C	-3.210698	0.162680	2.414619
B3LYP/6-31G** Geometry				C	-2.172398	0.951482	1.815221
				C	-0.801401	3.016291	-0.403173
C	2.308003	-1.539426	2.850401	C	0.267099	3.640994	-1.126971
C	1.021201	-1.535923	2.405204	C	0.315899	5.057794	-1.224265
B	0.766596	-1.545811	-0.097796	C	-0.660999	5.838092	-0.652460
C	-1.122009	-3.300900	-2.354600	C	-1.737498	5.226390	0.032740
C	-0.736906	-3.366907	-0.880702	H	1.137399	5.512196	-1.771764
H	-2.075210	-3.819799	-2.500901	H	-0.616298	6.919893	-0.735154
H	-0.354810	-3.814598	-2.951304	H	-2.519397	5.843889	0.464944
H	-0.735106	-4.421008	-0.570306	C	-1.359296	1.742077	2.676623
H	-1.504304	-2.851309	-0.287998	C	-1.587394	1.781571	4.033624
O	0.559994	-2.837409	-0.651001	C	-2.635893	1.028169	4.614022
H	2.703202	-2.431929	3.329496	H	-2.807891	1.074065	5.685222
H	2.736504	-0.603528	3.202904	C	-3.424795	0.231574	3.818220
C	3.048998	-1.804718	0.902498	H	-4.223195	-0.365627	4.251019
O	2.196197	-1.219513	0.085302	H	-0.954592	2.396668	4.666926
C	6.796800	0.298877	1.262501	H	-0.549596	2.320279	2.247624
C	6.549401	-0.825126	2.054296	C	-1.807699	3.856690	0.151533
C	5.339201	-1.503725	1.944796	H	-2.643098	3.402788	0.671333
C	4.350299	-1.067120	1.046600				
C	4.608699	0.059484	0.251904	B3LYP/6-31G** Energy = -6817.753381			
C	5.825799	0.731882	0.360005	B3LYP/6-31G** Free Energy = -6817.773604			
H	7.741901	0.827176	1.345802	M06-2X/LACVP** Derived Free Energy = -1700.366549			
H	7.299602	-1.173630	2.757794	Number of Imaginary Frequencies = 1 (-385.41)			
H	5.161701	-2.368528	2.575992				
H	3.877497	0.369488	-0.482993	B3LYP/6-31G** Geometry			
H	6.015499	1.594985	-0.271192				
C	3.114597	-3.322617	0.858591	C	-1.825803	3.316468	2.288866
H	3.507595	-3.599614	-0.125810	C	-1.197372	2.115686	2.442075
H	3.782198	-3.727621	1.619088	B	-1.750513	0.345962	0.724881
H	2.122597	-3.761017	0.950891	C	-4.393354	-2.060305	1.751176
C	0.098099	-1.497418	1.538405	C	-3.810191	-0.652989	1.648973
H	-0.976400	-1.459118	1.633207	H	-3.716441	-2.700883	2.335784
O	0.088396	-0.538308	-0.904790	H	-4.452637	-2.473512	0.739878
O	-2.647405	0.093598	-1.729882	H	-3.804512	-0.163484	2.640670
H	-2.452007	-0.797500	-2.109087	H	-4.445204	-0.051610	0.987366
O	-1.305409	-1.970997	-2.832594	O	-2.505985	-0.769957	1.132382
H	-0.542008	-1.446699	-2.526693	H	-2.697113	3.524847	2.907959
C	-0.839102	1.587991	-0.285779	H	-1.236526	4.188382	2.020165
C	0.146497	0.817892	-0.903684	C	-2.575478	2.805738	0.399363
C	1.138796	1.462995	-1.693383	O	-2.563441	1.494638	0.279670
C	1.222897	2.827696	-1.783577	C	0.220075	5.101902	-1.953930
Br	2.304093	0.381099	-2.745290	C	-0.922345	5.713573	-1.432640
H	1.994896	3.286798	-2.391577	C	-1.829030	4.976453	-0.674643
C	-2.775502	0.062992	-0.386782	C	-1.618794	3.605159	-0.438734
C	-1.963900	0.881488	0.399220	C	-0.473174	2.999589	-0.978524
C	-3.975000	-0.710516	1.598916	C	0.441811	3.744209	-1.721121

H	0.931963	5.682018	-2.533928	M06-2X/LACVP** Derived Free Energy =			-1700.374037
H	-1.106972	6.768868	-1.611447	Number of Imaginary Frequencies =			1 (-381.89)
H	-2.699246	5.480431	-0.269051				
H	-0.284246	1.946694	-0.810317	B3LYP/6-31G** Geometry			
H	1.336726	3.254832	-2.092114				
C	-3.995193	3.322100	0.582551	C	1.243195	-4.188500	1.338617
H	-4.515681	2.692290	1.305351	C	1.231392	-3.233199	2.307716
H	-4.042923	4.360800	0.908946	B	0.088995	-1.034700	1.743609
H	-4.515984	3.236881	-0.378352	C	-2.987013	-1.325097	3.738699
C	-0.876938	0.928193	2.149483	C	-2.136308	-1.728498	2.542702
H	-0.247721	0.184912	2.617291	H	-2.350616	-1.322896	4.639801
O	-0.760796	-0.031416	-0.274111	H	-3.780213	-2.065897	3.893598
O	2.039202	0.400652	-1.802595	H	-2.760505	-1.794499	1.641701
H	1.360621	-0.243468	-2.061296	H	-1.688809	-2.717098	2.724205
O	-5.714658	-2.056238	2.275567	O	-1.139808	-0.733798	2.362004
H	-5.658071	-1.795031	3.203967	H	0.514295	-4.995100	1.395816
C	0.822953	-1.775474	-0.441792	H	2.184197	-4.453601	0.864821
C	-0.469860	-1.292110	-0.658503	C	0.475201	-2.845302	-0.123787
C	-1.405232	-2.106039	-1.372404	O	-0.072601	-1.822301	0.494910
C	-1.077796	-3.372933	-1.780196	C	4.126108	-2.116305	-2.309276
Br	-3.113749	-1.412788	-1.855119	C	3.138510	-2.939006	-2.851678
H	-1.808676	-3.969855	-2.315598	C	1.961108	-3.188005	-2.145281
C	2.385301	0.149968	-0.514891	C	1.750604	-2.606603	-0.884683
C	1.824523	-0.884543	0.226710	C	2.751802	-1.779902	-0.349680
C	3.766570	0.828014	1.365614	C	3.927904	-1.538303	-1.053277
C	3.364973	0.998497	0.067011	H	5.041410	-1.925806	-2.861772
H	4.518649	1.484438	1.789816	H	3.278714	-3.386607	-3.830977
Br	4.130943	2.385614	-0.994191	H	1.202009	-3.817805	-2.594383
C	3.202493	-0.200196	2.163716	H	2.624198	-1.336501	0.628518
C	2.214420	-1.066926	1.590114	H	4.678402	-0.890803	-0.610174
C	1.191591	-3.089467	-0.885783	C	-0.573997	-3.762602	-0.722389
C	0.214617	-3.905096	-1.540885	H	-1.342000	-3.964102	0.025908
C	0.566056	-5.212289	-1.969976	H	-1.057394	-3.239303	-1.555492
C	1.835768	-5.701853	-1.767665	H	-0.159396	-4.706103	-1.079787
C	2.807842	-4.895624	-1.130363	C	0.984790	-2.106299	2.831213
H	-0.188224	-5.817012	-2.466177	H	1.181087	-1.682097	3.804814
H	2.095797	-6.702547	-2.099258	O	0.926695	0.141800	1.655710
H	3.810852	-5.283395	-0.978255	O	-0.457392	-0.392505	-2.138693
C	1.646242	-2.075837	2.418215	H	0.416407	-0.069905	-1.864991
C	2.041237	-2.221420	3.730519	O	-3.619812	-0.074797	3.547796
C	3.026711	-1.372391	4.287921	H	-2.931711	0.536802	3.245797
H	3.331008	-1.502077	5.322023	C	0.359201	1.569198	-0.244493
C	3.592288	-0.382679	3.516919	C	1.227098	1.053700	0.725210
H	4.346369	0.279743	3.933821	C	2.564298	1.574099	0.784614
H	1.592855	-2.997729	4.343620	C	3.014901	2.551498	-0.057485
H	0.890663	-2.732459	2.000914	Br	3.770093	0.842401	2.074420
C	2.496805	-3.623630	-0.702372	H	4.035101	2.910798	0.025218
H	3.250584	-3.014707	-0.216470	C	-1.387795	0.178997	-1.332397
				C	-1.065098	1.118697	-0.361298
B3LYP/6-31G** Energy =			-6817.753338	C	-3.749097	0.338197	-0.777705
B3LYP/6-31G** Free Energy =			-6817.771797	C	-2.739494	-0.214604	-1.520301

H	-4.775196	0.026697	-0.941108	H	5.450224	3.889089	-2.117212
Br	-3.133990	-1.537005	-2.841301	H	5.681225	2.114771	-0.445617
C	-3.462799	1.320799	0.205294	H	1.442380	1.360219	-0.674108
C	-2.102501	1.713899	0.422498	H	1.204483	3.187836	-2.278602
C	0.818605	2.600396	-1.142893	C	5.111713	0.115200	1.056278
C	2.158204	3.093997	-1.047589	H	5.749362	0.953362	1.337279
C	2.605307	4.108295	-1.933789	H	5.039375	-0.579198	1.894377
C	1.763211	4.630794	-2.888093	H	5.580880	-0.413725	0.218376
C	0.435912	4.154095	-2.984796	C	1.052632	0.392633	2.183191
H	3.627807	4.464895	-1.841485	H	0.059526	0.272990	2.591594
H	2.112113	5.406894	-3.562492	O	0.609171	-0.555635	-0.207011
H	-0.230786	4.570094	-3.734399	O	-1.212413	1.525176	-1.857300
C	-1.839404	2.700300	1.411298	H	-1.060068	0.592368	-2.077902
C	-2.865106	3.266901	2.136793	O	2.380432	-4.729442	1.410273
C	-4.208006	2.877801	1.916790	H	1.938351	-4.361015	0.630275
H	-5.004608	3.326702	2.501486	C	-1.730150	-0.894398	-0.459605
C	-4.496003	1.920900	0.971790	C	-0.414877	-1.342674	-0.597810
H	-5.521102	1.603600	0.802087	C	-0.176151	-2.586287	-1.260114
H	-2.640909	4.020102	2.886594	C	-1.202998	-3.378325	-1.699413
H	-0.813705	3.004500	1.587901	Br	1.617417	-3.128389	-1.612520
C	-0.024292	3.168695	-2.138696	H	-0.985855	-4.320137	-2.191716
H	-1.046692	2.820296	-2.224100	C	-1.718406	1.582602	-0.600198
B3LYP/6-31G** Energy =			-6817.760217	C	-1.983470	0.446615	0.156999
B3LYP/6-31G** Free Energy =			-6817.780305	C	-2.476717	3.029441	1.199408
M06-2X/LACVP** Derived Free Energy =			-1700.373818	C	-1.971430	2.874215	-0.064493
Number of Imaginary Frequencies =			1 (-384.57)	H	-2.663959	4.024450	1.588512
B3LYP/6-31G** Geometry				Br	-1.587244	4.402996	-1.137591
C	3.252110	1.721305	2.326189	C	-2.746881	1.896855	2.010406
C	2.004579	1.187077	2.437990	C	-2.490958	0.586541	1.487101
B	1.475459	-0.793788	0.937986	C	-2.822098	-1.695133	-0.939404
C	3.027998	-3.641381	2.042374	C	-2.550473	-2.964748	-1.542908
C	2.042160	-2.592226	2.547380	C	-3.626822	-3.767983	-2.003508
H	3.581475	-4.052616	2.895371	C	-4.927796	-3.337207	-1.883303
H	3.754623	-3.158121	1.370873	C	-5.200822	-2.077693	-1.300698
H	2.583807	-1.793959	3.074881	H	-3.401479	-4.729595	-2.456710
H	1.352234	-3.062588	3.258980	H	-5.744833	-3.958060	-2.238102
O	1.267687	-2.075578	1.476683	H	-6.228601	-1.737534	-1.214895
H	3.369966	2.711598	1.895791	C	-2.736521	-0.532947	2.330799
H	3.995196	1.455460	3.076785	C	-3.218107	-0.363223	3.610801
C	3.710637	0.536883	0.638484	C	-3.484231	0.930892	4.117705
O	2.897776	-0.498170	0.617383	H	-3.866821	1.048611	5.126906
C	3.314409	3.662214	-2.316307	C	-3.250569	2.035480	3.331008
C	4.568093	3.345440	-1.792112	H	-3.443309	3.035291	3.710911
C	4.696236	2.333630	-0.841815	H	-3.395256	-1.232314	4.237499
C	3.572995	1.603794	-0.413513	H	-2.531380	-1.528458	1.953195
C	2.320312	1.918768	-0.965709	C	-4.177773	-1.276954	-0.842599
C	2.191769	2.944978	-1.898905	H	-4.400417	-0.313043	-0.399796
H	3.213953	4.460922	-3.045404	B3LYP/6-31G** Energy =			-6817.763126
				B3LYP/6-31G** Free Energy =			-6817.780993
				M06-2X/LACVP** Derived Free Energy =			-1700.378417

Number of Imaginary Frequencies =				1 (-374.34)	Br	-3.460570	2.648305	0.877685
					C	0.516746	3.696735	0.065342
B3LYP/6-31G** Geometry					C	1.229508	2.513042	0.447414
					C	1.506000	-0.284523	2.622568
C	-1.903360	-2.570426	-3.005715	C	2.199354	-1.513612	2.871140	
C	-0.629318	-2.187576	-3.314428	C	2.498628	-1.891068	4.207730	
B	0.222528	-0.332201	-1.886814	C	2.135241	-1.089640	5.264648	
C	2.005856	1.759509	-3.661309	C	1.457286	0.128946	5.023775	
C	0.518612	1.402290	-3.717592	H	3.027118	-2.825534	4.377608	
H	2.162565	2.569779	-2.934198	H	2.370620	-1.386283	6.282439	
H	2.296787	2.135288	-4.650407	H	1.178075	0.762367	5.860689	
H	0.357612	0.682222	-4.533700	C	2.643706	2.509273	0.296893	
H	-0.045481	2.312862	-3.958570	C	3.307831	3.604799	-0.207400	
O	-0.026729	0.915339	-2.503491	C	2.597766	4.768092	-0.591772	
H	-2.722036	-2.293017	-3.665499	H	3.135164	5.623632	-0.989268	
H	-2.038567	-3.517018	-2.487928	C	1.229874	4.809755	-0.455052	
C	-2.109965	-1.150824	-1.473592	H	0.671977	5.697427	-0.741431	
O	-0.888323	-0.849878	-1.076005	H	4.388226	3.576370	-0.313116	
C	-4.214125	-3.632711	1.361302	H	3.197603	1.625201	0.591372	
C	-4.886580	-3.127312	0.247120	C	1.150314	0.519903	3.739886	
C	-4.216096	-2.323881	-0.672678	H	0.636225	1.458768	3.567207	
C	-2.857155	-2.012948	-0.495593					
C	-2.189301	-2.527746	0.627289	B3LYP/6-31G** Energy =				-6817.760009
C	-2.864486	-3.328577	1.546087	B3LYP/6-31G** Free Energy =				-6817.780136
H	-4.739290	-4.255358	2.079501	M06-2X/LACVP** Derived Free Energy =				-1700.373363
H	-5.936810	-3.356382	0.092832	Number of Imaginary Frequencies =				1 (-388.68)
H	-4.761463	-1.948501	-1.531465					
H	-1.146669	-2.281875	0.777277	B3LYP/6-31G** Geometry				
H	-2.332719	-3.710354	2.412474					
C	-2.873745	-0.068921	-2.217664	C	-2.805276	-2.587014	1.170316	
H	-3.813295	-0.429600	-2.636456	C	-1.624975	-2.525008	0.488818	
H	-2.257205	0.354716	-3.007467	B	-1.116392	-0.280512	-0.541899	
H	-3.097937	0.730496	-1.501549	C	-2.332982	-0.448849	-3.704201	
C	0.458460	-1.569311	-3.136036	C	-0.975882	-0.657631	-3.044295	
H	1.438153	-1.565623	-3.590450	H	-2.330075	-0.929156	-4.690297	
O	1.445240	-0.327362	-1.072631	H	-2.487991	0.630850	-3.857809	
O	-1.510227	0.425156	1.709123	H	-0.181883	-0.330629	-3.727895	
H	-2.460203	0.624070	1.737440	H	-0.838373	-1.731428	-2.850786	
O	2.849125	0.649103	-3.401738	O	-0.839491	0.098579	-1.858501	
H	2.688006	0.377609	-2.482039	H	-2.788378	-2.643305	2.256215	
C	1.218727	0.103631	1.275078	H	-3.640270	-3.100625	0.698017	
C	1.610113	-0.711901	0.214661	C	-3.189293	-0.553319	0.894198	
C	2.309570	-1.923089	0.490833	O	-2.603693	-0.215624	-0.240803	
C	2.592441	-2.318443	1.772523	C	-7.503693	-0.566759	0.697787	
Br	2.891118	-2.992739	-0.976992	C	-6.853492	-1.004145	1.854192	
H	3.130431	-3.243712	1.949101	C	-5.463393	-1.010032	1.914195	
C	-0.857409	1.471985	1.148129	C	-4.692793	-0.584933	0.818095	
C	0.516679	1.387021	0.966507	C	-5.356193	-0.145848	-0.337711	
C	-0.892948	3.727104	0.204263	C	-6.749794	-0.138861	-0.394014	
C	-1.543471	2.646375	0.734157	H	-8.588493	-0.560069	0.650884	
H	-1.449946	4.604076	-0.107715	H	-7.429691	-1.341542	2.710593	

H	-4.977591	-1.363620	2.818100				
H	-4.786894	0.196650	-1.192012	B3LYP/6-31G** Geometry			
H	-7.243494	0.206428	-1.297119				
C	-2.588002	0.013795	2.171295	C	-1.568911	-4.192196	0.080287
H	-3.172202	-0.260302	3.049496	C	-1.198013	-3.643491	-1.110312
H	-1.550499	-0.289394	2.300000	B	-0.596907	-1.192193	-1.053500
H	-2.594411	1.103395	2.061087	C	-2.905408	1.004923	-3.025582
C	-0.746677	-1.994807	-0.254584	C	-1.764109	0.007920	-2.871791
H	0.169427	-2.377102	-0.681379	H	-2.998110	1.271129	-4.091980
O	-0.335501	0.469202	0.422797	H	-2.657104	1.917320	-2.478078
O	2.377814	-0.613893	-1.887186	H	-0.851010	0.445220	-3.302892
H	2.565922	-1.349295	-2.492780	H	-1.992313	-0.907977	-3.447595
O	-3.395079	-1.032951	-2.967199	O	-1.589106	-0.290787	-1.510993
H	-3.257583	-0.786943	-2.038800	H	-2.607911	-4.464895	0.241988
C	1.897293	1.240819	0.120697	H	-0.843710	-4.817900	0.598381
C	0.525191	1.464607	0.105992	C	-1.448204	-2.342502	1.104796
C	0.044980	2.783101	-0.145919	O	-0.719803	-1.523499	0.369298
C	0.895572	3.825906	-0.403326	C	-5.661500	-1.609695	1.732312
Br	-1.836323	3.101185	-0.091027	C	-5.001901	-2.612000	2.448805
H	0.497964	4.817401	-0.591735	C	-3.647301	-2.847303	2.235799
C	2.590715	-1.031481	-0.614583	C	-2.916102	-2.080800	1.306502
C	2.391504	-0.136074	0.427910	C	-3.587202	-1.071494	0.599609
C	3.210726	-2.798562	0.959833	C	-4.948801	-0.847992	0.808114
C	2.978725	-2.368075	-0.319371	H	-6.720399	-1.429894	1.894716
H	3.503635	-3.825858	1.147342	H	-5.543700	-3.214603	3.172103
Br	3.096640	-3.601786	-1.786661	H	-3.165002	-3.642707	2.793994
C	3.056015	-1.897656	2.041925	H	-3.058003	-0.471692	-0.128689
C	2.629305	-0.554661	1.773814	H	-5.441001	-0.072288	0.229519
C	2.810284	2.309725	-0.142308	C	-0.649301	-2.807610	2.313391
C	2.298274	3.619218	-0.414920	H	-1.091602	-3.659911	2.828188
C	3.202565	4.682824	-0.675626	H	0.363798	-3.060410	1.995787
C	4.561766	4.470336	-0.669320	H	-0.590297	-1.969514	3.016295
C	5.072078	3.178343	-0.398909	C	-0.776413	-2.747087	-1.895108
H	2.798157	5.670720	-0.880034	H	-0.459916	-2.755183	-2.927109
H	5.244660	5.290441	-0.870325	O	0.737493	-0.728294	-1.387902
H	6.145979	3.015553	-0.394305	O	1.256499	2.193507	-1.751889
C	2.458494	0.324146	2.880006	H	0.858698	2.827911	-2.370284
C	2.702194	-0.099642	4.166711	O	-4.140507	0.547523	-2.488682
C	3.126005	-1.425836	4.425122	H	-4.350711	-0.294774	-2.913885
H	3.314605	-1.744727	5.445725	C	2.057701	0.425394	0.242400
C	3.297115	-2.304643	3.381729	C	1.854595	-0.630500	-0.649605
H	3.620024	-3.326138	3.565138	C	2.912393	-1.565501	-0.859213
H	2.568785	0.590863	4.994404	C	4.116395	-1.463308	-0.213615
H	2.135385	1.341742	2.692198	Br	2.646886	-2.995994	-2.097320
C	4.220486	2.127138	-0.142303	H	4.895892	-2.195209	-0.396323
H	4.620694	1.140442	0.064305	C	0.588703	2.262002	-0.576286
				C	0.962204	1.418696	0.465608
B3LYP/6-31G** Energy =		-6817.750209		C	-1.134291	3.305899	0.811824
B3LYP/6-31G** Free Energy =		-6817.768992		C	-0.474095	3.186504	-0.379978
M06-2X/LACVP** Derived Free Energy =		-1700.360445		H	-1.939589	4.023400	0.924330
Number of Imaginary Frequencies =		1 (-373.81)		Br	-0.996297	4.280212	-1.871071

C	-0.763390	2.481792	1.902019	H	2.827596	0.185292	-1.254599
C	0.281907	1.515991	1.723211	H	5.025193	-0.769011	-1.809804
C	3.323803	0.576788	0.899597	C	2.036104	2.637888	1.947006
C	4.357400	-0.390914	0.679589	H	2.004903	1.744986	2.581904
C	5.609302	-0.247420	1.335886	H	1.088604	3.160289	2.069908
C	5.851507	0.819375	2.168991	H	2.853505	3.271786	2.291405
C	4.844610	1.792777	2.371299	C	-0.070898	3.441196	-1.019791
H	6.376300	-0.996720	1.158280	H	-0.967398	3.717499	-1.552589
H	6.812709	0.922071	2.663588	O	-0.803103	0.980597	-1.101694
H	5.042414	2.644073	3.016203	O	0.413193	-1.251203	-2.128200
C	0.605909	0.684584	2.833206	H	-0.005906	-0.369302	-2.042997
C	-0.041787	0.820979	4.040908	O	-0.877193	4.021690	3.223412
C	-1.063184	1.786081	4.212617	H	-0.776792	4.000189	4.182912
H	-1.564381	1.882077	5.170918	C	-1.748205	-1.035203	-0.224197
C	-1.417186	2.593888	3.158721	C	-1.898004	0.227699	-0.789994
H	-2.204583	3.334689	3.269227	C	-3.196203	0.689301	-1.148992
H	0.235914	0.180874	4.873704	C	-4.317304	-0.069597	-0.943492
H	1.382107	-0.061917	2.717699	Br	-3.403101	2.417003	-1.942889
C	3.618608	1.675983	1.755702	H	-5.294003	0.313805	-1.217990
H	2.861211	2.433984	1.916208	C	0.557693	-1.748305	-0.877501
				C	-0.392306	-1.561905	0.127401
B3LYP/6-31G** Energy =		-6817.760660		C	2.004693	-2.979410	0.653396
B3LYP/6-31G** Free Energy =		-6817.779318		C	1.727292	-2.512307	-0.603304
M06-2X/LACVP** Derived Free Energy =		-1700.376192		H	2.904692	-3.557512	0.832694
Number of Imaginary Frequencies =		1 (-382.40)		Br	2.918090	-2.895607	-2.045206
				C	1.133595	-2.678211	1.731897
B3LYP/6-31G** Geometry				C	-0.075505	-1.954909	1.471500
				C	-2.906007	-1.876801	-0.057197
C	2.383803	3.945092	-0.466692	C	-4.202206	-1.372198	-0.399995
C	1.072402	3.952494	-0.852891	C	-5.350707	-2.190297	-0.224995
B	-0.149900	1.897795	-0.141993	C	-5.234208	-3.475398	0.248403
C	-1.953295	3.156193	2.869611	C	-3.954609	-3.994401	0.553901
C	-1.889697	2.884195	1.379311	H	-6.323306	-1.780894	-0.484792
H	-1.892296	2.198192	3.405210	H	-6.116309	-4.095796	0.375003
H	-2.925193	3.619894	3.103413	H	-3.859910	-5.018001	0.904199
H	-1.794596	3.843095	0.852512	C	-0.911403	-1.636408	2.577702
H	-2.835098	2.423897	1.061811	C	-0.580502	-2.027211	3.856300
O	-0.791799	2.038194	1.105908	C	0.601697	-2.763613	4.103998
H	3.128801	3.758492	-1.236894	H	0.847998	-3.070416	5.116097
H	2.708005	4.623389	0.319508	C	1.440295	-3.078113	3.059796
C	2.247501	2.159990	0.518604	H	2.358795	-3.632115	3.235294
O	1.255099	1.473893	-0.032895	H	-1.232201	-1.763712	4.684501
C	6.121197	0.541086	-0.488602	H	-1.812102	-1.059607	2.402704
C	6.018101	1.567884	0.451599	C	-2.825308	-3.220501	0.405801
C	4.770401	2.092085	0.780602	H	-1.855408	-3.642403	0.635099
C	3.603000	1.603388	0.169902				
C	3.717897	0.575590	-0.778000	B3LYP/6-31G** Energy =			-6817.768519
C	4.967496	0.046988	-1.097703	B3LYP/6-31G** Free Energy =			-6817.784844
H	7.093196	0.127184	-0.740505	M06-2X/LACVP** Derived Free Energy =			-1700.381961
H	6.908902	1.959582	0.933799	Number of Imaginary Frequencies =			1 (-396.03)
H	4.714804	2.890284	1.512903				

B3LYP/6-31G** Geometry

C	2.452130	3.844275	0.270238
C	1.213832	3.920189	-0.293064
B	0.026916	1.698501	-0.606585
C	0.102316	0.480328	-4.131794
C	0.472420	1.424416	-2.999386
H	0.577321	0.826031	-5.061090
H	-0.980784	0.486338	-4.276197
H	0.315429	2.456820	-3.352477
H	1.546319	1.327006	-2.773384
O	-0.316285	1.153714	-1.864490
H	3.322832	3.906573	-0.379458
H	2.604131	4.232366	1.274242
C	2.191613	1.797073	0.715022
O	1.420611	1.298687	-0.224284
C	6.267803	0.408044	0.440222
C	5.930708	1.396039	1.368629
C	4.619411	1.855648	1.456528
C	3.621909	1.344663	0.610122
C	3.969105	0.348868	-0.315585
C	5.281301	-0.116042	-0.395185
H	7.289600	0.045936	0.375922
H	6.689909	1.807928	2.026734
H	4.377615	2.627045	2.180934
H	3.201503	-0.091022	-0.939191
H	5.524797	-0.900039	-1.106190
C	1.598110	1.925767	2.106421
H	2.270613	2.441356	2.792527
H	0.633414	2.431775	2.074623
H	1.430402	0.913565	2.487413
C	0.128730	3.467501	-0.761770
H	-0.748365	3.919912	-1.199469
O	-0.943689	1.429600	0.422410
O	-0.765109	-1.891385	-1.681216
H	-0.233505	-1.595882	-2.458011
O	0.447905	-0.887076	-3.886504
H	1.399704	-0.958085	-3.722902
C	-2.073706	-0.686190	0.419790
C	-2.079694	0.699510	0.285101
C	-3.325689	1.364721	0.097803
C	-4.513594	0.683331	0.038994
Br	-3.349773	3.271823	-0.051982
H	-5.443889	1.222539	-0.104105
C	-0.098812	-1.854899	-0.515014
C	-0.759711	-1.372703	0.612888
C	1.850580	-2.418625	0.862088
C	1.235283	-2.335011	-0.359414
H	2.866276	-2.791234	0.937888
Br	2.231184	-2.846006	-1.921115
C	1.161179	-2.013729	2.032389

C	-0.159416	-1.470818	1.904289
C	-3.297211	-1.423281	0.363081
C	-4.533306	-0.727570	0.169383
C	-5.748811	-1.461060	0.118974
C	-5.750622	-2.829861	0.254364
C	-4.530628	-3.521972	0.445561
H	-6.678706	-0.918051	-0.028824
H	-6.684926	-3.381954	0.214156
H	-4.537836	-4.603073	0.549353
C	-0.821816	-1.038122	3.087691
C	-0.216420	-1.145537	4.319692
C	1.087476	-1.685447	4.440691
H	1.551772	-1.764759	5.419092
C	1.759875	-2.109144	3.317489
H	2.761472	-2.523952	3.395489
H	-0.744020	-0.814339	5.209393
H	-1.820612	-0.624413	3.003892
C	-3.337022	-2.838282	0.497570
H	-2.405827	-3.375290	0.640768

B3LYP/6-31G** Energy = -6817.760507
 B3LYP/6-31G** Free Energy = -6817.778252
 M06-2X/LACVP** Derived Free Energy = -1700.379614
 Number of Imaginary Frequencies = 1 (-392.06)

B3LYP/6-31G** Geometry

C	2.878640	3.326356	-1.256107
C	1.538643	3.579375	-1.268903
B	0.091222	1.915198	-0.009899
C	0.304360	4.096696	2.545799
C	0.048937	2.599900	2.422100
H	0.539665	4.311993	3.594498
H	-0.614833	4.646009	2.292501
H	-0.635264	2.309210	3.229502
H	0.983531	2.047586	2.562498
O	-0.585370	2.203508	1.205503
H	3.350933	2.994049	-2.175808
H	3.507250	3.939447	-0.613009
C	2.692317	1.542859	-0.217305
O	1.447315	1.380778	0.189698
C	3.975470	-1.141461	-3.339306
C	4.925482	-0.458574	-2.577009
C	4.519096	0.409532	-1.566208
C	3.153301	0.605753	-1.299105
C	2.205789	-0.085234	-2.070002
C	2.617274	-0.951640	-3.081303
H	4.293159	-1.820166	-4.125407
H	5.984979	-0.603189	-2.766611
H	5.273206	0.931623	-0.987511
H	1.150392	0.048681	-1.865100

H	1.870965	-1.490831	-3.656101				
C	3.620424	1.846647	0.947993	C	-2.601213	-3.021089	0.463868
H	3.630512	0.958648	1.591593	C	-1.515909	-2.496303	1.102672
H	4.641927	2.075432	0.642690	B	-1.219094	-0.018101	0.770300
H	3.214037	2.685453	1.516793	C	-3.212681	1.208887	2.940018
C	0.321642	3.387394	-0.981200	C	-1.692281	1.063177	2.989912
H	-0.608652	3.878806	-1.223199	H	-3.583777	1.440978	3.945721
O	-0.725491	1.069409	-0.868797	H	-3.662788	0.255693	2.630308
O	-0.193105	-0.410697	2.319203	H	-1.431586	0.162068	3.565801
H	-0.810797	0.239412	1.937904	H	-1.256675	1.929269	3.500520
O	1.415165	4.567180	1.790096	O	-1.104785	1.036587	1.700010
H	1.158862	4.530182	0.857396	H	-2.448919	-3.652680	-0.408539
C	-1.891517	-0.810574	0.050807	H	-3.474913	-3.272790	1.061468
C	-1.883899	0.475926	-0.487494	C	-3.082604	-1.196676	-0.446210
C	-3.131591	1.133844	-0.709191	O	-2.629397	-0.257788	0.354999
C	-4.328197	0.553661	-0.381588	C	-7.391305	-1.366948	-0.524502
Br	-3.155567	2.864643	-1.520392	C	-6.644513	-2.356946	-1.168014
H	-5.256390	1.084574	-0.563786	C	-5.253713	-2.312654	-1.136617
C	0.163279	-1.305303	1.369103	C	-4.584105	-1.283967	-0.453807
C	-0.605027	-1.554592	0.238404	C	-5.340997	-0.290369	0.187606
C	1.795954	-2.979027	0.689900	C	-6.734897	-0.336260	0.147809
C	1.379870	-2.015420	1.568800	H	-8.476505	-1.398742	-0.551899
H	2.727247	-3.507140	0.864498	H	-7.145819	-3.163436	-1.694922
Br	2.467080	-1.565435	3.072198	H	-4.688119	-3.094353	-1.634427
C	1.027747	-3.275516	-0.465398	H	-4.840291	0.527323	0.694114
C	-0.179443	-2.541499	-0.707096	H	-7.306591	0.443638	0.641719
C	-3.132324	-1.434655	0.415510	C	-2.376809	-1.371465	-1.782414
C	-4.363915	-0.739138	0.198013	H	-2.839015	-2.153256	-2.385921
C	-5.592324	-1.353320	0.559716	H	-2.466704	-0.414159	-2.307602
C	-5.611641	-2.608320	1.122317	H	-1.312610	-1.567073	-1.655819
C	-4.396950	-3.298337	1.345215	C	-0.757601	-1.568513	1.513381
H	-6.517116	-0.809807	0.385218	H	0.112200	-1.544025	2.153778
H	-6.554946	-3.070006	1.398120	O	-0.327995	0.166306	-0.355001
H	-4.415963	-4.287037	1.794115	O	2.291893	-0.927591	-2.129820
C	-0.914350	-2.834389	-1.889294	H	2.510387	-1.717986	-2.650029
C	-0.485166	-3.802496	-2.771094	O	-3.621477	2.264399	2.084830
C	0.702323	-4.531114	-2.522896	H	-3.034178	2.240804	1.312128
H	1.026811	-5.293718	-3.224497	C	1.832411	1.152993	-0.362695
C	1.441930	-4.267323	-1.392698	C	0.458011	1.249903	-0.540691
H	2.359623	-4.814136	-1.192600	C	-0.093182	2.482212	-1.000176
H	-1.065872	-4.010188	-3.665393	C	0.691024	3.574710	-1.260066
H	-1.826243	-2.282977	-2.090192	Br	-1.980282	2.606027	-1.286169
C	-3.190742	-2.729255	1.001411	H	0.240128	4.498616	-1.605954
H	-2.266550	-3.266168	1.181209	C	2.626195	-1.153907	-0.836723
				C	2.410604	-0.146816	0.096389
B3LYP/6-31G** Energy =			-6817.765618	C	3.544690	-2.620832	0.890858
B3LYP/6-31G** Free Energy =			-6817.785055	C	3.196888	-2.386415	-0.412938
M06-2X/LACVP** Derived Free Energy =			-1700.380198	H	3.983085	-3.570338	1.178446
Number of Imaginary Frequencies =			1 (-391.10)	Br	3.477276	-3.747302	-1.739955
				C	3.325799	-1.619142	1.869170
B3LYP/6-31G** Geometry				C	2.742906	-0.370634	1.468285

C	2.679617	2.273291	-0.637885	C	1.571391	-0.643414	2.421796
C	2.096124	3.502899	-1.084570	H	0.614186	-1.090204	2.687595
C	2.932930	4.618597	-1.353159	H	2.242290	-0.658920	3.280798
C	4.296329	4.532286	-1.192063	H	1.386002	0.400088	2.150496
C	4.878323	3.318278	-0.756378	C	0.169564	-3.588302	0.901997
H	2.473134	5.543704	-1.690848	H	-0.657942	-4.260794	0.737497
H	4.927434	5.391085	-1.400156	O	-0.951812	-1.241890	0.821093
H	5.955623	3.252970	-0.634481	O	-0.200087	0.780899	-1.968007
C	2.500214	0.607957	2.474397	H	0.552607	0.217691	-2.256406
C	2.830116	0.367840	3.789293	O	1.564796	-1.010820	-3.107503
C	3.420909	-0.859568	4.176878	H	1.669104	-0.456321	-3.893203
H	3.678811	-1.031382	5.217475	C	-2.083291	0.711120	0.043089
C	3.659201	-1.832159	3.234266	C	-2.067005	-0.652881	0.323091
H	4.104296	-2.781965	3.518955	C	-3.279713	-1.390868	0.185689
H	2.633822	1.128232	4.539402	C	-4.445606	-0.807657	-0.237613
H	2.032319	1.542963	2.189308	Br	-3.318032	-3.244267	0.655591
C	4.093117	2.219480	-0.487389	H	-5.348012	-1.402548	-0.328614
H	4.550412	1.293573	-0.156900	C	0.099818	1.475797	-0.849408
B3LYP/6-31G** Energy =			-6817.765960	C	-0.827083	1.512007	0.185791
B3LYP/6-31G** Free Energy =			-6817.782954	C	1.583031	2.983684	0.377192
M06-2X/LACVP** Derived Free Energy =			-1700.382044	C	1.305825	2.225185	-0.729807
Number of Imaginary Frequencies =			1 (-387.58)	H	2.509336	3.544875	0.437294
B3LYP/6-31G** Geometry				Br	2.554027	2.184472	-2.182305
C	2.464566	-3.259624	2.008600	C	0.648029	3.052194	1.442291
C	1.228662	-3.653811	1.592899	C	-0.575377	2.308506	1.345990
B	0.010782	-2.019001	0.076395	C	-3.286284	1.346431	-0.402614
C	0.695387	-2.111511	-3.425903	C	-4.482592	0.573643	-0.547415
C	0.449576	-2.929108	-2.169502	C	-5.676585	1.203555	-0.989518
H	-0.260410	-1.745702	-3.822105	C	-5.696171	2.546455	-1.285919
H	1.169682	-2.757217	-4.178902	C	-4.514463	3.314043	-1.153017
H	1.417173	-3.190017	-1.723501	H	-6.575591	0.600963	-1.090718
H	-0.041332	-3.864403	-2.478903	H	-6.613565	3.019162	-1.623921
O	-0.376818	-2.239599	-1.261505	H	-4.532152	4.372842	-1.394920
H	2.633567	-3.025423	3.056701	C	-1.487778	2.377617	2.435988
H	3.332063	-3.654732	1.484003	C	-1.210973	3.143415	3.546088
C	2.173987	-1.331021	1.209498	C	-0.006965	3.883203	3.632389
O	1.401887	-1.463915	0.152197	H	0.196739	4.484602	4.513289
C	6.252898	-0.365562	0.198204	C	0.902136	3.834493	2.601190
C	5.889994	-0.537958	1.536304	H	1.831941	4.394684	2.656692
C	4.576790	-0.859344	1.866802	H	-1.922974	3.180322	4.365487
C	3.603490	-1.017735	0.865500	H	-2.411184	1.811826	2.380187
C	3.976794	-0.849541	-0.476800	C	-3.342970	2.731432	-0.724315
C	5.293098	-0.521454	-0.801298	H	-2.442264	3.327923	-0.633215
H	7.276101	-0.108974	-0.060294	B3LYP/6-31G** Energy =			-6817.754671
H	6.630194	-0.422165	2.322405	B3LYP/6-31G** Free Energy =			-6817.770521
H	4.313887	-0.998541	2.910602	M06-2X/LACVP** Derived Free Energy =			-1700.370418
H	3.233795	-0.964734	-1.256200	Number of Imaginary Frequencies =			1 (-363.12)
H	5.566201	-0.381759	-1.842897	B3LYP/6-31G** Geometry			

C	-1.927131	-2.068882	-3.462876	C	4.465506	0.733081	-0.285817
C	-0.920029	-2.672389	-2.781084	C	5.707008	1.419274	-0.368524
B	-0.370409	-1.621894	-0.603186	C	5.785118	2.768274	-0.115322
C	-0.752796	-3.266596	2.399214	C	4.617823	3.482079	0.245086
C	-1.033708	-3.426493	0.910615	H	6.598004	0.850670	-0.621131
H	-0.541299	-4.267998	2.807511	H	6.739220	3.283068	-0.175028
H	-1.621691	-2.861293	2.925820	H	4.685331	4.541578	0.474087
H	-1.900011	-4.093088	0.792421	C	0.802508	2.927602	-1.618589
H	-0.175213	-3.934197	0.444709	C	0.244608	3.917805	-2.396983
O	-1.310405	-2.194991	0.286719	C	-0.979787	4.523111	-2.028273
H	-2.925733	-2.497676	-3.435370	H	-1.406687	5.306914	-2.646870
H	-1.675234	-1.540582	-4.378878	C	-1.628482	4.107113	-0.887870
C	-1.963312	-0.365283	-2.113273	H	-2.577477	4.551118	-0.598563
O	-0.908808	-0.457290	-1.330181	H	0.748103	4.234004	-3.306086
C	-5.926901	-0.404165	-0.416347	H	1.736903	2.470597	-1.920596
C	-5.758111	-0.490564	-1.801048	C	3.398221	2.847485	0.316694
C	-4.479015	-0.516670	-2.348257	H	2.517426	3.407689	0.605700
C	-3.339609	-0.480077	-1.523765	B3LYP/6-31G** Energy =			-6817.765778
C	-3.522099	-0.392079	-0.134763	B3LYP/6-31G** Free Energy =			-6817.784014
C	-4.805395	-0.349772	0.409446	M06-2X/LACVP** Derived Free Energy =			-1700.380160
H	-6.925199	-0.371960	0.010160	Number of Imaginary Frequencies =			1 (-399.67)
H	-6.623715	-0.532059	-2.455642	B3LYP/6-31G** Geometry			
H	-4.370323	-0.578270	-3.426657	C	2.707691	-3.313628	-1.498946
H	-2.666395	-0.346284	0.521231	C	1.416088	-3.678018	-1.248454
H	-4.911987	-0.255473	1.485947	B	0.057984	-1.950800	0.015519
C	-1.783114	0.705716	-3.174373	C	0.337851	-2.331370	3.554824
H	-0.803618	0.608613	-3.645180	C	0.046960	-3.033980	2.236928
H	-2.566419	0.675622	-3.932168	H	0.692142	-3.067166	4.285734
H	-1.826806	1.682017	-2.679971	H	-0.592850	-1.891362	3.945113
C	0.004376	-2.760094	-1.920291	H	-0.675445	-3.845975	2.411229
H	0.882674	-3.379199	-1.812597	H	0.974260	-3.481388	1.859340
O	0.860898	-1.349301	0.121306	O	-0.501228	-2.118486	1.300916
O	0.677723	0.288496	2.489109	H	3.486483	-3.726026	-0.860535
H	0.232418	-0.588001	2.593710	H	3.019301	-3.122938	-2.522544
O	0.333310	-2.380702	2.674208	C	2.397495	-1.383219	-0.822965
H	0.986204	-2.470404	1.959803	O	1.456087	-1.426507	0.100226
C	2.010508	0.771993	0.093400	C	6.311884	-0.663724	0.840962
C	1.974300	-0.612806	-0.088201	C	6.116796	-0.583835	-0.538740
C	3.194995	-1.313212	-0.312710	C	4.855299	-0.818734	-1.082149
C	4.397997	-0.673219	-0.442118	C	3.767490	-1.136821	-0.253056
Br	3.160885	-3.231513	-0.296513	C	3.970578	-1.214610	1.135047
H	5.305093	-1.240623	-0.619425	C	5.234775	-0.977812	1.671756
C	0.073121	1.100201	1.596714	H	7.294881	-0.479025	1.264469
C	0.743315	1.484699	0.436510	H	6.946303	-0.336245	-1.194635
C	-1.779675	2.609611	1.072129	H	4.724909	-0.750743	-2.156851
C	-1.221775	1.635807	1.855924	H	3.137371	-1.442600	1.791241
H	-2.763371	3.003416	1.303436	H	5.374065	-1.034002	2.747357
Br	-2.227569	0.874910	3.291330	C	2.033610	-0.703830	-2.135075
C	-1.078381	3.087809	-0.064475				
C	0.179014	2.492803	-0.414584				
C	3.269912	1.458286	0.030093				

H	1.033711	-0.999127	-2.452082	C	2.093297	-2.732101	-0.495667
H	2.032413	0.378672	-1.974985	B	1.383900	-0.332404	-0.722499
H	2.749915	-0.918440	-2.928667	C	-0.172210	0.592354	-3.883906
C	0.260984	-3.545909	-0.752166	C	0.655691	-0.441737	-3.134195
H	-0.620820	-4.165903	-0.714068	H	-0.766313	0.094144	-4.656098
O	-0.786303	-1.167504	-0.861296	H	0.483889	1.325447	-4.374119
O	-0.754677	1.762584	-2.239422	H	1.394689	-0.871647	-3.830491
H	-0.227569	2.217674	-2.916221	H	-0.002109	-1.250931	-2.803681
O	1.355357	-1.348976	3.438225	O	1.317496	0.180478	-2.047006
H	1.022666	-0.685880	2.815516	H	3.699001	-3.099385	0.814332
C	-2.067001	0.680710	-0.057724	H	4.074295	-3.333510	-0.961966
C	-1.981304	-0.629895	-0.520311	C	3.820100	-0.884703	-0.460099
C	-3.189206	-1.362591	-0.715815	O	2.730501	-0.232597	-0.118705
C	-4.419906	-0.826782	-0.439631	C	6.956510	-0.339665	2.450983
Br	-3.115909	-3.134598	-1.428599	C	7.198105	-1.108982	1.311092
H	-5.316207	-1.416780	-0.598634	C	6.191802	-1.294294	0.365499
C	-0.204187	2.005492	-1.025519	C	4.926104	-0.715490	0.547395
C	-0.816400	1.482005	0.106780	C	4.691409	0.056526	1.695985
C	1.538607	3.047595	0.339787	C	5.702012	0.243038	2.637178
C	0.983216	2.774687	-0.881815	H	7.742113	-0.193856	3.186478
H	2.444408	3.639691	0.410690	H	8.171204	-1.565385	1.156895
Br	1.832934	3.405268	-2.484914	H	6.397398	-1.902406	-0.509693
C	0.927394	2.545609	1.514685	H	3.720609	0.520530	1.822981
C	-0.253709	1.740214	1.395083	H	5.508515	0.849251	3.517171
C	-3.340801	1.274118	0.220859	C	4.203894	-0.865224	-1.932501
C	-4.532004	0.500723	0.040356	H	3.382893	-1.212832	-2.557493
C	-5.797203	1.080931	0.323940	H	4.411495	0.175372	-2.202516
C	-5.893700	2.380136	0.764627	H	5.093694	-1.461728	-2.135396
C	-4.720898	3.153531	0.934130	C	1.024298	-2.078703	-0.678273
H	-6.689305	0.476634	0.181837	H	-0.007304	-2.381602	-0.791366
H	-6.865301	2.815342	0.978315	O	0.470904	0.249611	0.251696
H	-4.800496	4.181735	1.275021	O	-2.192204	-0.903713	-1.706679
C	-0.830522	1.220227	2.589382	H	-1.921604	0.022084	-1.905793
C	-0.278932	1.496635	3.820785	O	-1.097806	1.266368	-3.029414
C	0.878071	2.305731	3.933288	H	-0.565604	1.740676	-2.372221
H	1.300763	2.511038	4.911690	C	-1.721996	1.146015	0.279791
C	1.468583	2.814117	2.801088	C	-0.344295	1.308610	0.103684
H	2.363586	3.426714	2.870790	C	0.157105	2.626206	-0.153237
H	-0.732142	1.084446	4.717084	C	-0.683594	3.707305	-0.276250
H	-1.708225	0.589631	2.511480	Br	2.036705	2.925002	-0.277047
C	-3.480499	2.617423	0.669346	H	-0.267093	4.689602	-0.472565
H	-2.591097	3.222920	0.800749	C	-2.423601	-1.145893	-0.397875
				C	-2.243795	-0.213080	0.617512
B3LYP/6-31G** Energy =			-6817.765302	C	-3.130497	-2.827770	1.225052
B3LYP/6-31G** Free Energy =			-6817.784284	C	-2.847001	-2.465788	-0.064455
M06-2X/LACVP** Derived Free Energy =			-1700.384485	H	-3.453698	-3.839667	1.444366
Number of Imaginary Frequencies =			1 (-376.26)	Br	-2.965308	-3.764708	-1.458536
				C	-2.992793	-1.889455	2.279137
B3LYP/6-31G** Geometry				C	-2.527792	-0.568860	1.975617
				C	-2.612394	2.260714	0.160778
C	3.421498	-2.885698	-0.215870	C	-2.083894	3.558609	-0.132343

C	-2.964992	4.665109	-0.262755	H	0.753090	-3.557314	0.605141	
C	-4.322092	4.502613	-0.113048	H	0.724185	-3.167588	-1.108553	
C	-4.851193	3.220718	0.172372	C	1.727503	-1.213054	2.941175	
H	-2.544492	5.642305	-0.484571	H	1.471507	-0.777468	3.894983	
H	-4.989792	5.352712	-0.215458	O	0.113102	0.454769	1.707807	
H	-5.924193	3.097020	0.284877	O	-0.326213	-0.677673	-1.854710	
C	-2.361687	0.342954	3.054804	H	0.351490	-0.115381	-1.446302	
C	-2.652883	-0.026927	4.349110	O	-2.966395	-2.367365	4.267773	
C	-3.122184	-1.329122	4.641530	H	-3.185292	-1.435767	4.404089	
H	-3.348880	-1.606408	5.666635	C	-0.595903	1.654201	-0.238371	
C	-3.284788	-2.240236	3.623643	C	0.300001	1.446883	0.811322	
H	-3.638289	-3.246532	3.832659	C	1.394803	2.351079	0.965933	
H	-2.518779	0.688685	5.155100	C	1.572003	3.429091	0.139350	
H	-1.999486	1.343151	2.846388	Br	2.672407	2.022954	2.342023	
C	-4.022094	2.130118	0.306384	H	2.416005	4.093787	0.289957	
H	-4.437994	1.152522	0.521899	C	-1.520510	-0.405780	-1.273201	
				C	-1.730905	0.701208	-0.459383	
B3LYP/6-31G** Energy =			-6817.759245	C	-3.836510	-1.101380	-1.014504	
B3LYP/6-31G** Free Energy =			-6817.778864	C	-2.587213	-1.307974	-1.537111	
M06-2X/LACVP** Derived Free Energy =			-1700.374358	H	-4.635613	-1.802775	-1.229112	
Number of Imaginary Frequencies =			1 (-371.77)	Br	-2.241519	-2.835857	-2.624937	
				C	-4.091605	0.020107	-0.182285	
B3LYP/6-31G** Geometry				C	-3.023903	0.931801	0.106026	
				C	-0.429903	2.776515	-1.119854	
C	3.370595	-2.712036	1.649745	C	0.664200	3.677910	-0.920243	
C	2.633200	-2.008149	2.552660	C	0.826399	4.789923	-1.788526	
B	0.597599	-0.906830	1.595584	C	-0.055505	5.009841	-2.821120	
C	-1.674797	-2.421558	3.675668	C	-1.136807	4.120647	-3.024930	
C	-1.650500	-1.721637	2.314579	H	1.662801	5.463219	-1.620818	
H	-0.904993	-1.992271	4.336672	H	0.075695	5.862552	-3.480407	
H	-1.437599	-3.481957	3.547650	H	-1.829810	4.297361	-3.842025	
H	-1.877797	-0.655039	2.435896	C	-3.299398	2.042888	0.949544	
H	-2.432503	-2.157826	1.682874	C	-4.558095	2.239782	1.473652	
O	-0.405003	-1.901230	1.664772	C	-5.610298	1.338789	1.185041	
H	3.265793	-3.794135	1.603629	H	-6.597496	1.506683	1.604647	
H	4.352395	-2.335434	1.374648	C	-5.377403	0.251801	0.373723	
C	2.165691	-2.062108	-0.006340	H	-6.175906	-0.449394	0.146514	
O	1.483095	-1.012813	0.413079	H	-4.745591	3.096072	2.115066	
C	5.348485	-0.883772	-2.656732	H	-2.499495	2.739183	1.177152	
C	4.738381	-2.126769	-2.817950	C	-1.319606	3.033734	-2.199046	
C	3.712583	-2.522779	-1.958852	H	-2.151908	2.359138	-2.363755	
C	3.278889	-1.673295	-0.931138					
C	3.898691	-0.419399	-0.775020	B3LYP/6-31G** Energy =				-6817.767832
C	4.925389	-0.033587	-1.630618	B3LYP/6-31G** Free Energy =				-6817.786331
H	6.148182	-0.577663	-3.324530	M06-2X/LACVP** Derived Free Energy =				-1700.386031
H	5.055577	-2.791456	-3.615761	Number of Imaginary Frequencies =				1 (-390.54)
H	3.242681	-3.488177	-2.107866					
H	3.580695	0.237289	0.027892	B3LYP/6-31G** Geometry				
H	5.398292	0.934810	-1.497303					
C	1.387887	-3.337402	-0.251958	C	-2.681977	3.728309	-0.463885	
H	2.042786	-4.183300	-0.463473	C	-1.469175	3.680107	-1.083382	

B	-0.221985	1.482300	-0.849494	C	5.925694	-2.207740	0.968496
C	0.016017	-0.166576	-4.155406	C	4.765590	-2.985936	1.195987
C	-0.768985	0.265318	-2.924204	H	6.686704	-0.270639	0.453712
H	0.495821	0.710625	-4.614897	H	6.908192	-2.660444	1.063795
H	-0.659083	-0.610069	-4.894511	H	4.866385	-4.033138	1.465880
H	-1.370289	-0.577982	-2.555813	C	0.515596	-0.410432	3.136594
H	-1.454880	1.084022	-3.187601	C	-0.226907	-0.340937	4.294393
O	0.165214	0.666207	-1.936799	C	-1.478910	-0.996232	4.390784
H	-2.798976	4.338403	0.428519	H	-2.054512	-0.931736	5.309283
H	-3.580375	3.630617	-1.069588	C	-1.957910	-1.717522	3.321278
C	-2.381887	1.834101	0.426403	H	-2.915813	-2.227319	3.382271
O	-1.596888	1.151303	-0.379001	H	0.151393	0.220655	5.143698
C	-6.472993	0.473219	0.287681	H	1.473198	0.093965	3.070800
C	-6.053992	1.310210	1.322388	C	3.512193	-2.429429	1.076687
C	-4.734590	1.756904	1.374696	H	2.629889	-3.034627	1.252581
C	-3.809890	1.372107	0.390895				
C	-4.240790	0.524917	-0.643513	B3LYP/6-31G** Energy =			-6817.771251
C	-5.559691	0.081723	-0.693719	B3LYP/6-31G** Free Energy =			-6817.789338
H	-7.501094	0.125924	0.248276	M06-2X/LACVP** Derived Free Energy =			-1700.384372
H	-6.753992	1.615707	2.094288	Number of Imaginary Frequencies =			1 (-379.50)
H	-4.432089	2.403497	2.190601				
H	-3.527689	0.210619	-1.395512	B3LYP/6-31G** Geometry			
H	-5.873892	-0.576170	-1.498524				
C	-1.786488	2.275288	1.749507	C	-2.780602	-2.811999	1.268093
H	-2.432288	2.969887	2.286410	C	-1.663902	-2.707498	0.491494
H	-1.641795	1.383683	2.368101	B	-1.214695	-0.388696	-0.374296
H	-0.808686	2.729385	1.592913	C	-2.835591	0.767020	-3.080992
C	-0.381576	3.152406	-1.458383	C	-1.727294	-0.252485	-2.822695
H	0.472327	3.501406	-2.017978	H	-3.579092	0.716318	-2.273292
O	0.750112	1.527688	0.215709	H	-3.339592	0.504325	-4.019193
O	1.146900	-2.230602	-1.310418	H	-1.041194	-0.265483	-3.676096
H	0.639202	-2.370794	-2.131720	H	-2.154697	-1.259184	-2.710900
O	0.987412	-1.156083	-3.835210	O	-0.953294	0.102409	-1.678794
H	1.537111	-0.766491	-3.136606	H	-2.672303	-2.923104	2.344793
C	2.058102	-0.454820	0.595698	H	-3.651403	-3.308395	0.846391
C	1.946809	0.893383	0.260107	C	-3.222796	-0.775397	1.089902
C	3.137413	1.649880	0.051216	O	-2.655896	-0.347693	-0.023796
C	4.383910	1.091773	0.162416	C	-7.508097	-1.104884	0.690799
Br	2.988323	3.505283	-0.386470	C	-6.938097	-0.968391	1.955800
H	5.267814	1.697470	-0.005878	C	-5.553997	-0.864996	2.097301
C	0.347298	-2.047707	-0.237118	C	-4.716897	-0.890192	0.971601
C	0.807299	-1.246916	0.801989	C	-5.302797	-1.027686	-0.298300
C	-1.692008	-2.558407	1.008073	C	-6.683198	-1.134781	-0.436400
C	-0.927605	-2.670202	-0.122926	H	-8.585498	-1.185381	0.582399
H	-2.662410	-3.039903	1.061266	H	-7.569598	-0.938992	2.838600
Br	-1.589405	-3.639988	-1.635835	H	-5.137898	-0.754400	3.091802
C	-1.210207	-1.818117	2.117379	H	-4.663597	-1.047884	-1.172499
C	0.053695	-1.149422	2.011787	H	-7.117297	-1.237776	-1.426401
C	3.347800	-1.061726	0.723598	C	-2.624096	-0.274704	2.392304
C	4.524703	-0.277230	0.500606	H	-1.552697	-0.467007	2.419104
C	5.804400	-0.880536	0.628905	H	-2.756093	0.812196	2.422508

H	-3.097297	-0.722406	3.265702	C	2.202748	-3.041825	-2.658542
C	-0.849800	-2.133798	-0.289503	C	1.442238	-1.724829	-2.631068
H	0.010599	-2.472997	-0.848805	H	2.961050	-3.005332	-3.448841
O	-0.326994	0.252698	0.579907	H	1.495955	-3.850434	-2.910931
O	1.692504	-0.878097	-1.915097	H	1.002940	-1.543350	-3.624472
H	0.991405	-0.204296	-1.810595	H	2.123131	-0.895321	-2.405178
O	-2.336289	2.082519	-3.233686	O	0.433936	-1.815021	-1.632469
H	-2.035887	2.360314	-2.356085	H	-3.360750	-3.751149	-1.675849
C	1.835009	1.155593	0.139111	H	-4.354862	-2.223854	-1.481578
C	0.458309	1.316796	0.268611	C	-2.150368	-2.083513	-0.044073
C	-0.094487	2.624899	0.129616	O	-1.500875	-1.001015	-0.428889
C	0.683215	3.722898	-0.123578	C	-5.274985	-1.106391	2.754800
Br	-1.985987	2.864503	0.265617	C	-4.887788	-0.191504	1.771186
H	0.225018	4.700700	-0.225475	C	-3.881183	-0.514111	0.866995
C	2.346403	-1.116404	-0.753398	C	-3.243674	-1.767006	0.931317
C	2.440005	-0.203409	0.291905	C	-3.643870	-2.682693	1.914832
C	3.663198	-2.746113	0.498696	C	-4.650476	-2.350885	2.822523
C	2.964700	-2.393606	-0.624803	H	-6.058989	-0.849885	3.460893
H	4.120895	-3.727214	0.566591	H	-5.373595	0.777691	1.708369
Br	2.750097	-3.652900	-2.042308	H	-3.596786	0.189177	0.091885
C	3.768400	-1.844118	1.587899	H	-3.162764	-3.650788	1.992449
C	3.136704	-0.561715	1.491404	H	-4.941473	-3.066975	3.585133
C	2.673012	2.287192	-0.140884	C	-1.334259	-3.350005	0.113651
C	2.086515	3.587095	-0.265679	H	-0.729454	-3.510916	-0.777644
C	2.912718	4.709293	-0.538974	H	-0.643563	-3.207386	0.952950
C	4.271218	4.560290	-0.693174	H	-1.958353	-4.223907	0.302163
C	4.855314	3.276588	-0.582379	C	-1.695764	-1.190259	-2.975586
H	2.448620	5.687795	-0.628570	H	-1.437364	-0.732572	-3.918593
H	4.895920	5.422890	-0.904170	O	-0.185882	0.524273	-1.714909
H	5.927414	3.161987	-0.712980	O	0.451815	-0.647465	1.729312
C	3.230406	0.312980	2.609408	H	-0.249189	-0.037575	1.457500
C	3.916005	-0.056227	3.745507	O	2.888346	-3.313799	-1.450135
C	4.546501	-1.319829	3.831302	H	2.255842	-3.196193	-0.726640
H	5.085100	-1.596834	4.732501	C	0.556302	1.758211	0.200372
C	4.469899	-2.194124	2.771798	C	-0.374892	1.507387	-0.810526
H	4.943997	-3.170725	2.824895	C	-1.511998	2.365677	-0.917945
H	3.971906	0.629569	4.585910	C	-1.701209	3.436289	-0.084463
H	2.748908	1.283081	2.559012	Br	-2.825392	1.983345	-2.245843
C	4.079911	2.170590	-0.313884	H	-2.577313	4.065480	-0.200676
H	4.539009	1.192288	-0.235188	C	1.604214	-0.303066	1.101410
B3LYP/6-31G** Energy =				C	1.742509	0.857421	0.351091
B3LYP/6-31G** Free Energy =				C	3.911321	-0.930458	0.654328
M06-2X/LACVP** Derived Free Energy =				C	2.696521	-1.200856	1.223629
Number of Imaginary Frequencies =				H	4.722325	-1.644250	0.741943
				Br	2.409330	-2.863144	2.119755
B3LYP/6-31G** Geometry				C	4.103715	0.265832	-0.083691
				C	3.002308	1.167621	-0.250910
				C	0.378291	2.872224	1.089054
C	-3.391358	-2.664751	-1.724968	C	-0.761815	3.724812	0.937036
C	-2.594160	-2.004360	-2.611376	C	-0.934126	4.829626	1.812517
B	-0.614173	-0.859628	-1.592988	C	-0.018732	5.088649	2.806216

C	1.107674	4.246860	2.963333	C	0.415625	3.009808	-1.715990
H	-1.804730	5.466717	1.681304	H	-0.446573	3.315219	-2.287285
H	-0.157740	5.935959	3.470702	O	-0.685383	1.503612	0.130609
H	1.826771	4.454379	3.750233	O	-1.220225	-2.348279	-1.181104
C	3.210003	2.346210	-1.018828	H	-0.691730	-2.584781	-1.964807
C	4.438302	2.618610	-1.579528	O	-0.932924	-1.537372	-3.684901
C	5.524308	1.727821	-1.409110	H	-1.508418	-1.053168	-3.072098
H	6.486208	1.954820	-1.858810	C	-2.088299	-0.388176	0.577906
C	5.355814	0.574632	-0.677592	C	-1.915889	0.939924	0.193111
H	6.179319	-0.121960	-0.544778	C	-3.068082	1.747136	-0.033083
H	4.574597	3.525602	-2.161243	C	-4.339086	1.245947	0.077419
H	2.382897	3.033702	-1.157642	Br	-2.826065	3.595735	-0.456778
C	1.301486	3.167847	2.129752	H	-5.194381	1.888156	-0.103076
H	2.167590	2.528356	2.257066	C	-0.423519	-2.095989	-0.116705
B3LYP/6-31G** Energy =			-6817.766395	C	-0.867007	-1.204089	0.852199
B3LYP/6-31G** Free Energy =			-6817.784631	C	1.603981	-2.545813	1.170986
M06-2X/LACVP** Derived Free Energy =			-1700.384639	C	0.838076	-2.733602	0.051189
Number of Imaginary Frequencies =			1 (-404.54)	H	2.564076	-3.041723	1.264882
B3LYP/6-31G** Geometry				Br	1.481860	-3.835804	-1.377118
C	2.763034	3.602783	-0.852195	C	1.134593	-1.712713	2.217691
C	1.523132	3.544396	-1.421691	C	-0.115702	-1.030200	2.055497
B	0.259612	1.400007	-0.955795	C	-3.403005	-0.936264	0.705108
C	0.085283	-0.614480	-4.054101	C	-4.541998	-0.109152	0.439815
C	0.828492	-0.085392	-2.837002	C	-5.847503	-0.656340	0.559417
H	0.772976	-1.140484	-4.724105	C	-6.029414	-1.968540	0.929013
H	-0.348011	0.232725	-4.606697	C	-4.906821	-2.788152	1.196706
H	1.593998	0.638502	-3.152502	H	-6.700998	-0.015731	0.353622
H	1.335586	-0.914699	-2.322307	H	-7.031318	-2.378130	1.016815
O	-0.131200	0.505614	-1.976997	H	-5.056031	-3.823851	1.487703
H	2.948643	4.313478	-0.051093	C	-0.566190	-0.199000	3.118202
H	3.627930	3.385776	-1.475798	C	0.170815	-0.060612	4.273300
C	2.422420	1.875882	0.263900	C	1.407208	-0.734124	4.427393
O	1.631211	1.107392	-0.458800	H	1.977813	-0.616433	5.343692
C	6.496207	0.463742	0.351082	C	1.877098	-1.540624	3.416490
C	6.052819	1.369643	1.314887	H	2.823393	-2.064734	3.521385
C	4.736323	1.828255	1.295193	H	-0.200376	0.570090	5.076003
C	3.840016	1.384668	0.310094	H	-1.512486	0.319310	3.009606
C	4.295204	0.469467	-0.653411	C	-3.629616	-2.286563	1.088704
C	5.610700	0.014755	-0.631617	H	-2.775922	-2.922972	1.293599
H	7.522004	0.107832	0.366977	B3LYP/6-31G** Energy =			-6817.762430
H	6.730825	1.719334	2.087585	B3LYP/6-31G** Free Energy =			-6817.783269
H	4.413933	2.531956	2.054096	M06-2X/LACVP** Derived Free Energy =			-1700.372326
H	3.602198	0.109476	-1.404111	Number of Imaginary Frequencies =			1 (-376.85)
H	5.945591	-0.695146	-1.382221	B3LYP/6-31G** Geometry			
C	1.820731	2.493783	1.514704	C	3.310293	-2.678593	-1.164316
H	2.417039	3.320576	1.900405	C	2.012994	-2.346490	-1.418715
H	0.806133	2.834993	1.313708	B	1.404697	0.031708	-0.816305
H	1.763625	1.716881	2.285601	C	0.836098	2.288221	-3.735295

C	0.469197	1.071818	-2.897700	H	-3.014096	5.425108	0.774519
H	0.106798	2.410225	-4.544295	H	-5.419096	4.873710	0.990018
H	1.822398	2.112522	-4.198197	H	-6.149699	2.490211	0.993609
H	0.415996	0.177421	-3.539303	C	-2.016102	-0.539203	3.040095
H	-0.514803	1.218118	-2.438799	C	-2.120402	-1.228607	4.226692
O	1.482698	0.921113	-1.912701	C	-2.507604	-2.590207	4.241987
H	3.524093	-3.266197	-0.274219	H	-2.585805	-3.120010	5.186484
H	3.994693	-2.842090	-1.993618	C	-2.781405	-3.237002	3.060084
C	3.804396	-0.701395	-0.621309	H	-3.077107	-4.282801	3.056280
O	2.709397	-0.153995	-0.146606	H	-1.902401	-0.723111	5.162794
C	6.651397	-1.561311	2.500387	H	-1.716401	0.502398	3.039099
C	7.023796	-1.712406	1.163685	C	-4.173400	1.712409	0.778005
C	6.111195	-1.439801	0.146487	H	-4.502001	0.678910	0.779401
C	4.809397	-1.011401	0.451090				
C	4.443097	-0.863706	1.798691	B3LYP/6-31G** Energy =			-6817.754700
C	5.358597	-1.135711	2.812389	B3LYP/6-31G** Free Energy =			-6817.772288
H	7.364097	-1.771916	3.292186	M06-2X/LACVP** Derived Free Energy =			-1700.372529
H	8.027195	-2.041607	0.910685	Number of Imaginary Frequencies =			1 (-381.75)
H	6.420695	-1.569198	-0.885113				
H	3.441198	-0.523905	2.032193	B3LYP/6-31G** Geometry			
H	5.062298	-1.010715	3.849689				
C	4.307396	-0.192691	-1.960907	C	-3.192574	3.240225	0.752897
H	4.634198	0.843208	-1.817203	C	-1.865680	3.536954	0.779791
H	5.149196	-0.772090	-2.339709	B	-0.226736	1.563292	0.913494
H	3.501796	-0.182587	-2.692306	C	-0.180237	2.104208	4.198092
C	0.987094	-1.604889	-1.408611	C	0.176286	0.925111	3.303296
H	-0.045006	-1.768586	-1.678611	H	0.605645	2.869625	4.111886
O	0.445998	0.284405	0.245897	H	-0.190325	1.755312	5.237294
O	-2.377304	-0.479483	-1.807605	H	-0.679198	0.240792	3.254302
H	-2.690105	-1.057880	-2.522707	H	1.008900	0.385232	3.769996
O	0.823701	3.484818	-2.981291	O	0.612475	1.272115	1.998793
H	1.332601	3.312414	-2.173692	H	-3.741480	3.351308	-0.177502
C	-1.801702	0.965007	0.505800	H	-3.776375	3.398916	1.657398
C	-0.451301	1.282707	0.353801	C	-2.823427	1.127832	0.742605
C	-0.067599	2.657606	0.424406	O	-1.556021	0.907062	0.995902
C	-0.991198	3.662606	0.551311	C	-4.219524	0.386883	-3.272287
Br	1.782901	3.133403	0.407907	C	-5.073916	0.187969	-2.188083
H	-0.660897	4.694906	0.590415	C	-4.626316	0.428785	-0.889385
C	-2.485304	-1.148887	-0.627307	C	-3.310326	0.857815	-0.653191
C	-2.202903	-0.475592	0.551495	C	-2.451333	1.043029	-1.750496
C	-2.950307	-3.213591	0.593085	C	-2.909632	0.817813	-3.046893
C	-2.844906	-2.523487	-0.584613	H	-4.570523	0.208171	-4.284484
H	-3.228708	-4.261691	0.591880	H	-6.091709	-0.154554	-2.349578
Br	-3.149708	-3.412479	-2.260017	H	-5.308211	0.267474	-0.062382
C	-2.682605	-2.553597	1.818287	H	-1.424939	1.350153	-1.586900
C	-2.295403	-1.172797	1.797292	H	-2.236239	0.976424	-3.884396
C	-2.784600	1.993208	0.646505	C	-3.704715	0.773218	1.927910
C	-2.371998	3.364408	0.649710	H	-3.709490	-0.318281	2.037115
C	-3.346096	4.390308	0.775815	H	-3.267822	1.207632	2.829206
C	-4.681197	4.082609	0.896114	H	-4.734123	1.115595	1.817012
C	-5.094299	2.728710	0.897609	C	-0.622675	3.309982	0.865187

H	0.261711	3.929002	0.834982	H	3.604005	1.421320	-3.947200
O	0.427564	1.362300	-0.362006	H	3.719206	1.437210	-2.174700
O	-0.225585	-1.198823	-2.039593	H	2.444404	-0.540784	-2.939711
H	-1.080781	-1.414743	-2.446489	H	1.327004	0.509823	-3.841704
O	-1.470150	2.661877	3.959594	O	1.126706	0.632611	-1.820803
H	-1.416364	3.158275	3.130591	H	2.389404	-3.259810	1.560674
C	1.948505	-0.504867	-0.468003	H	3.467803	-3.388603	0.084072
C	1.660675	0.853727	-0.583309	C	3.140305	-0.910407	0.838587
C	2.680454	1.735147	-1.048716	O	2.669806	-0.234500	-0.185209
C	3.929362	1.292473	-1.393918	C	7.420105	-1.435111	0.644481
Br	2.288512	3.600538	-1.206123	C	6.738406	-1.721917	1.827579
H	4.680646	1.993988	-1.739824	C	5.356206	-1.557516	1.900481
C	-0.184168	-1.740816	-0.799390	C	4.629606	-1.100209	0.789184
C	0.896129	-1.445688	0.024205	C	5.326505	-0.815402	-0.396615
C	-1.146729	-3.206729	0.902320	C	6.707105	-0.981203	-0.467016
C	-1.206847	-2.611436	-0.329083	H	8.497105	-1.562212	0.589679
H	-1.937414	-3.874845	1.226426	H	7.282606	-2.073623	2.699077
Br	-2.708944	-2.937775	-1.478176	H	4.850506	-1.790821	2.830580
C	-0.043132	-2.954501	1.754316	H	4.773705	-0.456096	-1.255612
C	0.984146	-2.054580	1.317008	H	7.228405	-0.750099	-1.391216
C	3.239015	-1.000140	-0.851805	C	2.475408	-0.662514	2.180489
C	4.242394	-0.086319	-1.309912	H	2.635009	0.392784	2.429894
C	5.522303	-0.575193	-1.685015	H	1.399807	-0.816012	2.112888
C	5.809133	-1.918786	-1.626510	H	2.887807	-1.284520	2.974185
C	4.816955	-2.829507	-1.192802	C	0.812504	-1.824094	-0.949117
H	6.270086	0.136523	-2.025220	H	-0.039897	-1.972789	-1.594017
H	6.789840	-2.283065	-1.917411	O	0.345407	0.329499	0.399396
H	5.041179	-3.891701	-1.158898	O	-2.301496	-0.373884	-1.994507
C	2.071444	-1.807352	2.202403	H	-2.535297	-0.967379	-2.726709
C	2.144762	-2.428645	3.428805	O	2.458908	2.839616	-3.059291
C	1.132183	-3.324164	3.850512	H	2.008708	2.954312	-2.208790
H	1.204697	-3.806959	4.820415	C	-1.895192	1.110402	0.309902
C	0.058585	-3.574592	3.029118	C	-0.526392	1.358700	0.304403
H	-0.729798	-4.255109	3.340224	C	-0.078190	2.712299	0.308710
H	2.988759	-2.227722	4.082401	C	-0.948989	3.768802	0.266517
H	2.843827	-1.111936	1.897596	Br	1.796710	3.067197	0.417411
C	3.569446	-2.384432	-0.816400	H	-0.570188	4.785201	0.265523
H	2.818763	-3.095448	-0.491894	C	-2.555296	-1.004090	-0.820610
B3LYP/6-31G** Energy =			-6817.765272	C	-2.370993	-0.305998	0.364794
B3LYP/6-31G** Free Energy =			-6817.786164	C	-3.225897	-3.010097	0.405179
M06-2X/LACVP** Derived Free Energy =			-1700.375062	C	-2.969797	-2.363590	-0.774317
Number of Imaginary Frequencies =			1 (-388.42)	H	-3.540898	-4.047896	0.404673
B3LYP/6-31G** Geometry				Br	-3.117199	-3.299980	-2.444723
				C	-3.065596	-2.319904	1.632583
				C	-2.623294	-0.955605	1.612590
				C	-2.830491	2.192303	0.273109
C	2.586503	-2.942404	0.538875	C	-2.347589	3.540203	0.239417
C	1.542803	-2.602498	-0.268522	C	-3.274187	4.615604	0.196423
B	1.252906	-0.111696	-0.642308	C	-4.628988	4.377906	0.187223
C	3.025606	1.543715	-3.023199	C	-5.111389	3.047907	0.222416
C	1.963505	0.448517	-2.950305	H	-2.890387	5.632104	0.170429

H	-5.329587	5.206807	0.153228	O	-0.681499	1.304500	-0.722099
H	-6.181990	2.865308	0.215015	O	-0.247703	-0.998700	-2.284001
C	-2.451792	-0.291112	2.859495	H	-0.520104	-0.087101	-2.077699
C	-2.707192	-0.936519	4.048190	O	1.948320	2.988511	3.019883
C	-3.147593	-2.282019	4.061883	H	1.613213	3.378709	2.198884
H	-3.346593	-2.776823	5.007681	C	-2.172591	-0.507504	-0.212789
C	-3.321595	-2.957011	2.876479	C	-1.946496	0.840097	-0.486091
H	-3.657396	-3.990711	2.872174	C	-3.053700	1.719894	-0.647885
H	-2.570991	-0.407824	4.987093	C	-4.346198	1.281590	-0.534577
H	-2.117190	0.740088	2.858900	Br	-2.746108	3.556894	-1.071788
C	-4.237491	1.984706	0.264709	H	-5.169200	1.977288	-0.655472
H	-4.616892	0.969106	0.290703	C	-0.154794	-1.672999	-1.108700
B3LYP/6-31G** Energy =				C	-1.020687	-1.447700	-0.040895
B3LYP/6-31G** Free Energy =				C	1.046719	-3.380194	0.146893
M06-2X/LACVP** Derived Free Energy =				C	0.869610	-2.652896	-0.999306
Number of Imaginary Frequencies =				H	1.836221	-4.121592	0.204489
				Br	2.036802	-2.923994	-2.485813
B3LYP/6-31G** Geometry				C	0.222325	-3.141695	1.275698
				C	-0.811878	-2.152898	1.192503
				C	-3.522589	-1.002107	-0.154580
C	2.943395	3.384210	-0.685924	C	-4.615893	-0.087510	-0.292374
C	1.672797	3.694407	-0.297915	C	-5.951591	-0.567014	-0.221165
B	0.246807	1.685604	0.357495	C	-6.210787	-1.905514	-0.045362
C	0.872425	2.270208	3.614190	C	-5.136283	-2.819811	0.055632
C	0.389423	1.085906	2.787594	H	-6.764893	0.146984	-0.319761
H	1.247032	1.898710	4.574788	H	-7.234585	-2.264018	0.003544
H	0.020724	2.935806	3.823095	H	-5.341979	-3.879812	0.171234
H	-0.302171	0.494704	3.399999	C	-1.591272	-1.908901	2.358209
H	1.238423	0.445408	2.524389	C	-1.374863	-2.614798	3.521308
O	-0.323785	1.479804	1.623798	C	-0.366059	-3.604296	3.590203
H	3.226989	3.518610	-1.726625	H	-0.208452	-4.155194	4.512502
H	3.749700	3.536813	0.027571	C	0.417136	-3.856094	2.488198
C	2.554001	1.329309	-0.667620	H	1.204537	-4.603992	2.527993
O	1.593907	1.110607	0.215387	H	-1.983957	-2.406900	4.396312
C	6.364214	-0.063880	0.776658	H	-2.359674	-1.145902	2.324713
C	6.033906	-0.218881	-0.568440	C	-3.831684	-2.382408	0.002923
C	4.807402	0.243215	-1.048933	H	-3.022883	-3.098906	0.072618
C	3.894505	0.860013	-0.182327	B3LYP/6-31G** Energy =			
C	4.229813	1.006216	1.175671	B3LYP/6-31G** Free Energy =			
C	5.457518	0.551119	1.645663	M06-2X/LACVP** Derived Free Energy =			
H	7.320717	-0.419777	1.147852	Number of Imaginary Frequencies =			
H	6.726703	-0.704680	-1.249044				
H	4.560096	0.093514	-2.093531	B3LYP/6-31G** Geometry			
H	3.532616	1.493713	1.851174				
H	5.708624	0.677121	2.694561	C	-1.385550	1.926151	-2.861418
C	2.198393	1.154007	-2.129917	C	-0.345832	1.052274	-2.749209
H	1.292289	1.713105	-2.366912	B	-0.893187	-1.051026	-1.460390
H	3.005587	1.484309	-2.784623	C	0.247173	-3.760415	-2.951764
H	2.003094	0.094907	-2.322815	C	-1.085935	-3.401337	-2.304468
C	0.510000	3.449004	0.140092	H	0.366697	-4.849712	-2.984653
H	-0.358200	4.048302	0.365797				

H	1.066864	-3.352691	-2.338467	H	2.457052	1.472011	5.363689
H	-1.108230	-3.711728	-1.257266	C	2.983937	-2.253521	0.653624
H	-1.901724	-3.898560	-2.842465	C	4.004755	-3.075703	0.233633
O	-1.318666	-1.998444	-2.431882	C	5.028845	-2.585089	-0.612171
H	-1.336972	2.863657	-2.312827	H	5.826460	-3.246574	-0.935863
H	-1.936050	1.974831	-3.798419	C	5.009817	-1.272193	-1.018683
C	-2.681325	0.710934	-1.678509	H	5.790909	-0.881882	-1.665786
O	-1.913909	-0.096443	-0.979400	H	4.026578	-4.112600	0.555642
C	-4.404195	3.838119	0.732560	H	2.206544	-2.637632	1.304028
C	-3.259681	3.159948	1.159768	C	1.733773	0.591878	3.557897
C	-2.705159	2.150552	0.377878	H	2.576066	0.936692	2.968694
C	-3.291250	1.803128	-0.851519				
C	-4.438764	2.490799	-1.275127	B3LYP/6-31G** Energy =			-6817.764792
C	-4.991387	3.499494	-0.486637	B3LYP/6-31G** Free Energy =			-6817.783994
H	-4.835613	4.623715	1.345853	M06-2X/LACVP** Derived Free Energy =			-1700.377939
H	-2.797488	3.415466	2.108666	Number of Imaginary Frequencies =			1 (-394.82)
H	-1.813947	1.630475	0.707684				
H	-4.911858	2.237780	-2.216925	B3LYP/6-31G** Geometry			
H	-5.883498	4.017572	-0.826043				
C	-3.499210	0.074906	-2.787503	C	2.695922	-2.876184	-0.130562
H	-2.873895	-0.595586	-3.375696	C	1.701618	-2.438981	0.694232
H	-4.281098	-0.532807	-2.316799	B	1.343698	0.076716	0.624796
H	-3.973526	0.812089	-3.435310	C	2.820892	0.868670	3.541084
C	0.247991	0.005091	-2.360399	C	2.370985	1.630748	2.300073
H	1.235000	-0.405289	-2.512095	H	1.962294	0.755072	4.220986
O	-0.199175	-1.635800	-0.341584	H	3.585688	1.454283	4.063976
O	0.872942	2.126833	0.649981	H	3.207184	1.738444	1.600572
H	1.014124	3.005532	0.261174	H	2.049878	2.635850	2.603760
O	0.312465	-3.283326	-4.286968	O	1.260890	1.013230	1.669784
H	-0.077455	-2.396734	-4.249477	H	2.427825	-3.368899	-1.062555
C	0.751998	-0.494062	1.526706	H	3.625024	-3.221270	0.316042
C	-0.266485	-1.249689	0.953312	C	3.162205	-0.917990	-0.813191
C	-1.342576	-1.697704	1.778315	O	2.710899	-0.089281	0.104298
C	-1.404383	-1.394294	3.112813	C	7.458708	-1.230153	-0.712388
Br	-2.730252	-2.752943	1.003623	C	6.775009	-1.475776	-1.902384
H	-2.236377	-1.749806	3.711216	C	5.383508	-1.384887	-1.944385
C	1.879459	1.309651	0.247190	C	4.657206	-1.038378	-0.795190
C	1.875389	-0.015145	0.665502	C	5.353705	-0.790655	0.402106
C	3.939269	0.957984	-1.017005	C	6.741405	-0.889643	0.437908
C	2.924151	1.775365	-0.597314	H	8.541808	-1.303643	-0.679988
H	4.718861	1.341795	-1.666007	H	7.322411	-1.736284	-2.803381
Br	2.856512	3.603859	-1.180031	H	4.874210	-1.572205	-2.882782
C	3.969498	-0.397612	-0.603192	H	4.801803	-0.535046	1.301704
C	2.927008	-0.890527	0.249612	H	7.265905	-0.699426	1.369705
C	0.715090	-0.169549	2.922003	C	2.424305	-0.937615	-2.137890
C	-0.382301	-0.623566	3.721507	H	2.799310	-1.710721	-2.808479
C	-0.424710	-0.300853	5.104203	H	1.355606	-1.074021	-1.977988
C	0.576473	0.442373	5.685097	H	2.553196	0.044679	-2.606304
C	1.665965	0.889289	4.900794	C	0.982312	-1.577179	1.279620
H	-1.265802	-0.654367	5.694705	H	0.165112	-1.611875	1.984220
H	0.534868	0.684782	6.742794	O	0.310495	0.249393	-0.378706

O	-2.642498	-0.654057	-2.142292	C	3.461859	-2.515631	-1.098816
H	-2.964092	-1.361968	-2.724081	C	2.206908	-2.445797	-1.638642
O	3.413903	-0.393031	3.255802	B	0.787346	-0.720452	-0.563325
H	2.749907	-0.927743	2.794810	O	0.248875	0.382572	-1.320371
C	-1.871511	1.164577	-0.207717	O	-0.093007	-1.217295	0.474170
C	-0.510613	1.324885	-0.441521	H	4.275276	-2.049656	-1.651838
C	-0.024524	2.610083	-0.824539	H	3.747613	-3.406819	-0.544896
C	-0.857233	3.691475	-0.945454	C	3.026392	-1.244044	0.422787
Br	1.833174	2.828693	-1.213843	O	2.108799	-0.397364	-0.021988
H	-0.455341	4.655374	-1.238768	C	6.860529	0.671249	0.907333
C	-2.772394	-1.058040	-0.855286	C	5.801241	1.345495	0.297533
C	-2.392700	-0.188322	0.159602	C	4.564892	0.723021	0.137432
C	-3.428579	-2.753622	0.778939	C	4.371189	-0.590884	0.593384
C	-3.289683	-2.340039	-0.518967	C	5.441442	-1.262534	1.205721
H	-3.829271	-3.736722	1.000553	C	6.676106	-0.635915	1.360878
Br	-3.801774	-3.505864	-1.957851	H	7.822168	1.160554	1.030578
C	-3.044686	-1.892804	1.837226	H	5.934629	2.364871	-0.052300
C	-2.515797	-0.596204	1.523707	H	3.740909	1.251499	-0.327599
C	-2.766121	2.273968	-0.335033	H	5.320856	-2.280130	1.561881
C	-2.246632	3.557566	-0.699852	H	7.492896	-1.169026	1.838166
C	-3.130340	4.663158	-0.818867	C	2.573912	-2.227831	1.492065
C	-4.478339	4.515850	-0.587564	H	2.339961	-1.649199	2.392144
C	-4.996829	3.249351	-0.227646	H	3.348407	-2.952985	1.743047
H	-2.719049	5.629757	-1.097681	H	1.666917	-2.750141	1.189919
H	-5.145746	5.367444	-0.680675	C	1.041212	-1.973006	-1.769640
H	-6.061928	3.137345	-0.046443	H	0.221232	-2.165998	-2.444866
C	-2.121503	0.244415	2.603696	C	-2.184538	-0.163120	-0.018911
C	-2.250099	-0.174167	3.909201	C	-1.418764	-1.304512	0.210393
C	-2.780888	-1.451467	4.213420	C	-2.030359	-2.588028	0.193323
H	-2.877585	-1.765053	5.248424	C	-3.364377	-2.744483	-0.075863
C	-3.167582	-2.291685	3.195632	Br	-0.948272	-4.123601	0.542739
H	-3.572173	-3.276486	3.414147	H	-3.811199	-3.732796	-0.074742
H	-1.939103	0.482547	4.716292	C	-1.523853	1.170545	0.088952
H	-1.696611	1.216116	2.381281	C	-0.345855	1.384304	-0.623918
C	-4.165120	2.158860	-0.105431	C	0.241144	2.679389	-0.654573
H	-4.572912	1.192960	0.171383	C	-0.288123	3.722680	0.057635
<u>TSs for Reaction of Cyclic, Lewis acid-activated Boronates</u>				Br	1.789553	2.958673	-1.734600
TS-4Si				H	0.172981	4.703456	0.013870
B3LYP/6-31G** Energy =				C	-2.040479	2.222858	0.921979
B3LYP/6-31G** Free Energy =				C	-1.420298	3.515234	0.885906
M06-2X/LACVP** Derived Free Energy =				C	-1.932498	4.564268	1.695844
M06-2X/LACVP** Derived Solution Free Energy =				C	-2.996229	4.350283	2.540420
M06-2X/LACV3P+** Derived Free Energy =				C	-3.585173	3.066391	2.612637
M06-2X/LACV3P+** Derived Solution Free Energy =				C	-3.122816	2.034451	1.826526
Number of Imaginary Frequencies =				H	-1.454752	5.539054	1.643420
B3LYP/6-31G** Geometry				H	-3.375257	5.157158	3.160388
				H	-4.407442	2.890011	3.299914
				H	-3.578885	1.055183	1.904332
				C	-4.158342	-1.615243	-0.399301
				C	-3.563967	-0.309917	-0.398295
				C	-4.371613	0.783369	-0.820913

C	-5.689186	0.602729	-1.177693	C	-1.030491	-1.487505	0.208303
C	-6.281405	-0.681023	-1.132324	C	-1.294087	-2.883306	0.124611
C	-5.525844	-1.765962	-0.755476	C	-2.537986	-3.355812	-0.202485
H	-3.933075	1.771967	-0.873179	Br	0.128918	-4.107099	0.464115
H	-6.278062	1.455164	-1.503360	H	-2.720782	-4.423712	-0.252478
H	-7.323719	-0.808141	-1.408868	C	-3.339494	-1.037716	-0.441295
H	-5.958960	-2.762563	-0.737009	C	-3.581990	-2.449217	-0.517789
TS-4Re				C	-4.854688	-2.923124	-0.935983
B3LYP/6-31G** Energy =				C	-5.849591	-2.047230	-1.301086
B3LYP/6-31G** Free Energy =				C	-5.602396	-0.654928	-1.270594
M06-2X/LACVP** Derived Free Energy =				C	-4.385597	-0.164522	-0.851898
M06-2X/LACVP** Derived Solution Free Energy =				H	-5.020686	-3.996525	-0.973878
Number of Imaginary Frequencies =				H	-6.816592	-2.419935	-1.625282
1 (-364.28)				H	-6.378900	0.035767	-1.585897
B3LYP/6-31G** Geometry				H	-4.212201	0.904278	-0.845304
C	3.817505	-1.282199	-1.842206	C	-2.392306	3.090795	1.145880
C	2.495605	-1.526504	-2.089203	C	-2.586201	1.673295	1.090187
B	0.948203	-0.364102	-0.524707	C	-3.570697	1.109096	1.949694
O	0.224408	-1.073799	0.499099	C	-4.332299	1.900598	2.780389
O	0.231599	0.746992	-1.136610	C	-4.162105	3.304598	2.799082
H	4.370908	-2.036294	-1.286103	C	-3.206207	3.883698	1.998477
H	4.407101	-0.742900	-2.579611	H	-3.707494	0.034896	1.960799
C	3.415501	0.199207	-0.508013	H	-5.067495	1.439599	3.433494
O	2.254403	-0.063593	0.070590	H	-4.774706	3.917299	3.453580
C	6.702409	-0.439067	2.210785	H	-3.047311	4.958798	2.013672
C	6.915804	0.253928	1.018480	TS-Re for Reaction of Boronate 2 and Propiophenone			
C	5.861301	0.465519	0.131682	B3LYP/6-31G** Energy =			
C	4.575303	-0.012284	0.427386	B3LYP/6-31G** Free Energy =			
C	4.369508	-0.709678	1.628891	M06-2X/LACVP** Derived Free Energy =			
C	5.425910	-0.919169	2.511589	Number of Imaginary Frequencies =			
H	7.524610	-0.601660	2.901384	1 (-342.05)			
H	7.904002	0.633730	0.777276	B3LYP/6-31G** Geometry			
H	6.050498	1.005914	-0.789423	C	3.700073	-1.469162	-1.775489
H	3.374310	-1.071680	1.858993	C	2.372839	-1.641936	-2.022250
H	5.250513	-1.455364	3.439493	B	0.831038	-0.457486	-0.471268
C	3.439096	1.402503	-1.430620	O	0.055523	-1.146732	0.529601
H	3.265794	2.294904	-0.822324	O	0.176200	0.702267	-1.070395
H	2.625195	1.345395	-2.153018	H	4.221740	-2.250476	-1.227261
H	4.388695	1.512203	-1.954822	H	4.309346	-0.927575	-2.494104
C	1.254105	-1.462408	-1.856001	C	3.326115	0.018358	-0.359790
H	0.390907	-1.950313	-2.284296	O	2.139304	-0.226921	0.164032
C	-1.765099	0.877893	0.215792	C	6.436111	-0.750515	2.538879
C	-0.675103	1.467994	-0.428613	C	6.778224	-0.568649	1.197354
C	-0.544008	2.887895	-0.396522	C	5.788614	-0.330234	0.246737
C	-1.379910	3.677295	0.347975	C	4.435247	-0.270235	0.620050
Br	0.792487	3.740793	-1.463428	C	4.101188	-0.470138	1.969452
H	-1.253813	4.754396	0.345471	C	5.095040	-0.702642	2.918860
C	-2.052795	-0.568710	0.000301	H	7.209176	-0.934162	3.279042

H	7.817830	-0.618215	0.887636	Number of Imaginary Frequencies =			1 (-352.02)
H	6.075640	-0.217545	-0.791816				
H	3.058669	-0.438576	2.260849	B3LYP/6-31G** Geometry			
H	4.817005	-0.848894	3.958288				
C	3.369212	1.277392	-1.227891	C	3.458726	-2.281963	-1.248567
H	3.000581	2.059056	-0.553127	C	2.195607	-2.210171	-1.756754
H	2.586252	1.180922	-1.983928	B	0.735622	-0.556483	-0.627206
C	1.129061	-1.525284	-1.809085	O	0.125706	0.549580	-1.324274
H	0.265151	-1.967980	-2.284288	O	-0.094632	-1.122871	0.420567
C	-1.842928	0.891298	0.242681	H	4.261648	-1.806741	-1.807738
C	-0.719994	1.447141	-0.376133	H	3.752608	-3.172399	-0.698316
C	-0.546891	2.862938	-0.334558	C	3.042203	-0.969951	0.299188
C	-1.365335	3.674269	0.405670	O	2.061234	-0.185516	-0.119163
Br	0.818077	3.685911	-1.391914	C	6.746267	1.244775	0.538150
H	-1.205480	4.746979	0.410562	C	5.537240	1.892527	0.285859
C	-2.186996	-0.537863	-0.003336	C	4.350354	1.166666	0.195702
C	-1.208244	-1.502915	0.203733	C	4.353378	-0.227415	0.368585
C	-1.528256	-2.884233	0.082532	C	5.580246	-0.872801	0.602093
C	-2.784036	-3.296009	-0.279524	C	6.763630	-0.143281	0.687273
Br	-0.165553	-4.174747	0.419716	H	7.669146	1.812994	0.607350
H	-3.009934	-4.353887	-0.358080	H	5.512899	2.970176	0.154018
C	-3.483317	-0.941789	-0.480073	H	3.419963	1.672730	-0.029679
C	-3.782891	-2.339679	-0.593584	H	5.624047	-1.951073	0.691972
C	-5.065352	-2.750361	-1.047465	H	7.701106	-0.661994	0.864275
C	-6.015227	-1.825727	-1.412274	C	2.628514	-1.931308	1.425357
C	-5.710861	-0.446172	-1.345116	H	2.219118	-1.257979	2.189741
C	-4.483647	-0.016718	-0.891220	H	1.771388	-2.507545	1.071210
H	-5.274830	-3.814775	-1.113015	C	1.016481	-1.760527	-1.860991
H	-6.989958	-2.150182	-1.764029	H	0.194446	-1.981473	-2.525940
H	-6.451169	0.283476	-1.659926	C	-2.266206	-0.243847	-0.063391
H	-4.266686	1.043556	-0.857067	C	-1.407850	-1.320050	0.151469
C	-2.406176	3.115664	1.186739	C	-1.910615	-2.649633	0.108858
C	-2.648731	1.706574	1.112726	C	-3.224272	-2.912275	-0.177947
C	-3.666256	1.168531	1.950311	Br	-0.711015	-4.097433	0.450752
C	-4.411991	1.977627	2.778433	H	-3.586763	-3.934370	-0.196010
C	-4.192068	3.374387	2.816038	C	-1.721799	1.136357	0.090222
C	-3.204117	3.927859	2.036237	C	-0.554116	1.469176	-0.594307
H	-3.841167	0.099781	1.946382	C	-0.071597	2.807241	-0.560651
H	-5.173316	1.536162	3.414863	C	-0.695600	3.777080	0.178302
H	-4.792543	4.001456	3.468168	Br	1.477355	3.252039	-1.581265
H	-3.007935	4.996450	2.065582	H	-0.311666	4.791449	0.181634
C	4.671108	1.763410	-1.863799	C	-2.336511	2.111997	0.949713
H	4.461201	2.684203	-2.416333	C	-1.823592	3.450535	0.972441
H	5.436459	1.994108	-1.119151	C	-2.433843	4.425050	1.807127
H	5.095105	1.052783	-2.580960	C	-3.491623	4.095492	2.621363
				C	-3.974569	2.766217	2.636851
TS-Si for Reaction of Boronate 2 and Propiophenone				C	-3.415597	1.804114	1.825348
				H	-2.036021	5.436417	1.798238
B3LYP/6-31G** Energy =				H	-3.946623	4.846068	3.260665
B3LYP/6-31G** Free Energy =				H	-4.791686	2.499007	3.300589
M06-2X/LACVP** Derived Free Energy =				H	-3.792158	0.789365	1.860825

C	-4.106424	-1.848358	-0.494424	C	-0.497994	0.924545	-1.040747
C	-3.623867	-0.498135	-0.462628	C	-1.959668	-0.666487	0.195252
C	-4.514973	0.531656	-0.876847	C	-0.975805	-1.466640	0.768610
C	-5.807728	0.247677	-1.256309	C	-3.271222	-1.231507	0.009164
C	-6.290480	-1.081929	-1.242048	C	-3.567327	-2.530644	0.544359
C	-5.451720	-2.106615	-0.872503	C	-4.865227	-3.081450	0.370960
H	-4.160122	1.554342	-0.904885	C	-5.836460	-2.405854	-0.330120
H	-6.462029	1.053528	-1.575656	C	-5.537463	-1.145612	-0.897963
H	-7.314675	-1.290667	-1.536168	C	-4.294722	-0.575611	-0.732383
H	-5.799760	-3.136171	-0.877181	H	-5.071482	-4.060914	0.795434
C	3.644680	-2.859803	2.092715	H	-6.822972	-2.840702	-0.461019
H	3.123471	-3.452570	2.850405	H	-6.294141	-0.623085	-1.476234
H	4.102546	-3.569794	1.395715	H	-4.081686	0.385475	-1.183997
H	4.444606	-2.312632	2.596380	C	-2.046086	3.164010	-0.332296
TS-5Re				C	-2.361925	1.869035	0.200060
B3LYP/6-31G** Energy =			-1445.348409	C	-3.391655	1.794660	1.180841
B3LYP/6-31G** Free Energy =			-1445.359671	C	-4.088167	2.915260	1.575897
M06-2X/LACVP** Derived Free Energy =			-1445.168203	C	-3.801809	4.180754	1.013571
Number of Imaginary Frequencies =			1 (-368.18)	C	-2.796352	4.296541	0.082444
B3LYP/6-31G** Geometry				H	-3.618383	0.837361	1.633699
C	3.939770	-2.025847	-1.387866	H	-4.862005	2.825861	2.333018
C	2.639999	-2.442565	-1.386079	H	-4.363744	5.055258	1.328064
B	1.040014	-0.819414	-0.359291	H	-2.547384	5.265218	-0.343906
O	0.319709	-1.048267	0.857454	C	-0.200827	2.203091	-1.574219
O	0.335849	-0.103026	-1.396046	H	0.643194	2.289678	-2.250199
H	4.607352	-2.437499	-0.633931	C	-0.969695	3.290712	-1.248216
H	4.419800	-1.777589	-2.331673	H	-0.745008	4.268808	-1.665543
C	3.441888	-0.134483	-0.673013	C	-1.275831	-2.744141	1.304448
O	2.348760	-0.264007	0.049403	H	-0.471932	-3.292156	1.785286
C	6.910225	0.593166	1.782904	C	-2.546668	-3.253049	1.216272
C	7.003148	0.729405	0.396921	H	-2.780062	-4.228528	1.634947
C	5.889340	0.494323	-0.407049	TS-5Si			
C	4.663355	0.119221	0.164748	B3LYP/6-31G** Energy =			-1445.348930
C	4.579366	-0.016419	1.560007	B3LYP/6-31G** Free Energy =			-1445.360603
C	5.694572	0.220241	2.359908	M06-2X/LACVP** Derived Free Energy =			-1445.168554
H	7.778278	0.778814	2.408375	Number of Imaginary Frequencies =			1 (-380.84)
H	7.943616	1.021178	-0.060782	B3LYP/6-31G** Geometry			
H	5.985150	0.602743	-1.482077	C	3.868725	-2.491205	-0.567231
H	3.629810	-0.295049	2.001215	C	2.605852	-2.681314	-1.053304
H	5.612362	0.117921	3.437863	B	1.016927	-0.843347	-0.459046
C	3.302793	0.606009	-1.992857	O	0.337322	-0.069808	-1.453854
H	3.089549	1.655818	-1.761310	O	0.263865	-1.145466	0.731521
H	2.462274	0.211120	-2.562367	H	4.637223	-2.166824	-1.265833
H	4.210618	0.565710	-2.594557	H	4.230187	-3.130866	0.234673
C	1.409975	-2.374750	-1.097158	C	3.350808	-0.785646	0.483707
H	0.572018	-3.047142	-1.211450	O	2.324860	-0.238411	-0.140210
C	-1.611170	0.717617	-0.231219	C	6.973901	1.480802	-0.099947

C	5.845224	1.728214	-0.884439	B3LYP/6-31G** Energy =			-6626.869999
C	4.679526	0.991694	-0.691052	B3LYP/6-31G** Free Energy =			-6626.886462
C	4.623076	-0.006794	0.294690	M06-2X/LACVP** Derived Free Energy =			-1509.509604
C	5.762012	-0.249027	1.078321	Number of Imaginary Frequencies =			1 (-361.34)
C	6.927325	0.490437	0.881943				
H	7.881842	2.056998	-0.250950	B3LYP/6-31G** Geometry			
H	5.871365	2.500878	-1.647070				
H	3.796867	1.184452	-1.288992	C	3.499192	-2.270556	-1.036985
H	5.748855	-1.014071	1.846887	C	2.208067	-2.340310	-1.515648
H	7.798428	0.293048	1.499470	B	0.708162	-0.665453	-0.476834
C	3.070327	-1.388339	1.850784	O	0.138789	0.388634	-1.281559
H	2.851862	-0.563922	2.538535	O	-0.177342	-1.173737	0.551077
H	3.917219	-1.950612	2.244224	H	3.841862	-3.131521	-0.462502
H	2.188597	-2.025481	1.810354	C	2.960938	-1.105682	0.497746
C	1.404976	-2.361473	-1.286379	O	2.000260	-0.282992	0.066044
H	0.595165	-2.803469	-1.846956	C	6.614767	1.055682	1.278416
C	-1.987912	-0.621578	0.069060	C	5.550160	1.673906	0.620985
C	-1.048031	-1.507105	0.588392	C	4.373094	0.972793	0.365144
C	-1.572094	0.772558	-0.253432	C	4.242423	-0.365193	0.770801
C	-0.440139	0.976338	-1.036506	C	5.319581	-0.980218	1.429687
C	-2.268109	1.928257	0.250184	C	6.495373	-0.275510	1.681183
C	-1.872015	3.238451	-0.182793	H	7.529680	1.605914	1.477340
C	-2.567133	4.377758	0.303257	H	5.632156	2.710615	0.308058
C	-3.594429	4.251473	1.209044	H	3.546023	1.458215	-0.139258
C	-3.960193	2.966842	1.673305	H	5.250133	-2.014373	1.749743
C	-3.318202	1.840637	1.207860	H	7.316445	-0.766641	2.194927
H	-2.258404	5.359355	-0.047868	C	2.530147	-2.135184	1.535981
H	-4.113632	5.131114	1.577995	H	3.331313	-2.831273	1.787370
H	-4.752451	2.866445	2.409758	H	1.656589	-2.694426	1.203670
H	-3.605688	0.866861	1.585194	H	2.248888	-1.592977	2.444597
C	-3.678430	-2.436258	0.249745	C	1.010306	-1.965162	-1.643487
C	-3.319610	-1.112323	-0.174952	H	0.177079	-2.247535	-2.267972
C	-4.303475	-0.355103	-0.872343	C	-2.295317	-0.207685	-0.009877
C	-5.566870	-0.855163	-1.096394	C	-1.493404	-1.314473	0.263231
C	-5.927613	-2.142570	-0.635106	C	-2.059807	-2.619008	0.266118
C	-4.996296	-2.914095	0.019490	C	-3.382125	-2.829647	-0.023259
H	-4.042918	0.628166	-1.244009	Br	-0.932455	-4.108483	0.667699
H	-6.292213	-0.255645	-1.639007	H	-3.793129	-3.833244	-0.005789
H	-6.929890	-2.521844	-0.811244	C	-1.685360	1.151279	0.074182
H	-5.249818	-3.914430	0.361659	C	-0.502757	1.387568	-0.623616
C	-0.058459	2.270509	-1.467170	C	0.040721	2.700812	-0.675587
H	0.806893	2.352467	-2.116420	C	-0.537460	3.742737	-0.000327
C	-0.772154	3.372075	-1.070455	Br	1.602535	3.006803	-1.728813
H	-0.484992	4.364912	-1.406849	H	-0.108560	4.737190	-0.059897
C	-1.408186	-2.810491	1.010256	C	-2.253922	2.205497	0.869851
H	-0.635870	-3.435357	1.447090	C	-1.678083	3.517358	0.811481
C	-2.698139	-3.255002	0.868720	C	-2.241775	4.568105	1.584131
H	-2.977221	-4.251328	1.201412	C	-3.313538	4.338505	2.414345
				C	-3.859161	3.037046	2.509182
				C	-3.346440	2.002317	1.758801
				H	-1.797035	5.557374	1.515158

TS-6*Si* Syn

H	-3.732066	5.147115	3.006014	H	0.314159	-2.003103	-2.452813
H	-4.687938	2.849568	3.185623	C	-2.271459	-0.268874	-0.010272
H	-3.769786	1.009928	1.853284	C	-1.410547	-1.337399	0.232917
C	-4.209351	-1.738158	-0.389349	C	-1.908150	-2.669424	0.223760
C	-3.661033	-0.413054	-0.411085	C	-3.221807	-2.944065	-0.049830
C	-4.498056	0.639520	-0.878076	Br	-0.699070	-4.103349	0.590331
C	-5.800932	0.402744	-1.255315	H	-3.580614	-3.967563	-0.041304
C	-6.348759	-0.899635	-1.187169	C	-1.732122	1.119287	0.088126
C	-5.563327	-1.946812	-0.767147	C	-0.573625	1.430228	-0.620865
H	-4.093709	1.641457	-0.948819	C	-0.105471	2.772427	-0.666676
H	-6.412628	1.224926	-1.614946	C	-0.730564	3.771743	0.030834
H	-7.380233	-1.070788	-1.480122	Br	1.412416	3.179056	-1.750202
H	-5.961198	-2.957494	-0.730359	H	-0.360490	4.789798	-0.023606
C	4.559165	-1.641151	-1.930918	C	-2.345723	2.130381	0.906037
H	5.482306	-1.471037	-1.373782	C	-1.843299	3.472510	0.857609
H	4.786987	-2.303987	-2.772450	C	-2.452224	4.480610	1.652406
H	4.209605	-0.686763	-2.331763	C	-3.497572	4.181823	2.494254
TS-6Si Anti				C	-3.970010	2.851375	2.578559
B3LYP/6-31G** Energy =				C	-3.412665	1.856135	1.806846
B3LYP/6-31G** Free Energy =				H	-2.063379	5.493617	1.590717
M06-2X/LACVP** Derived Free Energy =				H	-3.950999	4.958544	3.102694
Number of Imaginary Frequencies =				H	-4.777480	2.610101	3.263675
				H	-3.780244	0.841033	1.893203
				C	-4.109152	-1.891258	-0.387984
B3LYP/6-31G** Geometry				C	-3.630394	-0.539202	-0.396565
C	3.586512	-2.068851	-1.093358	C	-4.527433	0.474933	-0.836212
C	2.314981	-2.127692	-1.625061	C	-5.821484	0.176091	-1.199730
B	0.743140	-0.561636	-0.520099	C	-6.300246	-1.153748	-1.144071
O	0.113881	0.477163	-1.299251	C	-5.455688	-2.164584	-0.750526
O	-0.099442	-1.134514	0.505487	H	-4.176880	1.497563	-0.897057
H	4.255083	-1.392519	-1.630013	H	-6.479904	0.970484	-1.538738
C	3.017878	-0.904536	0.452500	H	-7.325525	-1.373975	-1.425764
O	2.023672	-0.129146	0.011819	H	-5.799900	-3.195087	-0.723814
C	6.636333	1.394030	0.979575	C	4.279525	-3.326581	-0.595195
C	5.570671	1.901532	0.232488	H	5.112685	-3.070524	0.064483
C	4.405261	1.157822	0.067460	H	3.591707	-3.991571	-0.069489
C	4.285677	-0.115327	0.651306	H	4.697188	-3.877322	-1.444656
C	5.356375	-0.611541	1.412319	TS-6Re Syn			
C	6.522416	0.137205	1.572641	B3LYP/6-31G** Energy =			
H	7.543152	1.977901	1.106604	B3LYP/6-31G** Free Energy =			
H	5.642999	2.887138	-0.217870	M06-2X/LACVP** Derived Free Energy =			
H	3.568895	1.567906	-0.486402	Number of Imaginary Frequencies =			
H	5.284680	-1.576420	1.900770				
H	7.337872	-0.261898	2.168495	B3LYP/6-31G** Geometry			
C	2.634274	-1.903921	1.532966	C	3.738989	-1.361670	-1.594596
H	2.343863	-1.327801	2.417865	C	2.420566	-1.530737	-1.953145
H	3.454251	-2.563852	1.812118	B	0.843461	-0.290126	-0.485751
H	1.773142	-2.500062	1.232569	O	0.132493	-0.987425	0.555740
C	1.107738	-1.788124	-1.754611				

O	0.090649	0.767467	-1.145882	H	-5.094482	3.916755	3.256716
H	4.391063	-0.887918	-2.328249	H	-3.364896	4.965557	1.824835
C	3.294351	0.276937	-0.520886	C	4.387242	-2.469533	-0.775990
O	2.129626	0.071629	0.094576	H	5.317967	-2.124105	-0.321823
C	6.545836	0.310625	2.316666	H	3.709188	-2.810402	0.010351
C	6.773400	0.703595	0.996478	H	4.620552	-3.324845	-1.419280
C	5.730021	0.694256	0.072507				
C	4.440420	0.290721	0.454383	TS-6Re Anti			
C	4.222664	-0.106581	1.783128				
C	5.267502	-0.093433	2.704947	B3LYP/6-31G** Energy =			-6626.861238
H	7.358724	0.321694	3.036628	B3LYP/6-31G** Free Energy =			-6626.878906
H	7.763857	1.021485	0.684787	M06-2X/LACVP** Derived Free Energy =			-1509.503011
H	5.930137	1.001443	-0.948551	Number of Imaginary Frequencies =			1 (-370.36)
H	3.225800	-0.408800	2.080744				
H	5.080277	-0.396460	3.730794	B3LYP/6-31G** Geometry			
C	3.287325	1.355723	-1.591857				
H	3.088586	2.311514	-1.099826	C	3.783075	-1.255794	-1.572403
H	2.481318	1.188973	-2.306155	C	2.464476	-1.509150	-1.883661
H	4.237001	1.425530	-2.123667	B	0.853826	-0.325227	-0.400265
C	1.172175	-1.430382	-1.793718	O	0.100761	-1.047420	0.592627
H	0.310286	-1.892159	-2.251011	O	0.140577	0.761034	-1.057858
C	-1.926707	0.873792	0.175911	H	4.206869	-1.975257	-0.868917
C	-0.843947	1.479287	-0.466497	C	3.307601	0.259880	-0.333676
C	-0.745530	2.901674	-0.462434	O	2.128790	-0.013607	0.228518
C	-1.619472	3.686867	0.241344	C	6.495564	-0.234680	2.535066
Br	0.610350	3.755994	-1.502540	C	6.688028	0.586650	1.425347
H	-1.519061	4.766541	0.218330	C	5.665322	0.757060	0.490600
C	-2.155703	-0.590116	0.008571	C	4.433174	0.106936	0.656096
C	-1.101137	-1.458970	0.265784	C	4.246551	-0.713755	1.781913
C	-1.305299	-2.866556	0.230858	C	5.269338	-0.882363	2.710073
C	-2.523513	-3.402760	-0.093990	H	7.291445	-0.365194	3.262244
Br	0.167874	-4.011950	0.633722	H	7.632873	1.103397	1.285763
H	-2.662410	-4.478442	-0.106848	H	5.831791	1.415415	-0.354511
C	-3.414964	-1.128879	-0.431898	H	3.288126	-1.201142	1.919826
C	-3.598693	-2.551389	-0.456664	H	5.107678	-1.516191	3.576933
C	-4.845070	-3.092311	-0.873013	C	3.314917	1.471723	-1.243676
C	-5.868959	-2.272537	-1.285299	H	3.096139	2.348327	-0.627430
C	-5.678605	-0.871198	-1.306466	H	2.518421	1.399075	-1.983973
C	-4.488960	-0.315749	-0.890903	H	4.268652	1.627665	-1.745218
H	-4.967154	-4.172244	-0.871462	C	1.216108	-1.461396	-1.709950
H	-6.815145	-2.696779	-1.607545	H	0.370361	-1.994133	-2.117147
H	-6.477435	-0.225506	-1.659254	C	-1.913369	0.865849	0.209195
H	-4.358440	0.758758	-0.924128	C	-0.810865	1.471077	-0.399014
C	-2.636671	3.093168	1.027989	C	-0.713699	2.894213	-0.383484
C	-2.789047	1.669308	1.009748	C	-1.595351	3.674041	0.316960
C	-3.774843	1.102104	1.865886	Br	0.641827	3.764974	-1.411077
C	-4.577775	1.894876	2.655494	H	-1.493544	4.753719	0.303298
C	-4.449564	3.303243	2.634818	C	-2.164418	-0.588455	0.000307
C	-3.492657	3.886342	1.838181	C	-1.134730	-1.485501	0.259571
H	-3.880088	0.025171	1.907756	C	-1.370152	-2.887018	0.185434
H	-5.313204	1.431654	3.306763	C	-2.591610	-3.386908	-0.182977

Br	0.061202	-4.078785	0.597912	C	3.011827	-0.570962	0.395894
H	-2.753280	-4.458602	-0.225039	C	2.680621	-1.566485	-0.520352
C	-3.424304	-1.087031	-0.484221	C	2.801174	-2.937015	-0.161451
C	-3.638434	-2.503706	-0.550706	C	3.202479	-3.311360	1.093903
C	-4.885352	-3.006286	-1.011198	Br	2.393188	-4.268478	-1.463895
C	-5.880786	-2.153718	-1.426405	H	3.297323	-4.362164	1.345306
C	-5.659798	-0.756872	-1.405624	C	2.973028	0.848077	-0.063134
C	-4.469196	-0.238743	-0.946933	C	1.821770	1.307749	-0.701047
H	-5.030470	-4.082954	-1.040752	C	1.720198	2.673011	-1.083654
H	-6.827608	-2.548336	-1.782625	C	2.740408	3.561145	-0.868875
H	-6.435611	-0.084667	-1.760232	Br	0.116986	3.260593	-1.941050
H	-4.315537	0.833102	-0.948636	H	2.634283	4.599702	-1.162980
C	-2.623893	3.075617	1.084664	C	4.094267	1.736515	0.083132
C	-2.784595	1.653665	1.040966	C	3.958957	3.112084	-0.300133
C	-3.788242	1.078575	1.870613	C	5.057062	3.999694	-0.139296
C	-4.597438	1.863434	2.661711	C	6.261959	3.551410	0.347694
C	-4.458861	3.271007	2.667610	C	6.416910	2.186044	0.683434
C	-3.486466	3.861128	1.895181	C	5.365847	1.305754	0.556358
H	-3.901511	0.001796	1.891734	H	4.927822	5.040395	-0.424599
H	-5.346021	1.394498	3.293603	H	7.097025	4.236268	0.460364
H	-5.108776	3.878194	3.290505	H	7.377599	1.825920	1.039651
H	-3.351748	4.939546	1.901719	H	5.507434	0.262108	0.807662
C	4.775014	-0.799250	-2.628241	C	3.454302	-2.328270	2.084430
H	5.136733	-1.666864	-3.190232	C	3.336189	-0.939567	1.747228
H	4.327177	-0.102287	-3.339052	C	3.505647	0.011330	2.792442
H	5.646021	-0.331002	-2.160876	C	3.814288	-0.384175	4.075076
TS-7Re				C	3.975040	-1.753533	4.390471
B3LYP/6-31G** Energy =				C	3.792565	-2.702927	3.412657
B3LYP/6-31G** Free Energy =				H	3.375257	1.063934	2.573101
M06-2X/LACVP** Derived Free Energy =				H	3.929540	0.364015	4.853900
Number of Imaginary Frequencies =				H	4.226477	-2.051298	5.404023
				H	3.889584	-3.760616	3.643098
				C	-2.130620	-0.284390	-1.415305
				H	-3.140364	-0.253197	-1.843532
B3LYP/6-31G** Geometry				H	-1.606649	0.647120	-1.645901
				Si	-3.379990	-0.065253	1.066858
C	-1.528200	-0.886405	-4.046921	C	-2.769041	-0.815587	2.720700
C	-0.289115	-0.334961	-3.999300	C	-1.513708	-0.025146	3.160234
B	0.968250	-0.618170	-1.872123	H	-1.729600	1.036230	3.315336
O	0.774130	0.484454	-0.946631	H	-1.133387	-0.429960	4.107662
O	2.257331	-1.250096	-1.771616	H	-0.710011	-0.102079	2.421031
H	-2.404861	-0.242484	-4.018186	C	-3.861176	-0.676938	3.802560
H	-1.661952	-1.824093	-4.583518	H	-4.144885	0.369724	3.961366
C	-1.375016	-1.479428	-2.011525	H	-4.768951	-1.235165	3.548773
O	-0.110063	-1.621240	-1.727786	H	-3.493515	-1.062491	4.762769
C	-2.114778	-2.796040	-2.059568	C	-2.363813	-2.298047	2.567786
H	-1.520785	-3.545477	-2.584995	H	-1.928974	-2.662115	3.508398
H	-3.100441	-2.696731	-2.517904	H	-3.213391	-2.949616	2.338600
H	-2.251647	-3.132726	-1.026021	H	-1.613111	-2.428166	1.783006
C	0.847247	-0.057830	-3.502366	C	-7.484220	-1.630626	-0.688213
H	1.704635	0.453344	-3.917924	C	-6.714837	-2.470135	0.118951

C	-5.514058	-2.010972	0.661283	H	0.340704	-4.294002	-0.002145
C	-5.048066	-0.702878	0.423766	C	3.802613	-0.140921	-0.077554
C	-5.846339	0.123186	-0.393568	C	3.355918	1.137976	0.249488
C	-7.045577	-0.331784	-0.945350	C	4.261574	2.234118	0.225057
H	-8.419613	-1.986026	-1.111266	C	5.570650	2.077992	-0.146726
H	-7.050188	-3.482312	0.327520	Br	3.621170	3.967364	0.714651
H	-4.935879	-2.687557	1.282057	H	6.244592	2.927819	-0.148416
H	-5.533075	1.144100	-0.593006	C	5.144449	-0.311744	-0.566082
H	-7.638655	0.330207	-1.570383	C	6.038656	0.809561	-0.573368
C	-3.497025	4.636349	1.343330	C	7.371539	0.645007	-1.037841
C	-4.575131	3.890126	1.824535	C	7.808793	-0.568264	-1.514099
C	-4.559768	2.497949	1.727746	C	6.918479	-1.666762	-1.553002
C	-3.463946	1.817109	1.162283	C	5.626845	-1.543407	-1.092080
C	-2.387313	2.590739	0.691907	H	8.035352	1.505425	-1.021981
C	-2.404285	3.984099	0.771612	H	8.827252	-0.681784	-1.873185
H	-3.512343	5.720719	1.410654	H	7.255081	-2.617261	-1.956493
H	-5.430283	4.392673	2.268254	H	4.957251	-2.392918	-1.140988
H	-5.419382	1.938302	2.088973	C	2.234675	-3.569006	0.771122
H	-1.521962	2.104087	0.254285	C	3.151535	-2.466705	0.795886
H	-1.564982	4.547367	0.374646	C	4.312245	-2.590776	1.610140
O	-2.167662	-0.503494	-0.018798	C	4.568160	-3.743027	2.319891
TS-8Si				C	3.681091	-4.842638	2.256684
B3LYP/6-31G** Energy =				C	2.536506	-4.750729	1.499955
				H	4.997690	-1.755057	1.680415
B3LYP/6-31G** Free Energy =				H	5.458049	-3.804947	2.939513
				H	3.898402	-5.748407	2.814885
M06-2X/LACVP** Derived Free Energy =				H	1.834055	-5.579050	1.456397
				C	-2.332391	1.980581	1.195416
Number of Imaginary Frequencies =				H	-2.730341	2.928503	1.580119
				H	-2.366217	1.252137	2.021930
B3LYP/6-31G** Geometry				Si	-4.449192	0.557380	0.128985
C	-1.057873	3.736277	-0.532748	C	-5.981834	1.720755	0.145309
C	0.027248	3.276420	-1.200801	C	-5.935684	2.702921	1.337052
B	1.029686	1.154280	-0.380600	H	-5.937293	2.199944	2.309007
O	2.070623	1.357345	0.615220	H	-5.047203	3.342311	1.295973
O	1.215873	-0.022073	-1.188352	H	-6.810823	3.366446	1.313268
H	-0.961672	4.604600	0.115096	C	-5.958599	2.552470	-1.158938
H	-2.045385	3.557682	-0.952889	H	-5.043077	3.147763	-1.245175
C	-0.851287	2.169652	0.885170	H	-6.030636	1.920030	-2.048853
O	-0.302563	1.151781	0.280424	H	-6.808047	3.248637	-1.174563
C	-0.074268	2.899063	1.964815	C	-7.296163	0.911197	0.182752
H	0.098624	2.191542	2.784341	H	-8.158576	1.589350	0.128634
H	-0.643011	3.747615	2.351493	H	-7.369494	0.224293	-0.666928
H	0.903365	3.227356	1.614699	H	-7.402276	0.320422	1.097955
C	0.963659	2.465984	-1.493102	C	-4.349563	-1.877453	-3.893620
H	1.680289	2.478162	-2.303040	C	-3.508090	-0.776896	-3.722949
C	2.846116	-1.279223	0.043896	C	-3.528860	-0.058474	-2.525671
C	1.601045	-1.167254	-0.571134	C	-4.388555	-0.423531	-1.474102
C	0.714824	-2.279458	-0.594926	C	-5.221091	-1.542522	-1.664796
C	1.027166	-3.454712	0.035934	C	-5.206210	-2.261418	-2.860597
Br	-0.931639	-2.100492	-1.536979	H	-4.331367	-2.438473	-4.823736

H	-2.828643	-0.482380	-4.517600	Br	-3.588233	4.273393	-0.673289
H	-2.854746	0.782322	-2.396327	H	-5.878802	3.507196	1.029046
H	-5.878639	-1.873335	-0.864176	C	-5.100072	0.149065	1.050595
H	-5.854730	-3.124451	-2.982647	C	-5.796920	1.363808	1.360551
C	-3.948220	-2.443845	3.735133	C	-6.904830	1.333150	2.249760
C	-4.963175	-1.488889	3.793683	C	-7.300939	0.158948	2.845303
C	-5.138433	-0.591047	2.739188	C	-6.590996	-1.034749	2.578135
C	-4.314818	-0.625595	1.598099	C	-5.524955	-1.040599	1.706255
C	-3.298771	-1.604793	1.560204	H	-7.425120	2.263847	2.460304
C	-3.115711	-2.497895	2.616232	H	-8.144853	0.147676	3.528546
H	-3.807784	-3.142272	4.555375	H	-6.886172	-1.957114	3.069817
H	-5.618250	-1.440747	4.659113	H	-4.988509	-1.963152	1.523328
H	-5.936071	0.140662	2.814982	C	-3.311829	-3.377820	-1.146418
H	-2.641665	-1.681167	0.698064	C	-3.991075	-2.140192	-0.905244
H	-2.322890	-3.238447	2.561867	C	-5.349761	-2.042547	-1.318309
O	-3.066473	1.532757	0.088070	C	-5.997788	-3.108716	-1.901399
TS-7Si				C	-5.330768	-4.339912	-2.101047
B3LYP/6-31G** Energy =				C	-4.012136	-4.465993	-1.732251
B3LYP/6-31G** Free Energy =				H	-5.874007	-1.103896	-1.186801
M06-2X/LACVP** Derived Free Energy =				H	-7.031185	-2.999856	-2.217382
Number of Imaginary Frequencies =				H	-5.855928	-5.174708	-2.555402
				H	-3.478173	-5.398599	-1.894790
B3LYP/6-31G** Geometry				C	1.939641	0.454058	-0.761376
				H	1.754552	-0.486188	-1.297666
				H	1.543991	0.317586	0.249002
				Si	4.562531	-0.209151	-0.189778
C	1.539827	3.175706	-0.268517	C	5.145454	-1.357483	-1.616099
C	0.409745	2.909142	0.425607	C	3.976026	-2.180738	-2.204503
B	-1.156218	1.178129	-0.462024	H	3.414206	-2.750669	-1.458388
O	-2.417046	1.501465	-1.083772	H	3.258795	-1.535531	-2.723296
O	-1.137449	-0.087024	0.267161	H	4.355913	-2.895755	-2.946611
H	1.546777	4.034156	-0.938282	C	5.720223	-0.473364	-2.747354
H	2.511539	2.854949	0.097466	H	4.974396	0.232829	-3.128023
C	1.124723	1.496829	-1.513156	H	6.590385	0.101881	-2.416968
O	-0.165544	1.304066	-1.568822	H	6.038039	-1.102403	-3.589626
C	1.704145	2.030968	-2.802174	C	6.265581	-2.299873	-1.121420
H	1.682065	1.216251	-3.537661	H	6.644790	-2.902320	-1.957664
H	2.737357	2.351590	-2.678246	H	7.113623	-1.737580	-0.714943
H	1.085309	2.844019	-3.184417	H	5.926327	-2.993884	-0.346663
C	-0.718550	2.375388	0.679653	C	7.992830	2.809094	0.953011
H	-1.411748	2.582552	1.484733	C	7.018320	3.177997	0.024165
C	-3.278976	-1.043890	-0.304420	C	5.994445	2.288798	-0.304877
C	-1.895839	-1.137868	-0.132789	C	5.915212	1.013957	0.285895
C	-1.264060	-2.403784	-0.315001	C	6.905649	0.667089	1.223874
C	-1.944615	-3.491953	-0.792844	C	7.934676	1.550721	1.553377
Br	0.568238	-2.612483	0.198568	H	8.790747	3.500017	1.210052
H	-1.435204	-4.441459	-0.917657	H	7.055598	4.158388	-0.442807
C	-3.989025	0.190158	0.137151	H	5.241389	2.591519	-1.026978
C	-3.528264	1.420453	-0.318398	H	6.867403	-0.300697	1.717835
C	-4.234290	2.612613	0.006591	H	8.685914	1.259506	2.282138
C	-5.350757	2.587734	0.800270	C	3.013310	-2.267598	3.762146

C	3.265277	-3.064626	2.645687	C	-8.239029	-0.727238	-0.702316
C	3.741557	-2.486505	1.467263	C	-7.643250	0.552592	-0.793291
C	3.979226	-1.102631	1.370472	C	-6.299400	0.722722	-0.545812
C	3.723033	-0.322428	2.516387	H	-7.901881	-2.811872	-0.335027
C	3.243627	-0.892858	3.695428	H	-9.301565	-0.845878	-0.892215
H	2.638926	-2.714726	4.678410	H	-8.251193	1.410105	-1.066467
H	3.088871	-4.135382	2.688869	H	-5.858474	1.708411	-0.629159
H	3.929008	-3.131964	0.615465	C	-3.258297	3.381304	1.073476
H	3.908378	0.748630	2.491693	C	-3.847270	2.076382	1.088812
H	3.051993	-0.265609	4.561335	C	-4.847259	1.818367	2.069017
O	3.315338	0.787397	-0.755241	C	-5.261170	2.798509	2.943255
TS-8Re				C	-4.705069	4.098059	2.891084
B3LYP/6-31G** Energy =				C	-3.718771	4.377884	1.975321
B3LYP/6-31G** Free Energy =				H	-5.276048	0.826525	2.137152
M06-2X/LACVP** Derived Free Energy =				H	-6.018728	2.567704	3.686499
Number of Imaginary Frequencies =				H	-5.046309	4.863265	3.581794
				H	-3.263450	5.363891	1.934324
B3LYP/6-31G** Geometry				C	2.517417	-1.326281	-0.534285
C	1.069470	-2.732271	-2.429335	H	3.280837	-1.667657	-1.243371
C	-0.275364	-2.553037	-2.449561	H	2.297123	-2.128647	0.178502
B	-1.228817	-0.863924	-0.858700	Si	4.506563	0.316610	0.501832
O	-1.938794	-1.304364	0.319065	C	4.331168	2.137357	1.074710
O	-1.705624	0.388517	-1.428236	C	3.591492	2.143636	2.433979
H	1.473275	-3.544167	-1.824908	H	4.135951	1.586837	3.202397
H	1.670269	-2.449262	-3.289768	H	3.478898	3.176818	2.788738
C	1.235709	-0.958587	-1.280257	H	2.588273	1.713180	2.350181
O	0.203890	-0.892625	-0.483640	C	5.733700	2.756046	1.263145
C	1.379401	0.041128	-2.402371	H	6.335625	2.188746	1.982195
H	0.472378	0.110189	-3.002147	H	6.294032	2.807062	0.323349
H	2.240427	-0.196799	-3.029917	H	5.645117	3.779650	1.650661
H	1.539724	1.018826	-1.943997	C	3.511226	2.997493	0.087846
C	-1.395202	-2.074303	-2.084262	H	3.402580	4.013109	0.492029
H	-2.401019	-2.356656	-2.365408	H	3.992951	3.098869	-0.889867
C	-3.384785	1.078692	0.160374	H	2.503799	2.602346	-0.071721
C	-2.262430	1.336756	-0.630158	C	7.140400	-0.536470	-3.331828
C	-1.718091	2.654562	-0.640195	C	6.475721	0.684597	-3.208293
C	-2.207712	3.649754	0.163771	C	5.715603	0.955376	-2.070023
Br	-0.285146	3.088161	-1.827930	C	5.600172	0.023238	-1.019549
H	-1.771957	4.642092	0.124134	C	6.281749	-1.201516	-1.171878
C	-4.060601	-0.245929	0.062904	C	7.039892	-1.481107	-2.310513
C	-3.285486	-1.390449	0.216964	H	7.733126	-0.748800	-4.217103
C	-3.906056	-2.670098	0.269159	H	6.549774	1.427320	-3.997713
C	-5.260682	-2.813245	0.116908	H	5.207834	1.911944	-2.004769
Br	-2.812741	-4.208769	0.543339	H	6.229086	-1.947311	-0.383841
H	-5.714188	-3.797344	0.166408	H	7.554464	-2.434136	-2.396661
C	-5.468422	-0.378494	-0.196653	C	6.014112	-2.333003	4.097794
C	-6.070320	-1.679260	-0.147299	C	6.940619	-1.652938	3.305464
C	-7.463688	-1.818801	-0.389514	C	6.504160	-0.884771	2.225061
				C	5.135953	-0.772470	1.911773
				C	4.221257	-1.464941	2.727692
				C	4.652473	-2.238503	3.806495

H	6.351870	-2.933388	4.937819	C	0.300136	-3.467203	-0.095104
H	8.001989	-1.722991	3.526946	C	-0.618012	1.342688	-0.077704
H	7.243492	-0.374221	1.612605	O	-1.054699	0.045183	-0.063404
H	3.157076	-1.391638	2.519545	C	-5.263789	-0.951658	2.401396
H	3.926428	-2.764817	4.419805	C	-4.195883	-1.590948	3.027896
O	2.927609	-0.153698	0.146794	C	-3.162977	-2.146737	2.269596
				C	-3.179178	-2.072238	0.871596
				C	-4.261884	-1.430548	0.253396
Catalytic Cycle				C	-5.291090	-0.872358	1.008196
				H	-6.065193	-0.516766	2.991396
Minima of Compound 5				H	-4.158982	-1.657247	4.111496
				H	-2.344073	-2.633529	2.787696
B3LYP/6-31G** Energy =			-6817.822869	H	-4.286585	-1.357748	-0.828604
B3LYP/6-31G** Free Energy =			-6817.842480	H	-6.115495	-0.373567	0.506796
M06-2X/LACVP** Derived Free Energy =			-1700.443475	C	1.193740	-3.877894	-0.796804
M06-2X/LACVP** Derived Solution Free Energy =			-1700.462998	H	2.017343	-4.187486	-1.396804
Number of Imaginary Frequencies =			0	C	-2.645758	-4.057832	-0.563804
				H	-2.910852	-4.734935	0.253096
B3LYP/6-31G** Geometry				H	-3.540960	-3.874441	-1.162704
				H	-1.889354	-4.533725	-1.193104
C	2.343703	-0.111583	-0.258504	C	-0.776669	-2.971614	0.759796
C	3.253213	-1.138374	0.117796	H	-0.464078	-2.038011	1.237896
C	3.434016	-1.504372	1.423896	H	-0.958362	-3.698216	1.559696
C	1.610196	0.546210	0.720296	O	2.183999	0.258415	-1.552904
Br	4.221821	-2.029365	-1.273904	H	2.633005	-0.371280	-2.142604
H	4.131724	-2.294865	1.677396	O	-0.958797	-0.129216	-2.420904
C	2.701610	-0.854380	2.448796	C	-0.938990	-0.903915	-3.624204
C	1.774800	0.181011	2.093796	H	-0.463280	-1.871411	-3.431904
C	1.042293	0.809304	3.139696	H	-1.961488	-1.083626	-3.979604
C	1.222597	0.438406	4.453196	C	-0.142597	-0.105308	-4.645204
C	2.142907	-0.579985	4.798696	H	-0.030892	-0.692006	-5.563304
C	2.865113	-1.212278	3.813696	H	-0.695907	0.812887	-4.898304
H	0.332986	1.589497	2.887496	H	1.036995	0.648604	-3.323704
H	0.651892	0.932700	5.233796	O	1.158900	0.196905	-4.173304
H	2.274810	-0.859984	5.839296	C	-2.107772	-2.730827	-0.006804
H	3.572821	-1.998071	4.063896	O	-1.842680	-1.926424	-1.174204
C	-1.124735	3.701283	-0.404404				
C	0.674285	1.643900	0.322796	B3LYP/6-31G** Energy =			-6817.820728
C	-1.516222	2.388279	-0.431804	B3LYP/6-31G** Free Energy =			-6817.841294
H	-1.825143	4.481976	-0.680704	M06-2X/LACVP** Derived Free Energy =			-1700.444437
Br	-3.300618	1.948861	-0.938704	M06-2X/LACVP** Derived Solution Free Energy =			-1700.464759
C	1.106472	3.010105	0.358996	Number of Imaginary Frequencies =			0
C	0.192862	4.048096	-0.013504				
C	0.621448	5.402000	0.019196	B3LYP/6-31G** Geometry			
C	1.902245	5.725913	0.401896				
C	2.808755	4.703322	0.768696	C	1.912506	0.370700	0.908804
C	2.422268	3.381818	0.748396	C	3.106807	-0.394700	0.810904
H	-0.083859	6.177893	-0.266104	C	3.828307	-0.468799	-0.349596
H	2.220635	6.763716	0.422196	C	1.434606	1.040500	-0.209196
H	3.819652	4.964032	1.067796	Br	3.675807	-1.376399	2.356504
H	3.125076	2.605725	1.029496	H	4.739607	-1.055399	-0.389696
B	-1.296192	-0.679019	-1.221204				

C	3.373406	0.206100	-1.508896	O	-1.916993	-0.296602	1.948704
C	2.154206	0.957200	-1.444196	C	-2.322693	-1.049702	3.095904
C	1.705906	1.601200	-2.631396	H	-3.020193	-0.418102	3.654904
C	2.424206	1.512000	-3.802296	H	-2.826093	-1.975202	2.800804
C	3.632206	0.776701	-3.857296	C	-1.086893	-1.341201	3.937304
C	4.093606	0.136801	-2.731196	H	-1.379393	-1.831601	4.872704
H	0.781906	2.167099	-2.604896	H	-0.436993	-2.040501	3.384504
H	2.059606	2.011400	-4.695096	H	-0.386694	0.389599	3.470704
H	4.188806	0.718101	-4.787596	O	-0.391793	-0.153001	4.275304
H	5.017507	-0.434899	-2.758696	C	-1.976692	-2.940102	-0.695096
C	-2.158695	3.448998	-0.096396	O	-2.027093	-2.178802	0.528804
C	0.193506	1.870899	-0.112096				
C	-2.230294	2.084698	-0.191496	B3LYP/6-31G** Energy =			-6817.819440
H	-3.065595	4.043598	-0.112596	B3LYP/6-31G** Free Energy =			-6817.839078
Br	-3.918094	1.225698	-0.401196	M06-2X/LACVP** Derived Free Energy =			-1700.440930
C	0.292305	3.297999	0.002304	M06-2X/LACVP** Derived Solution Free Energy =			-1700.463043
C	-0.900095	4.090999	0.018404	Number of Imaginary Frequencies =			0
C	-0.801096	5.502999	0.137004				
C	0.425304	6.116699	0.241604	B3LYP/6-31G** Geometry			
C	1.606004	5.337500	0.231604				
C	1.542205	3.967000	0.113404	C	2.308091	0.018863	-0.735600
H	-1.716096	6.089098	0.146004	C	3.326478	-0.883052	-0.319500
H	0.490504	7.196599	0.334104	C	3.651475	-1.057957	0.998900
H	2.572104	5.825500	0.320104	C	1.626903	0.761673	0.220500
H	2.453605	3.380200	0.110904	Br	4.271863	-1.853867	-1.678000
B	-1.722393	-0.864202	0.723704	H	4.437465	-1.750369	1.280700
C	-4.305193	-2.184503	-1.327096	C	2.965586	-0.324747	1.999000
C	-1.057694	1.277099	-0.170496	C	1.940300	0.598069	1.605700
O	-1.175993	-0.084001	-0.287596	C	1.274511	1.332179	2.627100
C	2.151508	-3.509100	-1.944996	C	1.609409	1.163874	3.951900
C	1.157808	-3.349500	-2.908396	C	2.622695	0.252058	4.334800
C	-0.168492	-3.132701	-2.527296	C	3.283384	-0.477552	3.375000
C	-0.524892	-3.071401	-1.175096	H	0.485022	2.019591	2.347500
C	0.486208	-3.233801	-0.216296	H	1.090418	1.738182	4.714000
C	1.809808	-3.447000	-0.592896	H	2.873193	0.130255	5.384100
H	3.182308	-3.674200	-2.244096	H	4.062073	-1.182464	3.654000
H	1.410408	-3.387600	-3.963996	C	-1.264953	3.689517	-1.117600
H	-0.915992	-3.011101	-3.303496	C	0.625018	1.774089	-0.236000
H	0.230108	-3.189601	0.837004	C	-1.635772	2.391723	-0.886300
H	2.571708	-3.542000	0.175004	H	-1.998842	4.413229	-1.455200
C	-5.465793	-2.103203	-1.001896	Br	-3.443681	1.851951	-1.157500
H	-6.488293	-2.033303	-0.711396	C	1.038839	3.126682	-0.476000
C	-2.500792	-4.333102	-0.311196	C	0.079353	4.092597	-0.919500
H	-2.480492	-4.998902	-1.178696	C	0.489974	5.431891	-1.154600
H	-1.868992	-4.765402	0.468204	C	1.797580	5.811571	-0.960500
H	-3.526192	-4.260802	0.058804	C	2.749565	4.861056	-0.522700
C	-2.909593	-2.284902	-1.752496	C	2.381445	3.555162	-0.287300
H	-2.529393	-1.288402	-1.998696	H	-0.251215	6.151402	-1.491900
H	-2.872992	-2.882702	-2.669496	H	2.101895	6.837866	-1.142700
O	1.228206	0.476200	2.075004	H	3.781170	5.165041	-0.371600
H	1.647506	-0.060500	2.769204	H	3.119934	2.835951	0.047900

B	-1.883214	-0.309673	0.765600	H	-1.694012	-4.452811	-0.190805
C	-4.703630	-1.374330	-1.203500	C	-2.088232	-2.679438	-1.378105
C	-0.696987	1.418309	-0.442000	C	-2.095928	-1.245838	-1.374905
O	-1.104207	0.117015	-0.294200	C	-2.441373	-0.578762	-2.583405
C	1.371731	-3.987323	-1.334900	C	-2.767425	-1.288084	-3.717105
C	1.016335	-3.692117	-0.017300	C	-2.766930	-2.703384	-3.711805
C	-0.243857	-3.175698	0.275400	C	-2.431784	-3.381861	-2.563905
C	-1.177854	-2.940484	-0.746000	H	-2.444446	0.504938	-2.602205
C	-0.810958	-3.236389	-2.064000	H	-3.027461	-0.755601	-4.627305
C	0.453534	-3.752409	-2.356100	H	-3.027893	-3.248501	-4.613805
H	2.357325	-4.379538	-1.561600	H	-2.421311	-4.468460	-2.545805
H	1.723032	-3.861628	0.789300	C	-1.796067	3.789082	-0.224905
H	-0.497754	-2.944794	1.305600	C	-1.783477	0.959583	-0.148505
H	-1.500855	-3.066579	-2.883000	C	-0.624420	3.090461	-0.350405
H	0.715131	-3.972113	-3.387400	H	-1.790140	4.872682	-0.270105
C	-5.826424	-1.009713	-0.946500	Br	1.010016	4.033271	-0.639905
H	-6.816319	-0.689098	-0.717900	C	-3.021024	1.668799	-0.005505
C	-3.381365	-3.661650	0.190200	C	-3.021521	3.100799	-0.038605
H	-3.484176	-4.434549	-0.576700	C	-4.247668	3.803317	0.106095
H	-2.857871	-4.101758	1.042800	C	-5.431223	3.125137	0.281795
H	-4.377260	-3.339935	0.504500	C	-5.434727	1.710737	0.319695
C	-3.352836	-1.816551	-1.547100	C	-4.262980	1.001516	0.178695
H	-2.778123	-0.964660	-1.923600	H	-4.231041	4.889518	0.077695
H	-3.425948	-2.546550	-2.360200	H	-6.362859	3.671474	0.393695
O	1.998894	0.196668	-2.041700	H	-6.371192	1.179874	0.463195
H	2.524985	-0.424040	-2.571700	H	-4.275907	-0.081985	0.212295
O	-1.991301	0.487929	1.863000	B	1.591318	1.034210	0.493195
C	-2.825607	0.150041	2.972100	C	5.542711	1.141676	-0.412905
H	-3.082292	1.090145	3.471500	C	-0.601324	1.668962	-0.292405
H	-3.755214	-0.309345	2.612900	O	0.581821	0.999542	-0.456705
C	-2.132921	-0.772369	3.966100	C	1.987766	-4.124264	-1.536305
H	-1.196414	-0.309484	4.299300	C	1.970326	-3.541365	-0.269305
H	-2.793522	-0.861759	4.844900	C	2.396438	-2.224436	-0.098305
H	-2.341042	-2.180866	2.636400	C	2.832586	-1.459107	-1.187505
O	-1.821640	-2.055874	3.444500	C	2.845926	-2.056006	-2.455505
C	-2.586446	-2.468762	-0.364200	C	2.430015	-3.376734	-2.627905
O	-2.521832	-1.525263	0.734100	H	1.657135	-5.149686	-1.673605
				H	1.604164	-4.095989	0.589595
B3LYP/6-31G** Energy =			-6817.821975	H	2.386108	-1.782837	0.891795
B3LYP/6-31G** Free Energy =			-6817.843234	H	3.178888	-1.493183	-3.321205
M06-2X/LACVP** Derived Free Energy =			-1700.444602	H	2.445145	-3.817533	-3.620505
M06-2X/LACVP** Derived Solution Free Energy =			-1700.464943	C	6.091840	2.192113	-0.179905
Number of Imaginary Frequencies =			0	H	6.574878	3.119545	0.023595
				C	3.090427	0.906311	-2.150905
B3LYP/6-31G** Geometry				H	3.687146	0.618451	-3.020505
				H	2.035828	0.896740	-2.425605
C	-1.420728	-1.244093	0.967095	H	3.373258	1.923430	-1.872405
C	-1.391633	-2.665091	0.930495	C	4.892697	-0.137768	-0.690605
C	-1.722385	-3.368813	-0.195905	H	5.030643	-0.813259	0.161395
C	-1.762476	-0.536516	-0.177605	H	5.367630	-0.619936	-1.553005
Br	-0.830470	-3.593853	2.511595	O	-1.128475	-0.553773	2.097795

H	-0.864734	-1.159756	2.811595	H	-2.536477	2.867441	2.020605
O	1.317281	1.582091	1.712395	B	1.139319	-0.785763	-0.975895
C	2.240084	1.543953	2.806195	C	4.630096	0.096829	1.047605
H	3.267592	1.424923	2.449995	C	0.415059	1.518318	-0.486395
H	2.144720	2.501547	3.327695	O	0.359790	0.344817	-1.197395
C	1.837761	0.402426	3.730695	C	1.062735	-5.195665	2.051505
H	2.022425	-0.556961	3.218295	C	0.594301	-3.902477	2.290605
H	2.457460	0.417868	4.634295	C	1.234173	-2.807160	1.712805
H	-0.008265	0.784302	3.343795	C	2.347577	-2.981731	0.877505
O	0.483453	0.513835	4.135795	C	2.810111	-4.282619	0.646605
C	3.361090	-0.035871	-0.970705	C	2.173440	-5.380736	1.229205
O	2.821854	0.507793	0.247695	H	0.565758	-6.050778	2.500405
B3LYP/6-31G** Energy =				H	-0.272103	-3.739700	2.924905
B3LYP/6-31G** Free Energy =				H	0.858346	-1.807270	1.904405
M06-2X/LACVP** Derived Free Energy =				H	3.667216	-4.451996	0.004005
M06-2X/LACVP** Derived Solution Free Energy =				H	2.546667	-6.381926	1.033405
Number of Imaginary Frequencies =				C	5.197970	1.111044	0.721005
B3LYP/6-31G** Geometry				H	5.694546	2.007457	0.431105
C	-2.500014	0.497042	-0.540095	C	3.914252	-2.038590	-0.935395
C	-3.435086	-0.570983	-0.433795	H	4.782969	-2.653367	-0.684595
C	-3.624168	-1.254588	0.739005	H	3.325966	-2.548905	-1.699595
C	-1.713423	0.825762	0.561705	H	4.276627	-1.089780	-1.335995
Br	-4.395673	-1.084208	-2.002995	C	3.927028	-1.123689	1.436505
H	-4.347147	-2.061607	0.789005	H	3.268423	-0.912907	2.286505
C	-2.864677	-0.919268	1.887505	H	4.642148	-1.882671	1.775405
C	-1.878804	0.119058	1.796705	O	-2.371433	1.214745	-1.680395
C	-1.075211	0.375279	2.944705	H	-2.255918	0.626948	-2.457595
C	-1.258292	-0.330226	4.113605	O	0.901948	-1.888569	-1.740395
C	-2.252466	-1.333752	4.205605	C	-0.313545	-2.153701	-2.453695
C	-3.034959	-1.621272	3.111205	H	-0.291516	-3.226300	-2.672295
H	-0.309531	1.140199	2.891405	H	-1.184150	-1.956824	-1.818195
H	-0.633298	-0.113109	4.974805	C	-0.464664	-1.399005	-3.771495
H	-2.392252	-1.874556	5.136605	H	0.475537	-1.468880	-4.337595
H	-3.795438	-2.396092	3.162605	H	-1.245151	-1.897525	-4.355495
C	1.498203	3.651647	-0.092395	H	-0.237212	0.406101	-3.071295
C	-0.626849	1.834791	0.373005	O	-0.880000	-0.042916	-3.644795
C	1.466235	2.437046	-0.727995	C	3.058645	-1.751012	0.303305
H	2.311085	4.343868	-0.282095	O	2.096318	-0.723438	-0.016995
Br	2.813647	1.982481	-1.996495	B3LYP/6-31G** Energy =			
C	-0.632983	3.112591	1.018405	B3LYP/6-31G** Free Energy =			
C	0.455593	4.018819	0.795005	M06-2X/LACVP** Derived Free Energy =			
C	0.454060	5.282919	1.444705	M06-2X/LACVP** Derived Solution Free Energy =			
C	-0.583150	5.650892	2.269105	Number of Imaginary Frequencies =			
C	-1.670727	4.768363	2.473105	B3LYP/6-31G** Geometry			
C	-1.695894	3.533863	1.864605	C	-1.597915	-1.309188	0.655600
H	1.288242	5.956941	1.270105	C	-1.831528	-2.697486	0.464000
H	-0.574575	6.620192	2.758305	C	-2.741932	-3.156177	-0.451900
H	-2.494834	5.070442	3.112505	C	-2.280206	-0.380281	-0.121700

Br	-0.795339	-3.934495	1.494800	O	-0.708810	-0.834296	1.556000
H	-2.902242	-4.221876	-0.574900	H	-0.266817	-1.544400	2.052100
C	-3.463423	-2.237770	-1.254400	O	1.823388	-0.979220	-0.917800
C	-3.218610	-0.831573	-1.102400	C	1.214182	-1.704214	-1.996200
C	-3.920102	0.062534	-1.959900	H	0.129583	-1.562304	-1.995800
C	-4.819506	-0.405558	-2.890600	H	1.622085	-1.330018	-2.942200
C	-5.071019	-1.792456	-3.023100	C	1.584168	-3.165317	-1.804200
C	-4.402428	-2.687162	-2.221700	H	1.134265	-3.522413	-0.863400
H	-3.734992	1.126732	-1.872900	H	1.164062	-3.760813	-2.622300
H	-5.341100	0.297247	-3.533600	H	3.368273	-2.664234	-1.267600
H	-5.785523	-2.145349	-3.760500	O	2.987966	-3.359030	-1.824900
H	-4.577438	-3.755360	-2.318500	C	3.157401	0.395368	1.279900
C	-1.339567	3.817910	0.267800	O	1.906305	0.784280	0.675000
C	-1.965993	1.070616	0.061100				
C	-0.443675	2.938001	-0.284800	B3LYP/6-31G** Energy =			-6817.821420
H	-1.100257	4.874608	0.316600	B3LYP/6-31G** Free Energy =			-6817.841383
Br	1.179231	3.615586	-1.022900	M06-2X/LACVP** Derived Free Energy =			-1700.441113
C	-2.906184	1.966524	0.663700	M06-2X/LACVP** Derived Solution Free Energy =			-1700.464323
C	-2.581271	3.357721	0.770500	Number of Imaginary Frequencies =			0
C	-3.512363	4.249830	1.367800				
C	-4.714667	3.791741	1.852900	B3LYP/6-31G** Geometry			
C	-5.034180	2.415844	1.761800				
C	-4.155988	1.527836	1.182800	C	3.038499	-0.708294	-0.635498
H	-3.252553	5.302728	1.436700	C	3.791799	-1.827294	-0.183798
H	-5.418261	4.481148	2.309800	C	3.775699	-2.235394	1.123202
H	-5.980784	2.057553	2.155300	C	2.254499	-0.002694	0.270402
H	-4.407998	0.475238	1.123800	Br	4.857699	-2.769094	-1.473898
B	1.300899	0.156985	-0.372100	H	4.365199	-3.089994	1.436802
C	1.984089	-0.932021	3.113700	C	2.984299	-1.539394	2.070202
C	-0.731588	1.549104	-0.363300	C	2.207299	-0.413194	1.637802
O	0.145904	0.675996	-0.938900	C	1.406099	0.257906	2.603102
C	6.322400	0.269739	-1.719300	C	1.387799	-0.157194	3.916302
C	6.269191	-0.714161	-0.734800	C	2.166199	-1.260694	4.341302
C	5.254191	-0.697851	0.226300	C	2.945299	-1.937994	3.433102
C	4.269600	0.299158	0.218900	H	0.788899	1.093106	2.291802
C	4.338209	1.285457	-0.776800	H	0.757699	0.364406	4.630202
C	5.349909	1.271148	-1.734400	H	2.141199	-1.572694	5.381002
H	7.109500	0.255931	-2.467200	H	3.542599	-2.791494	3.742802
H	7.016083	-1.502268	-0.708700	C	0.123599	3.374306	-1.387198
H	5.248884	-1.479351	0.977600	C	1.499299	1.187006	-0.233898
H	3.579916	2.059764	-0.809200	C	-0.403401	2.110806	-1.432098
H	5.375716	2.043947	-2.497300	H	-0.401801	4.200506	-1.853398
C	1.191588	-0.962714	4.026000	Br	-2.025901	1.798506	-2.389698
H	0.495188	-0.957507	4.832700	C	2.075099	2.497106	-0.176098
C	3.482912	1.531165	2.261200	C	1.365999	3.604706	-0.744198
H	4.438710	1.346956	2.760100	C	1.932199	4.905706	-0.677998
H	3.547720	2.477264	1.719700	C	3.152099	5.112706	-0.077398
H	2.694812	1.612172	3.013600	C	3.858399	4.020706	0.480102
C	2.979589	-0.948630	2.043500	C	3.336099	2.747706	0.430802
H	2.732381	-1.734328	1.322400	H	1.381999	5.735206	-1.113898
H	3.940386	-1.218839	2.494500	H	3.576199	6.111306	-0.031498

H	4.822599	4.189406	0.950702	C	-1.718004	0.103094	0.380206
H	3.884699	1.917406	0.861102	Br	-2.928813	-2.986202	-2.156794
B	-1.357201	-0.684494	-0.153298	H	-3.220515	-3.488802	0.738206
C	-2.215801	1.774806	3.207002	C	-2.497009	-1.750904	1.818106
C	0.260099	1.009306	-0.827098	C	-1.933006	-0.440805	1.687106
O	-0.281701	-0.241894	-0.911598	C	-1.624204	0.277794	2.874006
C	-6.579901	-1.423794	-0.301498	C	-1.866305	-0.266605	4.115906
C	-5.765901	-0.422994	-0.837398	C	-2.429509	-1.558104	4.241106
C	-4.592201	-0.045794	-0.183898	C	-2.735311	-2.283403	3.112506
C	-4.199801	-0.670794	1.009602	H	-1.190601	1.268393	2.791106
C	-5.026401	-1.668394	1.539402	H	-1.622104	0.301394	5.008906
C	-6.205801	-2.041494	0.890402	H	-2.618210	-1.973203	5.226606
H	-7.491901	-1.719894	-0.810798	H	-3.167714	-3.277202	3.193706
H	-6.043701	0.065006	-1.767098	C	-0.344292	4.180090	-0.146194
H	-3.960601	0.721706	-0.618498	C	-1.242400	1.512793	0.205306
H	-4.753601	-2.173094	2.459202	C	0.535605	3.132188	-0.190594
H	-6.826501	-2.823994	1.317102	H	0.010611	5.195089	-0.287994
C	-1.372801	2.338806	3.863902	Br	2.385706	3.460182	-0.522094
H	-0.627201	2.846706	4.430602	C	-2.184397	2.597095	0.249706
C	-2.370701	-1.213894	2.730902	C	-1.724293	3.942494	0.077906
H	-3.054701	-1.367494	3.570202	C	-2.656090	5.013397	0.126206
H	-2.193401	-2.173094	2.239802	C	-3.994191	4.771101	0.331906
H	-1.426501	-0.839194	3.129802	C	-4.453994	3.443402	0.495506
C	-3.287101	1.147206	2.435402	C	-3.574497	2.384400	0.455106
H	-3.627001	1.845406	1.662202	H	-2.290387	6.028096	-0.004794
H	-4.147601	0.963706	3.089802	H	-4.699688	5.595703	0.366606
O	3.066499	-0.302094	-1.927698	H	-5.512195	3.257605	0.653006
H	3.659299	-0.888494	-2.425698	H	-3.937000	1.370801	0.579306
O	-1.835901	-1.938394	-0.383998	B	1.516496	0.204085	-1.146794
C	-1.407901	-2.708094	-1.519498	C	5.099496	0.047874	1.602906
H	-0.346801	-2.533294	-1.724498	C	0.098201	1.790689	-0.008694
H	-1.558201	-3.758194	-1.253398	O	1.038298	0.789786	0.007806
C	-2.257601	-2.353594	-2.733498	C	0.899985	-3.483013	2.593606
H	-2.115501	-1.287194	-2.970198	C	1.696588	-2.488416	3.156506
H	-1.910501	-2.935294	-3.595198	C	2.495591	-1.679018	2.346106
H	-3.930301	-2.181394	-1.772398	C	2.510390	-1.854718	0.958206
O	-3.624701	-2.672994	-2.548998	C	1.704687	-2.860716	0.399806
C	-2.929501	-0.197394	1.731402	C	0.905685	-3.664714	1.209506
O	-1.887301	0.144306	0.791802	H	0.274384	-4.105712	3.225506
B3LYP/6-31G** Energy =			-6817.819410	H	1.696589	-2.333116	4.231306
B3LYP/6-31G** Free Energy =			-6817.839665	H	3.115093	-0.920720	2.810406
M06-2X/LACVP** Derived Free Energy =			-1700.445682	H	1.690587	-3.014116	-0.675194
M06-2X/LACVP** Derived Solution Free Energy =			-1700.468332	H	0.284383	-4.430312	0.754806
Number of Imaginary Frequencies =			0	C	6.013695	-0.098128	2.378906
B3LYP/6-31G** Geometry				H	6.819495	-0.233931	3.062606
				C	4.521190	-1.894524	-0.560094
				H	5.172189	-2.254526	0.238406
				H	4.103488	-2.759223	-1.081294
C	-2.024806	-0.652605	-0.746494	H	5.120092	-1.313026	-1.267794
C	-2.564010	-1.961203	-0.592194	C	3.999796	0.261977	0.664306
C	-2.804612	-2.491003	0.647606	H	4.360198	0.875876	-0.169194

H	3.203098	0.836380	1.144206	H	3.216425	6.215241	1.727396
O	-1.867505	-0.197105	-2.014594	H	4.524351	4.129757	2.116396
H	-1.110703	0.415292	-2.053294	H	3.534979	1.929245	1.633496
O	0.838297	0.443187	-2.311194	B	-0.937490	-0.480512	-1.200104
C	1.190295	-0.086214	-3.608294	C	-2.489052	-3.438232	1.858496
H	0.562797	0.461187	-4.316894	C	-0.268214	1.404496	0.196496
H	2.240196	0.142883	-3.821694	O	-0.896898	0.201888	0.002796
C	0.944891	-1.586214	-3.747794	C	-5.977302	0.451123	-0.031404
H	-0.018110	-1.835011	-3.277594	C	-5.366595	-0.041769	1.119896
H	0.851490	-1.811513	-4.817494	C	-4.269784	-0.901655	1.027196
H	2.379890	-1.926018	-2.485894	C	-3.765479	-1.284048	-0.220304
O	2.003389	-2.390417	-3.249594	C	-4.389686	-0.782156	-1.373004
C	3.402893	-1.026321	0.030006	C	-5.483197	0.075830	-1.282604
O	2.617594	-0.604518	-1.134494	H	-6.829510	1.120213	0.043296
B3LYP/6-31G** Energy =			-6817.822205	H	-5.739399	0.244026	2.099196
B3LYP/6-31G** Free Energy =			-6817.842246	H	-3.821880	-1.279649	1.938496
M06-2X/LACVP** Derived Free Energy =			-1700.445033	H	-4.002082	-1.052251	-2.350304
M06-2X/LACVP** Derived Solution Free Energy =			-1700.466170	H	-5.947902	0.453424	-2.189104
Number of Imaginary Frequencies =			0	C	-3.040743	-4.174039	2.642096
B3LYP/6-31G** Geometry				H	-3.532434	-4.820845	3.330996
C	2.672107	-0.221066	-0.159604	C	-3.018551	-3.540039	-1.063704
C	3.318723	-1.484758	-0.065704	H	-3.742444	-4.063648	-0.436604
C	3.128734	-2.317660	1.004796	H	-3.478453	-3.330245	-2.031804
C	1.789702	0.172223	0.839596	H	-2.153942	-4.191528	-1.223904
Br	4.444130	-2.020944	-1.520304	C	-1.800063	-2.551723	0.921896
H	3.632846	-3.277154	1.045696	H	-0.858457	-3.023111	0.615896
C	2.269729	-1.926871	2.062696	H	-1.528975	-1.618120	1.421496
C	1.589113	-0.667480	1.978896	O	2.888896	0.619937	-1.200904
C	0.728608	-0.299591	3.050496	H	3.429802	0.183043	-1.882104
C	0.551519	-1.130493	4.133996	O	-0.225496	0.009297	-2.254704
C	1.220934	-2.375585	4.209296	C	-0.151788	-0.645202	-3.526904
C	2.063239	-2.762074	3.193396	H	-0.683175	-1.601309	-3.505704
H	0.215796	0.654802	3.005596	H	-0.622996	0.013792	-4.264604
H	-0.108385	-0.827702	4.941596	C	1.317415	-0.839283	-3.870604
H	1.067643	-3.020887	5.068596	H	1.770324	-1.552478	-3.162804
H	2.585252	-3.714167	3.239196	H	1.405320	-1.268482	-4.874804
C	-0.439545	3.828294	0.245196	H	1.756793	0.850522	-3.060104
C	1.034586	1.451413	0.668096	O	2.020699	0.393125	-3.874504
C	-1.000229	2.604487	-0.014304	C	-2.573667	-2.234433	-0.390404
H	-1.011756	4.734087	0.075896	O	-1.632575	-1.647421	-1.326104
Br	-2.785027	2.473764	-0.662704	B3LYP/6-31G** Energy =			-6817.822205
C	1.636969	2.718021	0.955896	B3LYP/6-31G** Free Energy =			-6817.842243
C	0.886854	3.918811	0.738796	M06-2X/LACVP** Derived Free Energy =			-1700.445027
C	1.484438	5.175319	1.025896	M06-2X/LACVP** Derived Solution Free Energy =			-1700.466362
C	2.769237	5.249735	1.511096	Number of Imaginary Frequencies =			0
C	3.511252	4.064945	1.730796	B3LYP/6-31G** Geometry			
C	2.960668	2.832537	1.459696	C	2.672393	-0.221098	-0.159598
H	0.904527	6.078211	0.854896	C	3.318994	-1.484798	-0.065898

C	3.128894	-2.318098	1.004302	H	-0.859606	-3.022500	0.616702
C	1.789793	0.171901	0.839602	H	-1.530606	-1.617501	1.421902
Br	4.444694	-2.020497	-1.520498	O	2.889192	0.620102	-1.200598
H	3.632995	-3.277598	1.045002	H	3.430393	0.183502	-1.881698
C	2.269694	-1.927698	2.062202	O	-0.224707	0.008700	-2.254098
C	1.588993	-0.668299	1.978602	C	-0.151107	-0.645700	-3.526198
C	0.728393	-0.300599	3.050302	H	-0.681906	-1.602200	-3.504798
C	0.551193	-1.131899	4.133502	H	-0.623007	0.013000	-4.263798
C	1.220594	-2.376999	4.208502	C	1.318093	-0.838999	-3.870398
C	2.062994	-2.763198	3.192702	H	1.771594	-1.551999	-3.162998
H	0.215592	0.653800	3.005602	H	1.405893	-1.267899	-4.874798
H	-0.108807	-0.829300	4.941102	H	1.756892	0.850801	-3.059698
H	1.067194	-3.022499	5.067602	O	2.020692	0.393801	-3.874298
H	2.584995	-3.715298	3.238202	C	-2.574406	-2.234001	-0.390398
C	-0.439110	3.828200	0.245802	O	-1.632906	-1.647201	-1.325898
C	1.034792	1.451101	0.668402				
C	-1.000009	2.604500	-0.013798	B3LYP/6-31G** Energy =			-6817.819205
H	-1.011210	4.734100	0.076602	B3LYP/6-31G** Free Energy =			-6817.839771
Br	-2.784709	2.473999	-0.662198	M06-2X/LACVP** Derived Free Energy =			-1700.439565
C	1.637291	2.717701	0.956302	M06-2X/LACVP** Derived Solution Free Energy =			-1700.463031
C	0.887290	3.918501	0.739402	Number of Imaginary Frequencies =			0
C	1.485090	5.174901	1.026602				
C	2.769890	5.249102	1.511902	B3LYP/6-31G** Geometry			
C	3.511690	4.064202	1.731502				
C	2.960991	2.832002	1.460202	C	-2.279417	-0.570125	-0.690606
H	0.905189	6.077901	0.855702	C	-2.970955	-1.718102	-0.213906
H	3.217189	6.214602	1.728302	C	-3.268661	-1.891192	1.110994
H	4.524890	4.128903	2.117102	C	-1.894584	0.413862	0.210694
H	3.535192	1.928602	1.633902	Br	-3.487900	-3.047784	-1.496306
B	-0.937407	-0.480600	-1.199698	H	-3.800291	-2.777174	1.440494
C	-2.490605	-3.437701	1.858502	C	-2.878328	-0.910905	2.056894
C	-0.268108	1.404400	0.196902	C	-2.176389	0.254572	1.602894
O	-0.897007	0.201900	0.003202	C	-1.782057	1.218559	2.572694
C	-5.977908	0.451897	-0.033098	C	-2.074463	1.040968	3.906094
C	-5.482907	0.076997	-1.284098	C	-2.776001	-0.106408	4.348294
C	-4.389507	-0.781102	-1.373998	C	-3.166433	-1.061895	3.439594
C	-3.766207	-1.283402	-0.220998	H	-1.234327	2.095140	2.246394
C	-4.271307	-0.901402	1.026302	H	-1.762538	1.789358	4.628694
C	-5.368107	-0.041403	1.118502	H	-3.001105	-0.230101	5.403194
H	-6.830108	1.121096	0.041102	H	-3.702263	-1.949577	3.765594
H	-5.946908	0.454897	-2.190798	C	0.157434	3.911994	-1.290506
H	-4.001107	-1.051002	-2.350998	C	-1.200643	1.633339	-0.305706
H	-3.824207	-1.279802	1.937802	C	0.841395	2.763971	-0.989906
H	-5.741707	0.244097	2.097602	H	0.688563	4.778776	-1.668606
C	-3.042505	-4.173402	2.642102	Br	2.733093	2.698107	-1.256406
H	-3.534405	-4.820302	3.330802	C	-1.940703	2.818564	-0.621906
C	-3.019205	-3.539601	-1.063698	C	-1.248364	3.971641	-1.114706
H	-3.743405	-4.063102	-0.436698	C	-1.981425	5.148465	-1.423306
H	-3.478905	-3.329902	-2.031898	C	-3.345824	5.192211	-1.254606
H	-2.154605	-4.191201	-1.223598	C	-4.033762	4.054734	-0.770006
C	-1.801406	-2.551201	0.922202	C	-3.351000	2.899311	-0.462206

H	-1.441896	6.014647	-1.796906	C	-3.388997	-0.963637	-0.176010
H	-3.897293	6.096630	-1.493406	C	-3.644995	-1.141440	1.156890
H	-5.111360	4.094170	-0.640806	C	-1.768015	0.784180	0.272390
H	-3.886729	2.032329	-0.092306	Br	-4.309386	-2.028347	-1.480210
B	1.844915	0.367937	0.717494	H	-4.370587	-1.879947	1.480090
C	4.582883	-3.558755	-0.676806	C	-2.957903	-0.359932	2.118590
C	0.170856	1.612693	-0.489506	C	-2.002113	0.611878	1.671990
O	0.872718	0.460270	-0.261706	C	-1.315821	1.376485	2.656890
C	-0.437146	-4.421087	0.153394	C	-1.568619	1.193282	3.997590
C	0.020765	-4.093302	-1.121806	C	-2.518909	0.238672	4.433090
C	1.084995	-3.204238	-1.282106	C	-3.196401	-0.522135	3.509490
C	1.706514	-2.624958	-0.170206	H	-0.576929	2.101592	2.336090
C	1.239103	-2.964243	1.107894	H	-1.031825	1.787688	4.731190
C	0.177573	-3.852407	1.269694	H	-2.708008	0.108270	5.494390
H	-1.269569	-5.107459	0.274194	H	-3.926194	-1.261243	3.829590
H	-0.456249	-4.522986	-1.997206	C	1.047654	3.732909	-1.168010
H	1.425603	-2.965549	-2.282906	C	-0.808326	1.814390	-0.230610
H	1.704118	-2.520358	1.982494	C	1.428068	2.434013	-0.957810
H	-0.171035	-4.096195	2.269094	H	1.768547	4.459917	-1.526010
C	4.901151	-4.498866	-1.364906	Br	3.233273	1.914132	-1.307610
H	5.178423	-5.334375	-1.964806	C	-1.234040	3.164186	-0.451410
C	3.100965	-1.101605	-1.706706	C	-0.290450	4.132895	-0.923210
H	3.414639	-1.883016	-2.402406	C	-0.711764	5.471891	-1.140310
H	2.187181	-0.634275	-2.073006	C	-2.013368	5.847377	-0.902410
H	3.886991	-0.342432	-1.676706	C	-2.948958	4.893568	-0.436610
C	4.210221	-2.416542	0.151794	C	-2.570744	3.587872	-0.216910
H	5.024046	-1.680570	0.158294	H	0.015928	6.194599	-1.499810
H	4.071811	-2.738338	1.189794	H	-2.325979	6.873374	-1.071710
O	-1.995611	-0.398834	-2.003806	H	-3.975761	5.195257	-0.251810
H	-2.304337	-1.180124	-2.491206	H	-3.295137	2.864064	0.139190
O	1.837645	1.275937	1.728994	B	1.826096	-0.252482	0.583990
C	2.835248	1.348704	2.755394	C	4.700426	-3.110352	-0.371010
H	2.383167	1.926019	3.567994	C	0.504478	1.458504	-0.487310
H	3.078214	0.346596	3.127294	O	0.896992	0.154508	-0.360710
C	4.105271	2.040861	2.270594	C	-1.643862	-4.269519	-0.150710
H	3.808301	2.928771	1.690994	C	-0.863565	-3.969411	0.966690
H	4.676782	2.380442	3.142494	C	0.379828	-3.359497	0.810090
H	4.417025	0.660451	0.939894	C	0.868525	-3.035692	-0.464410
O	4.969143	1.198432	1.525294	C	0.077828	-3.343501	-1.577910
C	2.908446	-1.687199	-0.305406	C	-1.168465	-3.953314	-1.422510
O	2.799582	-0.615495	0.673494	H	-2.616757	-4.736529	-0.032810
				H	-1.223763	-4.205914	1.963690
B3LYP/6-31G** Energy =			-6817.819753	H	0.974526	-3.119891	1.686090
B3LYP/6-31G** Free Energy =			-6817.840684	H	0.424426	-3.102997	-2.576610
M06-2X/LACVP** Derived Free Energy =			-1700.440887	H	-1.772563	-4.171220	-2.297910
M06-2X/LACVP** Derived Solution Free Energy =			-1700.464765	C	5.849922	-2.743040	-0.424510
Number of Imaginary Frequencies =			0	H	6.861618	-2.409530	-0.443610
				C	2.552812	-1.802275	-1.970010
B3LYP/6-31G** Geometry				H	2.606220	-2.578574	-2.738610
				H	1.786405	-1.078683	-2.244710
C	-2.449107	-0.004627	-0.645510	H	3.518207	-1.294965	-1.939910

C	3.308330	-3.548167	-0.298310	C	-1.804542	3.927985	-0.214202
H	3.102335	-3.945369	0.701590	H	1.133938	5.950014	-1.766402
H	3.133639	-4.368469	-1.004410	H	-0.989973	7.084793	-1.192202
O	-2.207009	0.173575	-1.966310	H	-2.866360	5.780075	-0.198902
H	-2.739002	-0.466630	-2.466510	H	-2.625837	3.368278	0.218898
O	2.056587	0.565820	1.642390	B	1.754702	-0.656780	0.520898
C	3.016790	0.328930	2.677890	C	3.942836	-4.111959	0.171798
H	2.697283	0.953827	3.518090	C	0.770184	1.231710	-0.617702
H	2.997001	-0.720570	2.993590	O	0.925297	-0.115888	-0.451002
C	4.435986	0.706745	2.254590	C	-2.475266	-3.926821	-0.500702
H	4.371376	1.610344	1.627690	C	-1.820669	-3.610815	0.691098
H	5.012683	0.961651	3.151490	C	-0.465472	-3.286702	0.683398
H	4.593701	-0.735553	0.933590	C	0.264328	-3.269195	-0.513902
O	5.150497	-0.333948	1.616690	C	-0.400369	-3.593101	-1.702702
C	2.268219	-2.426178	-0.599910	C	-1.758866	-3.916114	-1.696502
O	2.476108	-1.450576	0.455090	H	-3.533264	-4.167931	-0.498602
B3LYP/6-31G** Energy =			-6817.823596	H	-2.366269	-3.611320	1.630098
B3LYP/6-31G** Free Energy =			-6817.844365	H	0.032425	-3.030897	1.613098
M06-2X/LACVP** Derived Free Energy =			-1700.439881	H	0.133431	-3.587496	-2.646602
M06-2X/LACVP** Derived Solution Free Energy =			-1700.462705	H	-2.255964	-4.157419	-2.631702
Number of Imaginary Frequencies =			0	C	5.139535	-4.001347	0.292098
B3LYP/6-31G** Geometry				H	6.194934	-3.899637	0.395898
C	-2.436308	0.406679	-0.553302	C	2.350320	-2.529074	-1.821602
C	-3.523901	-0.326931	-0.003602	H	2.329028	-3.351275	-2.542402
C	-3.715500	-0.443333	1.346898	H	1.798712	-1.683280	-2.232202
C	-1.537614	1.032388	0.301598	H	3.392318	-2.236764	-1.679602
Br	-4.744993	-1.164743	-1.222302	C	2.494637	-4.254473	0.033598
H	-4.559494	-1.005141	1.732198	H	2.059740	-4.525777	1.001998
C	-2.808506	0.172276	2.245098	H	2.261245	-5.074875	-0.655402
C	-1.701813	0.915986	1.716598	O	-2.258609	0.530781	-1.889802
C	-0.799619	1.518395	2.638198	H	-2.941304	0.009874	-2.343202
C	-0.989418	1.395893	3.996298	O	2.243894	0.175925	1.482998
C	-2.087811	0.667383	4.513098	C	3.162198	-0.258566	2.494698
C	-2.976205	0.067274	3.651898	H	2.605400	-0.414572	3.427598
H	0.053276	2.066303	2.254998	H	3.634107	-1.200062	2.199298
H	-0.287822	1.863700	4.680798	C	4.210688	0.826844	2.682998
H	-2.224310	0.582881	5.586898	H	3.703979	1.770639	2.943298
H	-3.822599	-0.497234	4.034298	H	4.855491	0.553850	3.525898
C	1.688164	3.339919	-1.427102	H	4.491185	1.158546	0.790398
C	-0.428422	1.842299	-0.290002	O	5.054386	0.977452	1.557898
C	1.820677	1.997321	-1.193302	C	1.767225	-2.971780	-0.475502
H	2.507758	3.901227	-1.862302	O	2.051315	-1.984377	0.537698
Br	3.454285	1.116236	-1.647402	B3LYP/6-31G** Energy =			-6817.817963
C	-0.598536	3.244797	-0.529902	B3LYP/6-31G** Free Energy =			-6817.838773
C	0.476257	4.000008	-1.101202	M06-2X/LACVP** Derived Free Energy =			-1700.444309
C	0.309144	5.391506	-1.332202	M06-2X/LACVP** Derived Solution Free Energy =			-1700.466088
C	-0.871662	6.020495	-1.012702	Number of Imaginary Frequencies =			0
C	-1.936155	5.278384	-0.448802	B3LYP/6-31G** Geometry			

C	-1.686528	-0.902164	-1.180804	H	3.579521	-3.090084	1.824096
C	-2.203159	-2.220152	-1.050804	C	1.331530	-2.734333	0.295196
C	-2.971167	-2.578034	0.025596	H	0.512243	-2.166214	-0.152804
C	-1.928207	0.039842	-0.186504	H	1.506310	-3.600037	-0.353404
Br	-1.752088	-3.512262	-2.378804	O	-0.946222	-0.642081	-2.286204
H	-3.352490	-3.590325	0.104396	H	-0.577202	0.251311	-2.212404
C	-3.251245	-1.641228	1.053096	O	1.364316	1.048866	2.318896
C	-2.707715	-0.318240	0.959396	C	2.188816	1.049847	3.491496
C	-2.960294	0.586966	2.026996	H	3.224311	0.803724	3.232996
C	-3.720103	0.208383	3.111596	H	2.153640	2.074348	3.877196
C	-4.268233	-1.093404	3.192496	C	1.688694	0.082159	4.560096
C	-4.033553	-1.998010	2.183096	H	2.114701	0.389349	5.522696
H	-2.541471	1.585856	1.980896	H	0.593797	0.186984	4.635896
H	-3.898787	0.916587	3.915296	H	1.790357	-1.558843	3.497196
H	-4.866539	-1.376391	4.053196	O	2.087363	-1.260050	4.369896
H	-4.439177	-3.004700	2.236796	C	2.615150	-1.859362	0.319696
C	-0.095517	3.935700	-0.591704	O	2.436074	-0.812558	1.309096
C	-1.323975	1.401528	-0.331604				
C	0.653657	2.831183	-0.280104	B3LYP/6-31G** Energy =			-6817.825354
H	0.385405	4.902089	-0.698004	B3LYP/6-31G** Free Energy =			-6817.847319
Br	2.541361	3.001939	-0.085104	M06-2X/LACVP** Derived Free Energy =			-1700.450153
C	-2.119649	2.542146	-0.684904	M06-2X/LACVP** Derived Solution Free Energy =			-1700.471736
C	-1.494320	3.825432	-0.798904	Number of Imaginary Frequencies =			0
C	-2.280594	4.958450	-1.138704				
C	-3.631797	4.834281	-1.364304	B3LYP/6-31G** Geometry			
C	-4.250926	3.566195	-1.262904				
C	-3.516151	2.449078	-0.932904	C	-0.881445	1.748283	-0.707795
H	-1.792172	5.925639	-1.220304	C	-0.552081	3.126692	-0.580295
H	-4.224777	5.705895	-1.624104	C	-1.061802	3.887978	0.437805
H	-5.316728	3.473120	-1.448804	C	-1.735729	1.154560	0.214305
H	-3.998874	1.481389	-0.858504	Br	0.639398	3.907323	-1.848595
B	1.556898	0.229262	1.254996	H	-0.792529	4.935785	0.515605
C	0.924319	-3.199224	1.619696	C	-1.929186	3.313355	1.402405
C	0.044128	1.552297	-0.130304	C	-2.268850	1.925846	1.295005
O	0.799203	0.442879	0.109996	C	-3.133335	1.368323	2.276205
C	3.686089	-0.149387	-3.533204	C	-3.633355	2.141510	3.300605
C	2.669067	-1.099364	-3.462404	C	-3.297392	3.512119	3.402105
C	2.297354	-1.650555	-2.233204	C	-2.461407	4.082941	2.470305
C	2.944263	-1.261570	-1.053904	H	-3.396007	0.318216	2.210305
C	3.963485	-0.300893	-1.137404	H	-4.291343	1.694393	4.040005
C	4.329898	0.252998	-2.361404	H	-3.698907	4.108608	4.215505
H	3.971099	0.278607	-4.489804	H	-2.193035	5.133848	2.537905
H	2.150860	-1.413352	-4.363704	C	-2.716018	-3.032466	-0.287195
H	1.481038	-2.363436	-2.217304	C	-2.095491	-0.288249	0.040305
H	4.461793	0.026995	-0.230704	C	-1.580528	-2.646835	0.373805
H	5.117715	0.999680	-2.400004	H	-2.941990	-4.086071	-0.410995
C	0.575810	-3.574016	2.714596	Br	-0.387994	-3.960804	1.073205
H	0.278103	-3.901709	3.683896	C	-3.291081	-0.668981	-0.657495
C	3.803931	-2.682590	0.835396	C	-3.601344	-2.058189	-0.816895
H	4.018812	-3.505595	0.148096	C	-4.785034	-2.434920	-1.505295
H	4.695245	-2.056110	0.910696	C	-5.631859	-1.481543	-2.021395

C	-5.326296	-0.108735	-1.869195				
C	-4.186506	0.288296	-1.205795	C	-1.895198	0.055821	-0.862597
H	-5.008306	-3.492526	-1.617395	C	-3.013353	-0.810508	-0.716497
H	-6.534151	-1.779267	-2.546795	C	-3.789152	-0.791459	0.410703
H	-5.997415	0.639148	-2.280795	C	-1.561542	0.934600	0.159303
H	-3.959334	1.342402	-1.093495	Br	-3.392332	-2.060984	-2.105597
B	1.131129	-1.045764	0.787005	H	-4.637794	-1.461405	0.495803
C	1.222363	-2.307861	-3.191795	C	-3.471496	0.078821	1.483803
C	-1.261365	-1.270927	0.551405	C	-2.334442	0.942049	1.367603
O	-0.160274	-0.928798	1.284005	C	-2.018189	1.780429	2.471603
C	5.294952	1.853447	-0.310395	C	-2.788189	1.771778	3.613603
C	3.989046	2.110912	-0.730995	C	-3.917443	0.926649	3.718203
C	3.127973	1.056989	-1.028595	C	-4.248195	0.096770	2.672303
C	3.548409	-0.275799	-0.905195	H	-1.153048	2.430374	2.408903
C	4.863215	-0.524265	-0.493595	H	-2.523548	2.419361	4.444303
C	5.729687	0.532458	-0.197395	H	-4.516342	0.931987	4.623803
H	5.967131	2.672265	-0.071895	H	-5.108637	-0.563575	2.740503
H	3.623419	3.129202	-0.824895	C	1.723035	3.733292	-0.214197
H	2.115668	1.279163	-1.347095	C	-0.426881	1.895028	-0.015897
H	5.222542	-1.542155	-0.390695	C	1.958851	2.401677	-0.002797
H	6.744193	0.318085	0.126105	H	2.552679	4.429240	-0.274997
C	0.389984	-3.097483	-3.569095	Br	3.737910	1.756364	0.204003
H	-0.343598	-3.793303	-3.904295	C	-0.694693	3.286945	-0.262497
C	3.032676	-2.802613	-0.841195	C	0.395265	4.210176	-0.361097
H	3.882684	-3.116191	-1.453995	C	0.131052	5.584093	-0.604597
H	3.323077	-2.835305	0.210305	C	-1.159219	6.036375	-0.755697
H	2.213094	-3.506635	-0.997995	C	-2.238577	5.126743	-0.670397
C	2.223637	-1.338435	-2.749995	C	-2.014062	3.789229	-0.428897
H	1.876610	-0.326844	-2.986095	H	0.970396	6.270740	-0.673097
H	3.157741	-1.484210	-3.305195	H	-1.351553	7.088287	-0.943897
O	-0.335027	1.078198	-1.754295	H	-3.255154	5.486207	-0.798297
H	-0.387102	0.121096	-1.594695	H	-2.849705	3.101982	-0.369197
O	2.176128	-1.017536	1.651605	B	1.748758	-0.645610	-0.679597
C	1.993926	-0.921841	3.072605	C	4.640810	-1.396893	1.417503
H	1.489801	0.019846	3.314405	C	0.888391	1.464645	0.083003
H	1.375648	-1.754457	3.428805	O	1.178108	0.143927	0.316203
C	3.379327	-0.955204	3.696205	C	-1.521236	-3.698402	2.145703
H	3.286825	-0.876306	4.784905	C	-1.226427	-3.554821	0.789203
H	3.849153	-1.926992	3.471005	C	0.048698	-3.162602	0.385503
H	4.207099	0.094818	2.301005	C	1.051415	-2.891065	1.329703
O	4.183298	0.126417	3.269205	C	0.745406	-3.043346	2.687403
C	2.556939	-1.400126	-1.230595	C	-0.529720	-3.444765	3.091603
O	1.288632	-1.148459	-0.565895	H	-2.514655	-4.002440	2.462503
				H	-1.991237	-3.718473	0.036203
B3LYP/6-31G** Energy =			-6817.826916	H	0.265904	-3.068616	-0.674297
B3LYP/6-31G** Free Energy =			-6817.844135	H	1.492618	-2.850893	3.449703
M06-2X/LACVP** Derived Free Energy =			-1700.448955	H	-0.745426	-3.551052	4.150903
M06-2X/LACVP** Derived Solution Free Energy =			-1700.469116	C	5.778625	-1.154765	1.091403
Number of Imaginary Frequencies =			0	H	6.782439	-0.947128	0.801303
				C	3.207756	-3.834802	0.483703
B3LYP/6-31G** Geometry				H	3.314516	-4.459609	1.374903

H	2.644920	-4.395666	-0.265797	C	-6.249997	-0.630536	-0.489700
H	4.200170	-3.604265	0.089203	C	-5.425291	-1.775732	-0.387400
C	3.273692	-1.689506	1.847303	C	-4.054292	-1.653026	-0.352400
H	2.741451	-0.752272	2.036803	H	-6.304107	1.508064	-0.627200
H	3.323057	-2.231409	2.797603	H	-7.329596	-0.742341	-0.517000
O	-1.214003	-0.023722	-2.037697	H	-5.879087	-2.760834	-0.334100
H	-0.331277	0.384622	-1.966097	H	-3.431288	-2.536523	-0.271000
O	1.619786	-0.197401	-1.970297	B	0.559692	1.784196	0.678000
C	2.095337	-0.968932	-3.086997	C	5.092686	3.026317	-0.944000
H	2.733379	-0.312272	-3.689797	C	-1.463205	1.059686	-0.409700
H	2.688984	-1.810069	-2.722597	O	-0.104605	1.224793	-0.403200
C	0.929705	-1.477658	-3.926297	C	4.236410	-2.084387	-0.855100
H	0.344959	-0.627421	-4.304297	C	3.713608	-1.625690	0.354000
H	1.349272	-1.997484	-4.797697	C	3.239702	-0.318492	0.461200
H	-0.626721	-1.895059	-2.837097	C	3.267398	0.551508	-0.637000
O	0.109947	-2.393506	-3.222097	C	3.793400	0.078811	-1.846700
C	2.459638	-2.538455	0.830103	C	4.275806	-1.225887	-1.953400
O	2.366583	-1.822649	-0.419397	H	4.607215	-3.101785	-0.941800
B3LYP/6-31G** Energy =				H	3.648411	-2.287090	1.212700
B3LYP/6-31G** Free Energy =				H	2.839100	0.027806	1.407500
M06-2X/LACVP** Derived Free Energy =				H	3.836097	0.729411	-2.712500
M06-2X/LACVP** Derived Solution Free Energy =				H	4.678508	-1.571185	-2.901400
Number of Imaginary Frequencies =				C	6.013186	3.148821	-1.716600
				H	6.830285	3.247725	-2.392900
B3LYP/6-31G** Geometry				C	2.178988	2.583203	-1.765800
				H	2.957087	2.792607	-2.503100
				H	1.446891	1.901500	-2.197900
C	-0.548591	-1.805009	0.880100	H	1.673684	3.523501	-1.528200
C	0.314714	-2.934305	0.917300	C	3.981787	2.901912	-0.005700
C	0.606517	-3.661904	-0.204200	H	3.566082	3.894010	0.209300
C	-1.105393	-1.407412	-0.328100	H	4.340789	2.495713	0.946700
Br	1.102816	-3.407202	2.600400	O	-0.850495	-1.106411	2.003800
H	1.269421	-4.517901	-0.143200	H	-0.318593	-1.426708	2.752100
C	0.051816	-3.288207	-1.453000	O	-0.139109	1.987693	1.830200
C	-0.806690	-2.142111	-1.519600	C	0.483489	2.381695	3.053800
C	-1.329891	-1.774913	-2.790900	H	1.406292	1.811000	3.206200
C	-1.028588	-2.503412	-3.919500	H	0.737084	3.449097	3.027300
C	-0.187483	-3.639208	-3.846000	C	-0.514809	2.085891	4.164100
C	0.341519	-4.019805	-2.635400	H	-0.055910	2.293893	5.136500
H	-1.973095	-0.905416	-2.862600	H	-1.385212	2.751587	4.053500
H	-1.439889	-2.202213	-4.878400	H	-1.264302	0.550387	3.276700
H	0.039720	-4.203807	-4.745100	O	-0.907303	0.724889	4.161700
H	0.993823	-4.886002	-2.563600	C	2.797991	2.001606	-0.488100
C	-3.674209	2.065476	-0.577000	O	1.880391	2.107002	0.621900
C	-2.007999	-0.214616	-0.375600	B3LYP/6-31G** Energy =			
C	-2.311410	2.195882	-0.527400	B3LYP/6-31G** Free Energy =			
H	-4.302013	2.945273	-0.666200	M06-2X/LACVP** Derived Free Energy =			
Br	-1.525618	3.932586	-0.642600	M06-2X/LACVP** Derived Solution Free Energy =			
C	-3.431798	-0.376223	-0.415700	Number of Imaginary Frequencies =			
C	-4.270803	0.780773	-0.513600				
C	-5.681703	0.620467	-0.551300				

B3LYP/6-31G** Geometry				H	5.221781	1.473803	0.065301
				H	4.279094	0.767186	-1.267199
C	-2.646572	-1.060943	-0.528399	H	3.781365	2.309476	-0.543299
C	-2.910847	-2.422348	-0.209899	C	3.330883	1.346568	2.046101
C	-2.511537	-2.984340	0.973401	H	2.644093	0.822255	2.719701
C	-1.961987	-0.268830	0.385101	H	4.334185	1.239787	2.475901
Br	-3.861028	-3.475365	-1.503699	O	-3.046083	-0.508650	-1.698199
H	-2.729917	-4.025444	1.185301	H	-3.508770	-1.184459	-2.220199
C	-1.811151	-2.202727	1.925601	O	2.201621	-0.676953	-1.696399
C	-1.529777	-0.828222	1.627401	C	1.734432	-1.282762	-2.908099
C	-0.820391	-0.064109	2.597701	H	0.681527	-1.042581	-3.085699
C	-0.423680	-0.628202	3.789901	H	2.337524	-0.882250	-3.730299
C	-0.705355	-1.985807	4.080101	C	1.946260	-2.785458	-2.791899
C	-1.383541	-2.754519	3.163301	H	1.291767	-3.179870	-1.997599
H	-0.588410	0.972495	2.381501	H	1.654769	-3.265563	-3.732799
H	0.110908	-0.024792	4.517801	H	3.562757	-2.657628	-1.747999
H	-0.386247	-2.414501	5.025101	O	3.302766	-3.115133	-2.561299
H	-1.606722	-3.797424	3.372501	C	3.312697	0.608368	0.673801
C	-1.079563	3.836786	-0.636099	O	1.941695	0.703242	0.229601
C	-1.681314	1.158475	0.039901				
C	-0.300044	2.807601	-1.094799	B3LYP/6-31G** Energy =			-6817.821357
H	-0.839082	4.860491	-0.901599	B3LYP/6-31G** Free Energy =			-6817.844354
Br	1.197449	3.182528	-2.215099	M06-2X/LACVP** Derived Free Energy =			-1700.445703
C	-2.519333	2.214459	0.521801	M06-2X/LACVP** Derived Solution Free Energy =			-1700.469802
C	-2.207058	3.570365	0.181101	Number of Imaginary Frequencies =			0
C	-3.035578	4.619550	0.661101				
C	-4.132173	4.348229	1.445901	B3LYP/6-31G** Geometry			
C	-4.446248	3.009824	1.781301	C	-2.640893	-0.967098	-0.346899
C	-3.661929	1.971038	1.332201	C	-2.813592	-2.350998	-0.065499
H	-2.786197	5.642954	0.393701	C	-2.335892	-2.926697	1.081601
H	-4.759188	5.157518	1.807501	C	-1.948794	-0.169297	0.556401
H	-5.315344	2.801208	2.398101	Br	-3.722591	-3.419599	-1.373599
H	-3.912110	0.948534	1.592401	H	-2.483591	-3.985498	1.264401
B	1.460105	0.163633	-0.925799	C	-1.636892	-2.137897	2.028701
C	2.965957	2.760361	1.980901	C	-1.430794	-0.744097	1.759101
C	-0.592019	1.456295	-0.762099	C	-0.698994	0.018804	2.713601
O	0.154600	0.445809	-1.297999	C	-0.214294	-0.561896	3.864401
C	4.316974	-3.554914	1.446801	C	-0.427693	-1.936596	4.128801
C	3.080664	-3.032037	1.831201	C	-1.123792	-2.705897	3.226001
C	2.770439	-1.698542	1.570601	H	-0.525295	1.071004	2.520701
C	3.687124	-0.858925	0.919601	H	0.338806	0.040905	4.578601
C	4.927234	-1.390702	0.545601	H	-0.040092	-2.378596	5.041501
C	5.238759	-2.728897	0.804301	H	-1.292591	-3.762897	3.413801
H	4.558093	-4.595409	1.642701	C	-1.173897	3.959203	-0.460499
H	2.350676	-3.662450	2.330701	C	-1.716295	1.268003	0.218901
H	1.799832	-1.308660	1.859701	C	-0.481697	2.935204	-1.052899
H	5.658822	-0.769389	0.040801	H	-0.956798	4.988004	-0.726599
H	6.203466	-3.122979	0.498001	Br	0.853503	3.322005	-2.360299
C	2.674835	3.931656	1.940901	C	-2.466796	2.317902	0.838201
H	2.409016	4.962251	1.899401	C	-2.182897	3.680103	0.496001
C	4.213883	1.329384	-0.333999				

C	-2.923298	4.723402	1.113901	B3LYP/6-31G** Geometry			
C	-3.908898	4.440301	2.030501				
C	-4.197097	3.095801	2.365101				
C	-3.495896	2.062502	1.785401				
H	-2.696699	5.751702	0.845201	C	-2.491602	-0.799079	-0.197694
H	-4.469498	5.245301	2.496101	C	-2.656020	-2.815277	1.168706
H	-4.980696	2.878100	3.084801	C	-1.828496	-0.129285	0.823306
H	-3.725495	1.035101	2.045001	Br	-3.766721	-3.043468	-1.458394
B	1.231906	0.236905	-1.168499	H	-2.970828	-3.846775	1.284606
C	4.814905	1.598508	1.984201	C	-2.004114	-2.153283	2.239406
C	-0.745495	1.579204	-0.719799	C	-1.583002	-0.793887	2.065406
O	-0.096695	0.574604	-1.378499	C	-0.925097	-0.152892	3.151906
C	4.243909	-3.485292	1.047801	C	-0.701102	-0.818194	4.336406
C	3.026608	-2.930793	1.449901	C	-1.119814	-2.159991	4.503606
C	2.733507	-1.597993	1.162401	C	-1.757719	-2.811385	3.474006
C	3.644307	-0.796293	0.457301	H	-0.602688	0.875805	3.035506
C	4.864507	-1.359692	0.067801	H	-0.198898	-0.307599	5.152706
C	5.162108	-2.692591	0.360701	H	-0.936418	-2.670792	5.444006
H	4.472210	-4.524092	1.267101	H	-2.084028	-3.841682	3.588806
H	2.301209	-3.532594	1.989301	C	-0.448962	3.908204	0.123206
H	1.784507	-1.178694	1.480701	C	-1.371084	1.276312	0.593706
H	5.591207	-0.765291	-0.473999	C	0.379129	2.833196	-0.070894
H	6.112608	-3.111091	0.042701	H	-0.086053	4.913300	-0.062294
C	5.941805	1.672009	2.412701	Br	2.170131	3.097881	-0.662094
H	6.934204	1.729910	2.795601	C	-2.253775	2.383619	0.805806
C	4.093805	1.293508	-0.977699	C	-1.782063	3.714715	0.566106
H	5.136405	1.450309	-0.692199	C	-2.657054	4.813623	0.778306
H	4.053705	0.662308	-1.867299	C	-3.947656	4.612834	1.209406
H	3.649704	2.263107	-1.219099	C	-4.416667	3.299238	1.447806
C	3.452405	1.522007	1.466001	C	-3.592776	2.213731	1.251306
H	3.079904	2.528407	1.239501	H	-2.285545	5.817719	0.592206
H	2.784705	1.101707	2.226601	H	-4.608548	5.459639	1.367806
O	-3.125594	-0.401998	-1.477199	H	-5.436468	3.147146	1.788506
H	-3.568193	-1.087999	-2.003599	H	-3.959785	1.210534	1.437806
O	1.819006	-0.668894	-1.997099	B	1.041303	-0.165509	-1.182894
C	1.107907	-1.346495	-3.042599	C	4.342872	-3.749438	-0.163694
H	0.257206	-0.748095	-3.384399	C	-0.073382	1.506300	0.163706
H	1.817607	-1.472994	-3.865599	O	0.804609	0.463493	0.025606
C	0.647408	-2.709795	-2.541799	C	5.780614	1.064650	1.016106
H	-0.112292	-2.571496	-1.755099	C	5.179207	0.228855	1.955306
H	0.168109	-3.250195	-3.366199	C	4.189199	-0.674636	1.564206
H	2.188708	-3.003194	-1.412799	C	3.782698	-0.756733	0.227806
O	1.725409	-3.509594	-2.096599	C	4.398005	0.086162	-0.708894
C	3.295705	0.667407	0.170701	C	5.384913	0.989753	-0.320294
O	1.884005	0.802306	-0.113899	H	6.549220	1.768743	1.321306
				H	5.477007	0.278053	2.998806
				H	3.735693	-1.314932	2.312006
				H	4.091805	0.041065	-1.749194
				H	5.845619	1.635549	-1.062494
				C	5.079667	-4.421044	0.518206
				H	5.738062	-5.006250	1.117106
B3LYP/6-31G** Energy =			-6817.822042				
B3LYP/6-31G** Free Energy =			-6817.844022				
M06-2X/LACVP** Derived Free Energy =			-1700.445193				
M06-2X/LACVP** Derived Solution Free Energy =			-1700.466498				
Number of Imaginary Frequencies =			0				

C	1.846285	-2.327516	0.868206	C	3.989226	-1.852477	-0.110902
H	2.420179	-2.972021	1.537806	C	5.392928	-2.053465	-0.033402
H	1.386292	-1.526212	1.446606	C	6.252518	-0.982957	0.050298
H	1.054279	-2.933409	0.418606	C	5.738306	0.334638	0.061898
C	3.446079	-2.949830	-0.992594	C	4.382104	0.561526	-0.017502
H	2.660474	-3.588023	-1.415694	H	5.773837	-3.071061	-0.037402
H	3.998883	-2.526935	-1.838794	H	7.324220	-1.145747	0.111598
O	-2.756896	-0.133177	-1.348394	H	6.420499	1.176245	0.136398
H	-3.045402	-0.753474	-2.039894	H	3.999295	1.575223	-0.003602
O	0.345607	0.247597	-2.280894	B	-0.984577	-1.506223	0.748298
C	0.395901	-0.458804	-3.523394	C	-5.599174	-1.814065	-1.085102
H	1.418501	-0.473612	-3.919894	C	1.201922	-1.418603	-0.238402
H	0.069792	-1.494401	-3.371494	O	-0.155679	-1.252215	-0.335002
C	-0.545993	0.257904	-4.478094	C	-3.100415	2.659858	-1.883302
H	-0.153584	1.266301	-4.682094	C	-2.969712	2.339359	-0.531602
H	-0.586298	-0.284795	-5.428494	C	-2.968300	1.005559	-0.128502
H	-1.802889	0.732315	-3.095094	C	-3.082590	-0.034142	-1.062402
O	-1.867393	0.317116	-3.969294	C	-3.213793	0.300157	-2.415502
C	2.740889	-1.775024	-0.244494	C	-3.225105	1.635857	-2.821202
O	1.922994	-1.198417	-1.291994	H	-3.100524	3.697658	-2.203302
				H	-2.844119	3.117660	0.215098
B3LYP/6-31G** Energy =			-6817.824556	H	-2.865098	0.772260	0.925698
B3LYP/6-31G** Free Energy =			-6817.844027	H	-3.309086	-0.478544	-3.163502
M06-2X/LACVP** Derived Free Energy =			-1700.448609	H	-3.324608	1.872856	-3.876502
M06-2X/LACVP** Derived Solution Free Energy =			-1700.469989	C	-6.465774	-1.807473	-1.926302
Number of Imaginary Frequencies =			0	H	-7.232674	-1.791280	-2.665602
				C	-2.678268	-2.514038	-1.623602
B3LYP/6-31G** Geometry				H	-3.407567	-2.578745	-2.433802
				H	-1.700670	-2.262729	-2.035102
C	0.891295	1.614794	0.891698	H	-2.611259	-3.497338	-1.150202
C	0.376283	2.939990	0.854298	C	-4.557474	-1.836355	-0.063002
C	0.477476	3.711991	-0.271302	H	-4.506565	-2.832255	0.394498
C	1.477800	1.067300	-0.242002	H	-4.805980	-1.131058	0.737898
Br	-0.525224	3.618881	2.392298	O	0.792001	0.956093	2.076398
H	0.081566	4.721687	-0.272802	H	0.875209	-0.008406	1.965098
C	1.067880	3.188896	-1.449502	O	-0.391676	-1.591517	1.981398
C	1.555493	1.842200	-1.445602	C	-1.142273	-1.893924	3.172798
C	2.107197	1.328705	-2.651202	H	-1.937667	-2.606731	2.930798
C	2.182690	2.106906	-3.785102	H	-0.435469	-2.363918	3.861998
C	1.711678	3.440602	-3.780002	C	-1.741985	-0.652530	3.827598
C	1.163773	3.966797	-2.633202	H	-2.412789	-0.152536	3.113298
H	2.468607	0.306909	-2.672302	H	-2.364881	-0.998635	4.662698
H	2.606494	1.691110	-4.694502	H	-0.438898	0.790282	3.651698
H	1.779673	4.042602	-4.681002	O	-0.780193	0.228979	4.364898
H	0.790764	4.987293	-2.615602	C	-3.126677	-1.486842	-0.580502
C	3.093636	-2.950086	-0.182602	O	-2.330876	-1.624035	0.624198
C	2.044312	-0.317195	-0.192002				
C	1.742634	-2.735598	-0.239402	B3LYP/6-31G** Energy =			-6817.821022
H	3.484045	-3.962082	-0.184902	B3LYP/6-31G** Free Energy =			-6817.843147
Br	0.550748	-4.222609	-0.323102	M06-2X/LACVP** Derived Free Energy =			-1700.439696
C	3.464814	-0.519982	-0.111302	M06-2X/LACVP** Derived Solution Free Energy =			-1700.462220

Number of Imaginary Frequencies =				0	H	-1.876221	-2.124070	4.807092	
					C	0.628846	-4.464805	1.573692	
B3LYP/6-31G** Geometry					H	0.003635	-5.262096	1.162092	
					H	1.675842	-4.730720	1.411592	
C	-2.098984	0.478433	-0.908708		H	0.446547	-4.384902	2.648192	
C	-3.347092	-0.034049	-0.460008		C	-1.152029	-2.705580	1.189992	
C	-3.909986	0.352759	0.727592		H	-1.383916	-1.793977	0.630892	
C	-1.398372	1.367023	-0.100908		H	-1.826940	-3.485971	0.820392	
Br	-4.205910	-1.360337	-1.551908		O	-1.556590	0.114126	-2.093808	
H	-4.862392	-0.060028	1.041892		H	-2.122299	-0.556266	-2.509208	
C	-3.235473	1.282649	1.557492		O	2.025409	-0.011025	2.011592	
C	-1.954066	1.782131	1.148192		C	2.634003	-0.443433	3.234792	
C	-1.274554	2.676122	2.022792		H	1.920405	-0.305123	4.056992	
C	-1.839548	3.064530	3.216092		H	2.895388	-1.503937	3.173992	
C	-3.111155	2.580948	3.608192		C	3.878914	0.399249	3.460492	
C	-3.790667	1.704957	2.794992		H	3.589029	1.462253	3.489392	
H	-0.297048	3.047408	1.736792		H	4.308211	0.145943	4.436392	
H	-1.302639	3.748722	3.866592		H	4.486913	0.303541	1.623092	
H	-3.543250	2.898554	4.552192		O	4.884111	0.156435	2.495092	
H	-4.762673	1.317471	3.087992		C	0.311465	-3.128501	0.886592	
C	2.539244	2.508268	-1.461408		O	1.201578	-2.175213	1.505992	
C	-0.043966	1.807804	-0.552508						
C	2.295527	1.268972	-0.929308		B3LYP/6-31G** Energy =				-6817.820458
H	3.532548	2.760954	-1.816108		B3LYP/6-31G** Free Energy =				-6817.842013
Br	3.705909	-0.018448	-0.871108		M06-2X/LACVP** Derived Free Energy =				-1700.440328
C	0.177852	3.101401	-1.121708		M06-2X/LACVP** Derived Solution Free Energy =				-1700.463417
C	1.492757	3.458783	-1.565308		Number of Imaginary Frequencies =				0
C	1.717075	4.747680	-2.118908						
C	0.687188	5.651494	-2.237808		B3LYP/6-31G** Geometry				
C	-0.614917	5.298712	-1.810208						
C	-0.864034	4.057916	-1.268208		C	-2.436606	-0.405799	-0.900395	
H	2.719779	5.004866	-2.449608		C	-3.448406	-1.315399	-0.484795	
H	0.869102	6.634192	-2.662308		C	-3.961606	-1.302099	0.784205	
H	-1.425507	6.014324	-1.912208		C	-1.946306	0.527501	0.003605	
H	-1.865038	3.795230	-0.944808		Br	-4.094806	-2.583699	-1.773695	
B	1.339797	-0.855715	1.193592		H	-4.735706	-2.006699	1.068105	
C	-1.419926	-2.483176	2.609692		C	-3.474106	-0.369699	1.733305	
C	1.007622	0.909290	-0.447808		C	-2.447006	0.551501	1.342405	
O	0.770504	-0.343607	0.037792		C	-1.961106	1.466501	2.318005	
C	1.196159	-3.575513	-3.350308		C	-2.470006	1.472201	3.597105	
C	2.219460	-3.495927	-2.404108		C	-3.491406	0.568001	3.975705	
C	1.914662	-3.337423	-1.054408		C	-3.979806	-0.334899	3.060305	
C	0.584563	-3.245004	-0.619308		H	-1.168806	2.153701	2.044405	
C	-0.433838	-3.315290	-1.577608		H	-2.082306	2.178001	4.325805	
C	-0.129240	-3.482694	-2.930908		H	-3.884606	0.588601	4.987605	
H	1.430957	-3.702216	-4.403008		H	-4.762106	-1.036799	3.337505	
H	3.257659	-3.556242	-2.717308		C	1.019894	3.380001	-1.326095	
H	2.717263	-3.263734	-0.327708		C	-0.927606	1.518801	-0.461895	
H	-1.476136	-3.220175	-1.292208		C	1.384994	2.144401	-0.862295	
H	-0.935041	-3.537983	-3.657908		H	1.777294	4.085101	-1.650695	
C	-1.663023	-2.293673	3.777392		Br	3.235794	1.674501	-0.810095	

C	-1.338806	2.800401	-0.954295	M06-2X/LACVP** Derived Solution Free Energy =			-1700.464208
C	-0.349506	3.741101	-1.387195	Number of Imaginary Frequencies =			0
C	-0.756606	5.012801	-1.871395				
C	-2.088706	5.349901	-1.929595	B3LYP/6-31G** Geometry			
C	-3.069806	4.423501	-1.504095				
C	-2.706006	3.183301	-1.029395	C	2.100206	0.041944	0.856698
H	0.006694	5.714801	-2.195995	C	2.912826	-1.128441	0.909498
H	-2.390206	6.324501	-2.301395	C	3.350438	-1.757334	-0.227002
H	-4.120406	4.694201	-1.552995	C	1.677097	0.509637	-0.385202
H	-3.465406	2.480701	-0.705595	Br	3.396039	-1.824133	2.624998
B	1.495494	-0.280299	1.161405	H	3.983253	-2.635423	-0.151502
C	-0.349206	-3.066199	1.638705	C	2.991429	-1.257940	-1.504302
C	0.418794	1.197701	-0.422995	C	2.124909	-0.118955	-1.586402
O	0.814294	-0.049799	-0.025295	C	1.751600	0.346538	-2.877802
C	4.270794	-2.295399	-3.004795	C	2.227211	-0.263954	-4.016102
C	3.033594	-2.934699	-3.046295	C	3.097431	-1.377338	-3.930302
C	2.262394	-3.055799	-1.887995	C	3.465939	-1.864532	-2.697802
C	2.712894	-2.538699	-0.667795	H	1.086885	1.200026	-2.954102
C	3.961394	-1.899599	-0.639595	H	1.933704	0.113041	-4.991502
C	4.731894	-1.776900	-1.793595	H	3.471339	-1.843132	-4.837302
H	4.869394	-2.199700	-3.905795	H	4.130955	-2.720820	-2.617502
H	2.659994	-3.340099	-3.982195	C	-0.993263	3.914390	-0.339602
H	1.302894	-3.556299	-1.954995	C	0.760677	1.691721	-0.408202
H	4.326194	-1.488599	0.295905	C	-1.471340	2.637081	-0.207902
H	5.694194	-1.275000	-1.746795	H	-1.675478	4.756877	-0.305402
C	-1.009206	-3.068699	2.650105	Br	-3.336935	2.342048	0.057698
H	-1.598106	-3.046099	3.537305	C	1.284253	3.018330	-0.546202
C	2.603293	-3.790299	1.504205	C	0.394233	4.139714	-0.519402
H	2.617793	-4.743799	0.968805	C	0.917810	5.452423	-0.664402
H	3.633994	-3.507899	1.730805	C	2.268006	5.657347	-0.826502
H	2.055393	-3.914299	2.441805	C	3.152226	4.552563	-0.847102
C	0.440794	-3.059699	0.409505	C	2.674449	3.268754	-0.709402
H	0.009494	-2.347299	-0.299995	H	0.228795	6.292711	-0.643302
H	0.388593	-4.051699	-0.053695	H	2.658589	6.664654	-0.936502
O	-1.934906	-0.418799	-2.160095	H	4.218023	4.720382	-0.970802
H	-2.398606	-1.101899	-2.671795	H	3.358964	2.428366	-0.724102
O	1.602794	0.746401	2.050405	B	-1.527486	-0.430420	0.923798
C	2.294594	0.618601	3.297405	C	-4.954580	-0.776181	0.265898
H	1.825094	1.333201	3.979805	C	-0.604620	1.510096	-0.248302
H	2.178994	-0.393999	3.699505	O	-1.152398	0.252087	-0.216302
C	3.770994	0.959401	3.130205	C	-0.115532	-3.482395	-3.325602
H	4.256294	0.916901	4.112205	C	-1.315943	-2.886216	-3.704102
H	4.247594	0.196201	2.494405	C	-2.216450	-2.435432	-2.736302
H	3.623594	2.269301	1.720905	C	-1.931248	-2.571927	-1.372802
O	3.976394	2.263901	2.623505	C	-0.718837	-3.173606	-1.005202
C	1.936594	-2.704799	0.645205	C	0.180171	-3.622890	-1.968702
O	2.033194	-1.502099	1.437705	H	0.588674	-3.824983	-4.077202
				H	-1.557245	-2.764220	-4.756202
B3LYP/6-31G** Energy =			-6817.819499	H	-3.139759	-1.972248	-3.065502
B3LYP/6-31G** Free Energy =			-6817.838664	H	-0.476636	-3.280101	0.047298
M06-2X/LACVP** Derived Free Energy =			-1700.441162	H	1.116679	-4.075773	-1.659102

C	-5.749786	-0.422395	1.103698	Br	-0.484443	4.259010	-0.229006
H	-6.450192	-0.110107	1.843198	C	3.185047	1.352172	0.322194
C	-3.579933	-3.450656	0.292098	C	3.393901	2.765964	0.230594
H	-4.113523	-3.983666	-0.499902	C	4.714720	3.284914	0.290594
H	-2.816721	-4.117443	0.699798	C	5.793789	2.443974	0.432394
H	-4.285837	-3.189069	1.084298	C	5.592536	1.046481	0.518894
C	-4.010572	-1.191664	-0.770302	C	4.323716	0.513729	0.464894
H	-3.528188	-0.304055	-1.192002	H	4.855361	4.360009	0.219794
H	-4.572264	-1.673174	-1.578302	H	6.800204	2.849036	0.476294
O	1.766493	0.753138	1.950198	H	6.448211	0.386949	0.627594
H	1.637703	0.206836	2.755998	H	4.180775	-0.558365	0.530494
O	-1.146994	0.051087	2.143698	B	-1.214466	0.989138	-1.035506
C	-1.494983	-0.593019	3.359598	C	-5.939686	0.455316	0.467994
H	-1.904997	0.175973	4.029398	C	0.783361	1.699263	0.116194
H	-2.270170	-1.350233	3.201398	O	-0.510757	1.242311	0.122694
C	-0.282872	-1.245798	4.010198	C	-2.403601	-2.594517	2.722994
H	-0.607363	-1.747604	4.934198	C	-2.413607	-2.740717	1.334794
H	0.151442	-2.002190	3.350298	C	-2.734066	-1.659505	0.517094
H	0.417599	0.448114	4.720898	C	-3.046219	-0.408593	1.072694
O	0.784312	-0.334579	4.285798	C	-3.034614	-0.273094	2.464794
C	-2.921855	-2.180345	-0.269502	C	-2.715355	-1.357706	3.283594
O	-2.230165	-1.599832	0.856698	H	-2.147733	-3.435327	3.360094
B3LYP/6-31G** Energy =				H	-2.168443	-3.697526	0.883794
B3LYP/6-31G** Free Energy =				H	-2.732571	-1.794005	-0.560706
M06-2X/LACVP** Derived Free Energy =				H	-3.272578	0.679715	2.923394
M06-2X/LACVP** Derived Solution Free Energy =				H	-2.707550	-1.230006	4.362094
Number of Imaginary Frequencies =				C	-6.856787	0.445050	1.253394
				H	-7.665788	0.424281	1.946194
				C	-3.431523	2.127821	0.804194
B3LYP/6-31G** Geometry				H	-4.227321	2.196451	1.548894
				H	-2.473315	2.346185	1.274494
C	1.574944	-1.395467	-0.827906	H	-3.619795	2.885328	0.038494
C	1.467890	-2.813563	-0.762706	C	-4.838086	0.474974	-0.489506
C	1.430666	-3.470062	0.438994	H	-5.014056	1.250681	-1.245106
C	1.628872	-0.653769	0.347394	H	-4.799322	-0.482727	-1.021206
Br	1.356653	-3.794759	-2.392606	O	1.651965	-0.838270	-2.062606
H	1.354225	-4.551959	0.461894	H	1.260898	0.053245	-2.042706
C	1.475293	-2.744364	1.657294	O	-0.518068	0.943212	-2.213006
C	1.563547	-1.315367	1.615194	C	-1.099377	0.703533	-3.512706
C	1.602174	-0.608668	2.847694	H	-1.962952	1.363166	-3.652906
C	1.561848	-1.278467	4.050394	H	-0.323866	0.986704	-4.229806
C	1.479795	-2.690164	4.088294	C	-1.509332	-0.748351	-3.738506
C	1.436268	-3.405162	2.913394	H	-1.595038	-0.905848	-4.821306
H	1.663114	0.474029	2.830994	H	-0.708457	-1.407781	-3.373806
H	1.592669	-0.717468	4.979894	H	-2.882123	-0.525299	-2.384406
H	1.451876	-3.205263	5.043794	O	-2.766244	-1.084404	-3.167806
H	1.373127	-4.490160	2.927994	C	-3.441575	0.745822	0.150594
C	2.274933	3.622706	0.072594	O	-2.561275	0.756889	-1.018806
C	1.849228	0.825522	0.262994	B3LYP/6-31G** Energy =			
C	1.010513	3.100254	0.014894				
H	2.425173	4.693801	-0.008206	B3LYP/6-31G** Free Energy =			

M06-2X/LACVP** Derived Free Energy =				-1700.445543	H	5.415588	0.651725	2.879595
M06-2X/LACVP** Derived Solution Free Energy =				-1700.467826	C	5.106704	-4.348876	0.858895
Number of Imaginary Frequencies =				0	H	5.780106	-4.866774	1.501695
					C	1.858597	-2.258387	1.051495
B3LYP/6-31G** Geometry					H	2.449499	-2.826185	1.773895
					H	1.393094	-1.410789	1.554295
C	-2.576708	-0.658702	-0.112705	H	1.070299	-2.915390	0.672895	
C	-2.988304	-1.998403	0.130995	C	3.435800	-3.045682	-0.761405	
C	-2.723502	-2.632502	1.315895	H	2.648602	-3.727985	-1.105305	
C	-1.844010	0.019001	0.854195	H	3.971599	-2.705480	-1.654505	
Br	-3.898501	-2.921106	-1.279705	O	-2.878110	-0.013303	-1.266205	
H	-3.049098	-3.655403	1.471895	H	-3.285908	-0.624304	-1.905005	
C	-2.020004	-1.952200	2.341795	O	0.323290	0.028108	-2.319305	
C	-1.567008	-0.612298	2.105895	C	0.387192	-0.738392	-3.527205	
C	-0.849610	0.044804	3.143895	H	0.680490	-0.055191	-4.331405	
C	-0.600808	-0.586495	4.341995	H	1.128495	-1.538790	-3.444605	
C	-1.050304	-1.909297	4.570495	C	-0.999206	-1.301397	-3.806005	
C	-1.744602	-2.575899	3.588195	H	-0.994204	-1.836296	-4.762205	
H	-0.503714	1.059305	2.979395	H	-1.266104	-2.026197	-3.019205	
H	-0.054910	-0.063693	5.121795	H	-1.810611	0.313801	-3.145405	
H	-0.846002	-2.393496	5.520495	O	-1.971209	-0.272000	-3.902305	
H	-2.094399	-3.591900	3.750495	C	2.734096	-1.807884	-0.120105	
C	-0.308923	3.927006	-0.169805	O	1.899494	-1.336087	-1.206505	
C	-1.328315	1.385802	0.533695					
C	0.462081	2.802308	-0.311805	B3LYP/6-31G** Energy =				-6817.821161
H	0.090374	4.896707	-0.446605	B3LYP/6-31G** Free Energy =				-6817.843524
Br	2.237380	2.939314	-0.986305	M06-2X/LACVP** Derived Free Energy =				-1700.444452
C	-2.149119	2.546900	0.697895	M06-2X/LACVP** Derived Solution Free Energy =				-1700.465914
C	-1.628323	3.832101	0.340295	Number of Imaginary Frequencies =				0
C	-2.442027	4.984899	0.505195					
C	-3.719426	4.878995	1.004095	B3LYP/6-31G** Geometry				
C	-4.236522	3.610593	1.359695					
C	-3.473018	2.474795	1.209595	C	-0.430913	-1.806793	0.948497	
H	-2.034230	5.953500	0.228995	C	0.597983	-2.786797	0.905097	
H	-4.333329	5.766193	1.126395	C	0.909680	-3.458899	-0.246103	
H	-5.245722	3.533790	1.753495	C	-1.104511	-1.470190	-0.218003	
H	-3.876015	1.506294	1.484695	Br	1.598982	-3.104202	2.509097	
B	1.019391	-0.294590	-1.191005	H	1.699677	-4.201602	-0.248503	
C	4.353102	-3.753179	0.126895	C	0.211682	-3.170196	-1.445103	
C	-0.039115	1.519407	0.040695	C	-0.796914	-2.151192	-1.436603	
O	0.786288	0.428809	-0.036505	C	-1.460613	-1.857389	-2.660303	
C	5.771786	1.156826	0.815795	C	-1.150816	-2.538990	-3.815403	
C	5.405887	0.901824	-0.507105	C	-0.159020	-3.548894	-3.817003	
C	4.419490	-0.040079	-0.791305	C	0.508079	-3.854097	-2.654003	
C	3.775892	-0.743581	0.237195	H	-2.222810	-1.086386	-2.671703	
C	4.152091	-0.481380	1.558795	H	-1.672915	-2.299288	-4.737203	
C	5.141188	0.461624	1.845895	H	0.073978	-4.077095	-4.736503	
H	6.540084	1.891028	1.039895	H	1.276175	-4.622700	-2.641903	
H	5.889585	1.436726	-1.319605	C	-3.963798	1.775121	-0.175103	
H	4.134590	-0.223280	-1.822605	C	-2.113707	-0.366486	-0.182703	
H	3.675793	-1.009981	2.376295	C	-2.622897	2.008616	-0.332603	

H	-4.665094	2.602624	-0.182203	B3LYP/6-31G** Free Energy =			-6817.839679
Br	-1.991590	3.791913	-0.591603	M06-2X/LACVP** Derived Free Energy =			-1700.443998
C	-3.509408	-0.636980	-0.015703	M06-2X/LACVP** Derived Solution Free Energy =			-1700.467775
C	-4.442203	0.450523	-0.007303	Number of Imaginary Frequencies =			0
C	-5.826605	0.180829	0.161797				
C	-6.278210	-1.108769	0.319297	B3LYP/6-31G** Geometry			
C	-5.359514	-2.185173	0.313497				
C	-4.011813	-1.956478	0.150097	C	2.528996	0.143594	-0.566505
H	-6.522701	1.015132	0.165997	C	3.594593	-0.659310	-0.075505
H	-7.338411	-1.304064	0.449397	C	3.801092	-0.813811	1.269695
H	-5.722319	-3.200871	0.440997	C	1.685498	0.796296	0.324595
H	-3.313417	-2.785981	0.149197	Br	4.753390	-1.519014	-1.319605
B	0.463902	1.826903	0.386297	H	4.623790	-1.427414	1.621295
C	4.365908	3.225487	0.145297	C	2.951394	-0.176108	2.209895
C	-1.681501	0.943012	-0.323603	C	1.876197	0.643096	1.734195
O	-0.357500	1.207706	-0.542303	C	1.046199	1.285999	2.693395
C	4.450988	-1.682714	-1.444803	C	1.268999	1.122998	4.043095
C	3.868989	-1.279511	-0.243903	C	2.330396	0.312294	4.509595
C	3.226895	-0.044008	-0.154603	C	3.152494	-0.323609	3.607795
C	3.139798	0.803692	-1.263803	H	0.220302	1.897502	2.348995
C	3.732096	0.389889	-2.465503	H	0.622301	1.623000	4.758395
C	4.384391	-0.839413	-2.554903	H	2.493496	0.194494	5.576495
H	4.952984	-2.643316	-1.517003	H	3.972992	-0.947811	3.951895
H	3.891087	-1.927311	0.627597	C	-1.354893	3.456407	-1.239605
H	2.800696	0.271293	0.789497	C	0.635601	1.713300	-0.225305
H	3.685299	1.025290	-3.344803	C	-1.642698	2.143208	-0.977805
H	4.834290	-1.140215	-3.496803	H	-2.125391	4.113810	-1.627905
C	5.073808	3.183584	1.122797	Br	-3.395300	1.466614	-1.301005
H	5.705508	3.136581	1.979097	C	0.958406	3.088899	-0.495605
C	1.562205	2.474199	-2.380303	C	-0.051291	3.964903	-1.009505
H	2.172906	2.699696	-3.258903	C	0.269314	5.322101	-1.278405
H	0.912701	1.630801	-2.612103	C	1.536915	5.803797	-1.047705
H	0.934109	3.343701	-2.167803	C	2.536112	4.943294	-0.535705
C	3.521608	3.302890	-1.044303	C	2.256308	3.621794	-0.266705
H	4.149108	3.278688	-1.942803	H	-0.507784	5.973004	-1.669905
H	2.989112	4.262293	-1.049803	H	1.772919	6.842896	-1.256005
O	-0.779410	-1.181792	2.099897	H	3.534314	5.329290	-0.352505
H	-0.200311	-1.453794	2.832897	H	3.027805	2.971192	0.128595
O	0.009303	1.982605	1.662997	B	-1.810507	-0.492191	0.730795
C	0.857705	2.399901	2.740997	C	-4.338012	-1.901683	-1.362005
H	1.797706	2.813098	2.363897	C	-0.652201	1.254305	-0.467605
H	0.314108	3.172304	3.294497	O	-0.961405	-0.064694	-0.285705
C	1.107500	1.194900	3.637997	C	1.956482	-3.846604	-0.874605
H	1.699497	0.445798	3.084697	C	1.140082	-3.646902	-1.985405
H	1.692601	1.498498	4.513197	C	-0.198516	-3.282597	-1.823005
H	-0.697003	0.597608	3.342697	C	-0.741716	-3.103195	-0.546105
O	-0.105303	0.630905	4.111097	C	0.090983	-3.303898	0.565295
C	2.454204	2.171095	-1.163803	C	1.424382	-3.670703	0.404295
O	1.711504	2.258098	0.059697	H	3.001381	-4.107308	-1.003205
				H	1.543682	-3.768103	-2.986305
B3LYP/6-31G** Energy =			-6817.819328	H	-0.804316	-3.132495	-2.709605

H	-0.308916	-3.157297	1.563695	C	-1.359701	-2.904401	0.263601
H	2.051082	-3.812205	1.279695	H	-2.411501	-4.487401	-0.701099
C	-5.497511	-1.604878	-1.192005	Br	-0.200401	-4.088501	1.209901
H	-6.519510	-1.352375	-1.025005	C	-3.087900	-1.131301	-1.067999
C	-2.941819	-3.989387	0.268995	C	-3.208301	-2.546501	-1.255099
H	-2.905722	-4.814988	-0.447305	C	-4.220501	-3.053801	-2.113199
H	-2.458820	-4.314989	1.192595	C	-5.085101	-2.203400	-2.761799
H	-3.985118	-3.747184	0.484895	C	-4.972300	-0.805200	-2.575599
C	-2.936213	-2.253987	-1.580705	C	-4.000300	-0.283101	-1.752199
H	-2.405610	-1.379389	-1.970805	H	-4.299701	-4.129501	-2.245499
H	-2.887216	-3.036488	-2.345605	H	-5.855901	-2.601500	-3.414799
O	2.401196	0.250794	-1.911705	H	-5.660100	-0.138400	-3.087299
H	1.617498	0.790397	-2.098305	H	-3.924000	0.789499	-1.612499
O	-2.094004	0.384310	1.728195	B	1.070600	-1.042101	1.129101
C	-2.977805	0.108413	2.822695	C	4.139299	-2.251102	-2.572399
H	-2.853408	-0.922888	3.169595	C	-1.218801	-1.502101	0.450901
H	-2.671702	0.790412	3.622695	O	-0.301300	-1.015101	1.337401
C	-4.444604	0.350518	2.465795	C	4.484600	2.530198	-0.454199
H	-4.993103	0.566820	3.389795	C	3.197800	2.257098	-0.922699
H	-4.498301	1.245118	1.825195	C	2.718900	0.948398	-0.927199
H	-4.645308	-0.995881	1.057995	C	3.506200	-0.111902	-0.452699
O	-5.095508	-0.761880	1.882995	C	4.798500	0.171098	0.003201
C	-2.215515	-2.761490	-0.299905	C	5.283800	1.482198	0.002001
O	-2.335011	-1.752090	0.732495	H	4.858600	3.549498	-0.441099
				H	2.551600	3.056598	-1.271399
B3LYP/6-31G** Energy =			-6817.823919	H	1.714600	0.745399	-1.285799
B3LYP/6-31G** Free Energy =			-6817.845040	H	5.434000	-0.626202	0.371301
M06-2X/LACVP** Derived Free Energy =			-1700.443857	H	6.287000	1.681698	0.367601
M06-2X/LACVP** Derived Solution Free Energy =			-1700.467226	C	5.208299	-2.400802	-3.114899
Number of Imaginary Frequencies =			0	H	6.149899	-2.528202	-3.596399
				C	3.665999	-2.525802	0.435301
B3LYP/6-31G** Geometry				H	4.650499	-2.761902	0.024601
				H	3.779199	-2.132702	1.446501
C	-1.228600	1.593199	-0.963199	H	3.082599	-3.449502	0.484201
C	-1.041500	2.990099	-0.768899	C	2.845399	-2.077702	-1.918999
C	-1.492000	3.635799	0.350901	H	2.311899	-3.035002	-1.877599
C	-1.892000	0.849499	0.004501	H	2.217999	-1.395502	-2.503299
Br	-0.124500	3.968199	-2.143299	O	-0.759800	0.959499	-2.069999
H	-1.329000	4.701299	0.471001	H	-0.366300	1.622199	-2.662099
C	-2.173800	2.907199	1.357901	O	1.896600	-0.615801	2.122201
C	-2.381200	1.498899	1.181701	C	1.429900	0.006599	3.327201
C	-3.077700	0.794399	2.202401	H	0.373300	-0.220401	3.500401
C	-3.534500	1.443399	3.327201	H	2.029100	-0.405901	4.144901
C	-3.322400	2.832499	3.498601	C	1.656500	1.509599	3.230201
C	-2.656600	3.547199	2.531001	H	1.035000	1.913999	2.414901
H	-3.247700	-0.269401	2.081301	H	1.327000	1.982799	4.162001
H	-4.064600	0.883699	4.092101	H	3.317400	1.410398	2.245001
H	-3.687700	3.329899	4.391801	O	3.022100	1.838298	3.062101
H	-2.489000	4.614499	2.648001	C	2.924899	-1.529702	-0.461799
C	-2.321101	-3.414601	-0.569299	O	1.532599	-1.477301	-0.075599
C	-2.067000	-0.621901	-0.203099				

B3LYP/6-31G** Energy =				-6817.820896	H	-0.849874	2.942478	2.286596
B3LYP/6-31G** Free Energy =				-6817.841439	H	-1.183985	3.337769	-1.981104
M06-2X/LACVP** Derived Free Energy =				-1700.441497	H	-3.588071	2.850402	-1.836404
M06-2X/LACVP** Derived Solution Free Energy =				-1700.463904	C	0.758157	5.447622	-2.954904
Number of Imaginary Frequencies =				0	H	0.539335	6.246116	-3.625204
					C	0.907872	4.886127	0.756996
B3LYP/6-31G** Geometry					H	0.405951	5.665813	0.180996
					H	0.524972	4.901616	1.779896
C	-1.859861	-1.133550	-0.863004	H	1.980667	5.100756	0.783396	
C	-3.178266	-0.975986	-0.353104	C	1.322512	3.441938	-1.285704	
C	-3.484359	-1.212695	0.959996	H	2.405013	3.426168	-1.116904	
C	-0.845650	-1.546822	-0.008704	H	1.073439	2.486931	-1.756704	
Br	-4.546481	-0.408024	-1.570704	O	-1.562968	-0.907442	-2.164304	
H	-4.500563	-1.084023	1.316296	H	-2.365176	-0.596864	-2.615404	
C	-2.469148	-1.623767	1.858996	O	2.218893	0.518263	1.765296	
C	-1.131643	-1.789130	1.369696	C	2.960076	1.135883	2.823796	
C	-0.126632	-2.192602	2.294796	H	3.983571	1.322211	2.473296	
C	-0.431326	-2.418810	3.620096	H	2.500850	2.089171	3.101396	
C	-1.755730	-2.257547	4.095796	C	2.966502	0.184483	4.008196	
C	-2.750541	-1.869674	3.229896	H	3.435928	-0.765004	3.703896	
H	0.890571	-2.315774	1.939896	H	3.575990	0.614500	4.810496	
H	0.353282	-2.712989	4.310296	H	1.114217	-0.345468	3.818296	
H	-1.978925	-2.437853	5.142596	O	1.670508	-0.018852	4.541096	
H	-3.770545	-1.740303	3.582296	C	0.662910	3.509320	0.123396	
C	3.131365	-2.089312	-1.614404	O	1.373136	2.586739	0.987696	
C	0.527856	-1.748784	-0.563504					
C	2.713031	-0.867224	-1.158604	B3LYP/6-31G** Energy =				-6817.821217
H	4.132668	-2.206984	-2.014104	B3LYP/6-31G** Free Energy =				-6817.843986
Br	3.908790	0.620909	-1.235904	M06-2X/LACVP** Derived Free Energy =				-1700.443583
C	0.938491	-3.036773	-1.037904	M06-2X/LACVP** Derived Solution Free Energy =				-1700.467120
C	2.258296	-3.205236	-1.567704	Number of Imaginary Frequencies =				0
C	2.666931	-4.482625	-2.035704					
C	1.810561	-5.557549	-1.984704	B3LYP/6-31G** Geometry				
C	0.505756	-5.395785	-1.461704					
C	0.080522	-4.169796	-1.001404	C	-2.784788	-0.973434	-0.422503	
H	3.671434	-4.593497	-2.435404	C	-3.051171	-2.341738	-0.137203	
H	2.132288	-6.530140	-2.344504	C	-2.609663	-2.945532	1.009797	
H	-0.166620	-6.247803	-1.424204	C	-2.053098	-0.218125	0.485897	
H	-0.921581	-4.055724	-0.603604	Br	-4.063558	-3.342450	-1.424403	
B	1.534573	1.243944	0.833796	H	-2.829150	-3.991135	1.196497	
C	1.000282	4.545429	-2.188604	C	-1.863073	-2.201723	1.957197	
C	1.406226	-0.680360	-0.627504	C	-1.579090	-0.821019	1.691997	
O	0.992792	0.568429	-0.250204	C	-0.824299	-0.096410	2.657897	
C	-3.594866	2.644002	0.306496	C	-0.384592	-0.702604	3.813897	
C	-2.815266	2.672024	1.463996	C	-0.668075	-2.066308	4.070597	
C	-1.449674	2.935361	1.381696	C	-1.391665	-2.797617	3.157797	
C	-0.833480	3.176378	0.144096	H	-0.596713	0.946393	2.468797	
C	-1.624279	3.143357	-1.010304	H	0.185601	-0.128897	4.538697	
C	-2.993372	2.879419	-0.928404	H	-0.314869	-2.529003	4.986997	
H	-4.658160	2.431473	0.363796	H	-1.616852	-3.844720	3.341797	
H	-3.268761	2.485311	2.433296	C	-1.168650	3.898186	-0.496503	

C	-1.765016	1.213679	0.165897				
C	-0.438137	2.867195	-1.026303	B3LYP/6-31G** Energy =			-6817.824580
H	-0.933963	4.923589	-0.761003	B3LYP/6-31G** Free Energy =			-6817.843427
Br	0.974759	3.241313	-2.254803	M06-2X/LACVP** Derived Free Energy =			-1700.442232
C	-2.552329	2.271869	0.723197	M06-2X/LACVP** Derived Solution Free Energy =			-1700.463997
C	-2.240746	3.630473	0.392097	Number of Imaginary Frequencies =			0
C	-3.017360	4.681163	0.949597				
C	-4.064056	4.408650	1.799297	B3LYP/6-31G** Geometry			
C	-4.378339	3.067746	2.124697				
C	-3.643626	2.027555	1.601397	C	2.074414	1.168992	-0.406501
H	-2.768873	5.706466	0.688897	C	2.425516	2.426992	0.159099
H	-4.651866	5.218942	2.219697	C	2.981216	2.529091	1.407799
H	-5.208437	2.858235	2.792797	C	2.261513	0.013992	0.344799
H	-3.893013	1.003152	1.854797	Br	2.057818	4.007292	-0.857301
B	1.312397	0.228517	-1.019703	H	3.236217	3.502891	1.811799
C	4.708680	1.562260	2.338697	C	3.222715	1.363391	2.177799
C	-0.722620	1.513492	-0.695903	C	2.848613	0.086391	1.643299
O	-0.019507	0.505001	-1.290003	C	3.072311	-1.068209	2.443799
C	4.225244	-3.499346	1.220997	C	3.641311	-0.963410	3.692999
C	3.033336	-2.933061	1.677397	C	4.015713	0.298690	4.214199
C	2.746220	-1.595264	1.414097	C	3.808115	1.436590	3.469999
C	3.640909	-0.795853	0.686897	H	2.791110	-2.039409	2.051299
C	4.837117	-1.370138	0.241997	H	3.806510	-1.858210	4.285899
C	5.126334	-2.712134	0.504897	H	4.464213	0.364689	5.200799
H	4.448357	-4.543443	1.419697	H	4.087916	2.411490	3.860399
H	2.319744	-3.532470	2.235097	C	0.684608	-3.633206	-1.353901
H	1.809814	-1.171876	1.762997	C	1.761211	-1.270907	-0.231601
H	5.552909	-0.776929	-0.315903	C	-0.073491	-2.836605	-0.535501
H	6.057939	-3.139523	0.145397	H	0.261506	-4.537505	-1.777601
C	5.813379	1.632574	2.822097	Br	-1.873392	-3.330402	-0.131801
H	6.786078	1.686587	3.252997	C	2.575110	-2.085308	-1.079301
C	4.134482	1.349253	-0.656103	C	2.027308	-3.282407	-1.644401
H	5.161580	1.499866	-0.315803	C	2.839907	-4.093409	-2.481301
H	4.140890	0.757353	-1.572803	C	4.141208	-3.740810	-2.753301
H	3.692870	2.324047	-0.880103	C	4.684709	-2.557511	-2.197901
C	3.372881	1.488943	1.754197	C	3.922410	-1.750710	-1.383801
H	3.000068	2.498239	1.541197	H	2.412506	-4.999208	-2.903001
H	2.675886	1.039835	2.470397	H	4.754107	-4.367511	-3.394001
O	-3.227196	-0.379340	-1.555403	H	5.712510	-2.284613	-2.418101
H	-3.711188	-1.035846	-2.083003	H	4.343811	-0.844911	-0.961801
O	1.981007	-0.622774	-1.843803	B	-1.208387	0.076697	0.683599
C	1.359615	-1.238982	-2.979803	C	-1.069784	2.351597	-3.051401
H	0.483322	-1.810493	-2.656003	C	0.453710	-1.646205	0.032699
H	1.034005	-0.473786	-3.694703	O	-0.300889	-0.940004	0.924699
C	2.394827	-2.163569	-3.599303	C	-6.400087	0.271304	-0.100101
H	1.956533	-2.667074	-4.467803	C	-6.071185	1.623604	-0.015401
H	3.245019	-1.559758	-3.957203	C	-4.765385	2.049102	-0.267001
H	3.130934	-2.722860	-1.905103	C	-3.762786	1.131900	-0.607401
O	2.812139	-3.173264	-2.701403	C	-4.107188	-0.224799	-0.703601
C	3.290091	0.672942	0.428497	C	-5.410788	-0.651397	-0.444401
O	1.890189	0.793325	0.077997	H	-7.412987	-0.061295	0.105099

H	-6.828584	2.353005	0.256399	C	3.850448	-1.815808	-0.351304
H	-4.534783	3.105302	-0.183301	C	2.041007	0.352641	-0.143304
H	-3.349189	-0.959600	-0.951601	C	2.506643	-2.003571	-0.538704
H	-5.650690	-1.708597	-0.510301	H	4.535625	-2.651227	-0.446304
C	-0.142283	2.940795	-3.557101	Br	1.851095	-3.738953	-0.993604
H	0.670617	3.458394	-4.012001	C	3.441713	0.572203	0.069096
C	-1.942283	2.914398	-0.282101	C	4.352683	-0.528522	-0.033204
H	-2.519882	3.745699	-0.695501	C	5.740189	-0.310759	0.179396
H	-2.106983	2.866798	0.794999	C	6.217023	0.942028	0.486996
H	-0.888383	3.126997	-0.473201	C	5.320353	2.031152	0.595296
C	-2.250385	1.687498	-2.499501	C	3.970348	1.852489	0.390896
H	-2.325886	0.670398	-2.899001	H	6.417966	-1.156078	0.096396
H	-3.137584	2.229500	-2.847201	H	7.279127	1.097899	0.649896
O	1.579114	1.032193	-1.654001	H	5.701280	3.017242	0.843796
H	1.158815	1.848594	-1.976001	H	3.291471	2.692907	0.479696
O	-1.911387	0.564698	1.744499	B	-0.530454	-1.875788	0.236996
C	-1.833087	-0.025302	3.052199	C	-4.524485	-3.037780	0.048396
H	-0.818488	-0.385604	3.251199	C	1.583972	-0.927146	-0.418204
H	-2.079786	0.771098	3.760099	O	0.253166	-1.146510	-0.646904
C	-2.842189	-1.159801	3.174199	C	-4.395051	1.889117	-1.381104
H	-2.576190	-1.955301	2.461699	C	-4.362073	1.090216	-2.524704
H	-2.782390	-1.582301	4.183799	C	-3.760007	-0.166700	-2.485404
H	-4.227588	-0.329899	2.108499	C	-3.183720	-0.653116	-1.302804
O	-4.175888	-0.717799	2.994099	C	-3.231898	0.153385	-0.160704
C	-2.333685	1.587098	-0.942801	C	-3.826364	1.415501	-0.199804
O	-1.377887	0.565397	-0.581301	H	-4.859124	2.870729	-1.412304
B3LYP/6-31G** Energy =				H	-4.800263	1.446228	-3.452804
B3LYP/6-31G** Free Energy =				H	-3.743224	-0.768701	-3.388804
M06-2X/LACVP** Derived Free Energy =				H	-2.808008	-0.208226	0.768296
M06-2X/LACVP** Derived Solution Free Energy =				H	-3.824147	2.027901	0.696596
Number of Imaginary Frequencies =				C	-5.217184	-2.980761	1.035796
				H	-5.830282	-2.919044	1.904696
B3LYP/6-31G** Geometry				C	-1.724367	-2.369856	-2.506504
				H	-2.361471	-2.522839	-3.381604
				H	-1.025945	-1.560875	-2.718104
C	0.303144	1.706989	1.032896	H	-1.149692	-3.285072	-2.339404
C	-0.619227	2.788814	1.062996	C	-3.701888	-3.130402	-1.155004
C	-0.762903	3.649818	0.008996	H	-4.339586	-3.046285	-2.042604
C	1.074438	1.494668	-0.101904	H	-3.224315	-4.117415	-1.194804
Br	-1.702621	2.998943	2.631196	O	0.454321	0.874585	2.093696
H	-1.474581	4.466237	0.062796	H	-0.208873	1.073203	2.776496
C	0.011292	3.466197	-1.163304	O	-0.004063	-2.208203	1.448396
C	0.934562	2.371072	-1.225004	C	-0.794778	-2.783381	2.492996
C	1.680857	2.196351	-2.423904	H	-1.772965	-2.293555	2.534696
C	1.527481	3.057255	-3.487104	H	-0.954408	-3.852377	2.304396
C	0.620910	4.141580	-3.417004	C	-0.026073	-2.569202	3.788696
C	-0.121484	4.338200	-2.276504	H	-0.630182	-2.912786	4.635196
H	2.377135	1.368532	-2.492904	H	0.895711	-3.171727	3.767496
H	2.108276	2.901940	-4.391604	H	0.757473	-0.906324	3.219996
H	0.512128	4.812183	-4.263904	O	0.264965	-1.198910	4.002596
H	-0.826062	5.162720	-2.209304	C	-2.573359	-2.057933	-1.261804

O	-1.805964	-2.237754	-0.062504	H	7.296998	0.673271	-0.084702
				H	5.443805	2.170679	-0.807702
B3LYP/6-31G** Energy =			-6817.823340	H	3.202401	1.251189	-1.239202
B3LYP/6-31G** Free Energy =			-6817.843480	H	4.639683	-2.689317	-0.282702
M06-2X/LACVP** Derived Free Energy =			-1700.442917	H	6.869687	-1.763527	0.173998
M06-2X/LACVP** Derived Solution Free Energy =			-1700.464544	C	0.167984	-2.606397	-3.808902
Number of Imaginary Frequencies =			0	H	-0.628519	-3.133894	-4.281102
				C	2.086583	-2.743106	-0.600302
B3LYP/6-31G** Geometry				H	2.723980	-3.486009	-1.088402
				H	2.263083	-2.774307	0.475698
C	-2.057210	-1.162187	-0.498002	H	1.049382	-3.022901	-0.796302
C	-2.343816	-2.476786	-0.033602	C	2.230789	-1.316906	-2.706702
C	-2.875017	-2.705984	1.208898	H	2.230894	-0.269306	-3.025602
C	-2.278405	-0.083086	0.350398	H	3.139187	-1.771511	-3.119302
Br	-1.919322	-3.952688	-1.177502	O	-1.590909	-0.901589	-1.737102
H	-3.079521	-3.720383	1.534298	H	-1.134612	-1.666891	-2.128402
C	-3.156912	-1.619482	2.074998	O	1.988493	-0.569805	1.617598
C	-2.844406	-0.287884	1.644598	C	1.965395	-0.050105	2.956098
C	-3.105501	0.785717	2.540498	H	2.058600	1.040494	2.927198
C	-3.652602	0.554020	3.782198	H	1.016994	-0.308001	3.442698
C	-3.966008	-0.761679	4.200898	C	3.141592	-0.665411	3.694998
C	-3.720513	-1.824280	3.362798	H	3.144594	-0.304711	4.729398
H	-2.869997	1.797016	2.227098	H	3.012687	-1.760110	3.724498
H	-3.846998	1.389121	4.448898	H	4.351493	-0.549916	2.191998
H	-4.398109	-0.928177	5.182998	O	4.384594	-0.299916	3.127198
H	-3.953317	-2.839379	3.673698	C	2.356389	-1.338107	-1.150402
C	-0.826588	3.758707	-0.999102	O	1.337493	-0.428702	-0.674102
C	-1.824199	1.264012	-0.110902				
C	-0.041892	2.912304	-0.259902	B3LYP/6-31G** Energy =			-6817.823109
H	-0.434884	4.714005	-1.331502	B3LYP/6-31G** Free Energy =			-6817.843449
Br	1.740711	3.412896	0.204698	M06-2X/LACVP** Derived Free Energy =			-1700.439024
C	-2.664795	2.128115	-0.879702	M06-2X/LACVP** Derived Solution Free Energy =			-1700.461509
C	-2.156690	3.391013	-1.327002	Number of Imaginary Frequencies =			0
C	-2.995786	4.249117	-2.087302				
C	-4.283887	3.879823	-2.397502	B3LYP/6-31G** Geometry			
C	-4.787593	2.631925	-1.958702				
C	-3.999497	1.778421	-1.220302	C	2.024520	1.057054	-0.734200
H	-2.599081	5.204515	-2.420002	C	3.323014	0.809120	-0.209000
H	-4.916684	4.543126	-2.979502	C	3.622418	1.001013	1.112800
H	-5.804994	2.346030	-2.208902	C	1.023932	1.511780	0.114800
H	-4.390101	0.822623	-0.888202	Br	4.672597	0.183986	-1.419400
B	1.208595	-0.043902	0.631098	H	4.623913	0.805787	1.480200
C	1.076186	-2.007201	-3.280502	C	2.619430	1.452139	2.006700
C	-0.529097	1.655406	0.186998	C	1.300337	1.704873	1.503700
O	0.257199	0.889002	0.998598	C	0.306248	2.143598	2.423000
C	6.312696	0.265475	-0.293302	C	0.605753	2.327691	3.754200
C	5.273100	1.103480	-0.699502	C	1.911746	2.085757	4.244200
C	4.007598	0.580186	-0.960102	C	2.895435	1.654831	3.385300
C	3.751792	-0.791313	-0.812202	H	-0.700648	2.318024	2.061800
C	4.802688	-1.624718	-0.407602	H	-0.169139	2.662411	4.437700
C	6.072090	-1.100324	-0.147802	H	2.131950	2.238351	5.296400

H	3.901430	1.461606	3.748400	C	-0.704396	-3.432776	0.172100
C	-2.887547	2.330581	-1.542700	O	-1.352971	-2.472559	1.043700
C	-0.324761	1.809415	-0.458200				
C	-2.539880	1.072972	-1.127400	B3LYP/6-31G** Energy =			-6817.823553
H	-3.873542	2.516206	-1.954400	B3LYP/6-31G** Free Energy =			-6817.843888
Br	-3.804816	-0.352296	-1.291300	M06-2X/LACVP** Derived Free Energy =			-1700.444278
C	-0.656027	3.133023	-0.895900	M06-2X/LACVP** Derived Solution Free Energy =			-1700.464694
C	-1.955520	3.393857	-1.439200	Number of Imaginary Frequencies =			0
C	-2.284686	4.707665	-1.867300				
C	-1.369760	5.729642	-1.767200	B3LYP/6-31G** Geometry			
C	-0.083966	5.476008	-1.233500				
C	0.264301	4.213199	-0.809700	C	-1.401123	1.655879	0.707608
H	-3.274681	4.888991	-2.277100	C	-1.095743	3.037483	0.562208
H	-1.630234	6.730648	-2.097300	C	-1.208453	3.682882	-0.638792
H	0.635055	6.286490	-1.158800	C	-1.817012	0.926673	-0.398092
H	1.251997	4.028074	-0.403000	Br	-0.479457	3.986793	2.107908
B	-1.478936	-1.128556	0.872800	H	-0.963568	4.736385	-0.717692
C	-1.125722	-4.443665	-2.137900	C	-1.633942	2.970175	-1.787492
C	-1.259187	0.794839	-0.576200	C	-1.936221	1.573371	-1.669292
O	-0.931620	-0.486970	-0.229900	C	-2.343711	0.877365	-2.841692
C	3.600019	-2.849687	0.376500	C	-2.450121	1.526763	-4.051192
C	2.994213	-3.077371	-0.857800	C	-2.156641	2.906868	-4.160692
C	1.611209	-3.251835	-0.946200	C	-1.756052	3.610774	-3.049192
C	0.810210	-3.197115	0.200400	H	-2.571295	-0.180338	-2.771692
C	1.431016	-2.966031	1.437400	H	-2.763112	0.973659	-4.931892
C	2.810721	-2.794166	1.526400	H	-2.246348	3.404966	-5.121192
H	4.674623	-2.708214	0.439400	H	-1.522967	4.669877	-3.119092
H	3.597112	-3.115087	-1.760100	C	-2.721049	-3.291441	-0.049492
H	1.166704	-3.445124	-1.915500	C	-2.139790	-0.526832	-0.246392
H	0.823818	-2.910015	2.335400	C	-1.433456	-2.856122	-0.219892
H	3.268125	-2.613278	2.494900	H	-2.932633	-4.353244	0.013208
C	-0.962646	-5.367369	-2.899400	Br	-0.015037	-4.121501	-0.378092
H	-0.815067	-6.185073	-3.566100	C	-3.494784	-0.957352	-0.063492
C	-1.039631	-4.795267	0.794800	C	-3.783363	-2.356656	0.040808
H	-0.578152	-5.600979	0.221100	C	-5.126257	-2.781776	0.224408
H	-0.670032	-4.837377	1.821900	C	-6.149370	-1.866192	0.306208
H	-2.123535	-4.945639	0.807800	C	-5.868391	-0.482987	0.206808
C	-1.348693	-3.311059	-1.241100	C	-4.577197	-0.039968	0.026108
H	-2.426090	-3.191931	-1.080600	H	-5.328941	-3.846579	0.301008
H	-1.007169	-2.386968	-1.715200	H	-7.172365	-2.201107	0.448508
O	1.735615	0.877661	-2.044900	H	-6.679601	0.235701	0.275508
H	2.525006	0.529241	-2.490800	H	-4.371413	1.022035	-0.046592
O	-2.148717	-0.367738	1.784300	B	1.144819	-1.146183	0.469308
C	-2.790231	-0.912922	2.942800	C	2.408275	1.847735	-0.589992
H	-2.889259	-1.998019	2.846900	C	-1.126076	-1.470017	-0.302892
H	-2.171325	-0.686938	3.820500	O	0.169218	-1.081298	-0.519792
C	-4.159814	-0.266087	3.082000	C	7.314502	0.018308	-0.376392
H	-4.618723	-0.605275	4.017500	C	6.772199	0.181100	-1.652192
H	-4.033386	0.826710	3.149700	C	5.406102	0.001080	-1.860692
H	-4.635017	-0.362674	1.202200	C	4.552707	-0.343133	-0.801892
O	-5.044024	-0.628964	2.039600	C	5.106410	-0.502525	0.472108

C	6.475307	-0.323804	0.682408	H	4.270492	-0.290611	5.177401
H	8.378900	0.157724	-0.211692	H	4.951290	-1.740013	3.287101
H	7.412495	0.448210	-2.487992	C	-0.676100	3.669298	-0.310199
H	5.007700	0.131674	-2.863092	C	1.117896	1.508395	0.086601
H	4.459513	-0.768034	1.298008	C	-1.139702	2.394299	-0.129699
H	6.883909	-0.452098	1.680908	H	-1.373198	4.487400	-0.455499
C	2.396362	2.729935	0.234908	Br	-3.018803	2.057303	-0.115099
H	2.325750	3.499234	0.968308	C	1.628798	2.837794	-0.113099
C	2.842027	-1.682858	-2.079492	C	0.718801	3.925196	-0.313499
H	3.288423	-1.429851	-3.044792	C	1.225203	5.236995	-0.512999
H	3.319141	-2.595251	-1.712992	C	2.580204	5.472692	-0.522099
H	1.777930	-1.877674	-2.224492	C	3.483402	4.400890	-0.332399
C	2.406991	0.772835	-1.579592	C	3.021999	3.118691	-0.132099
H	2.944586	1.093143	-2.478992	H	0.520205	6.050396	-0.661199
H	1.376994	0.559320	-1.883292	H	2.959106	6.478391	-0.677199
O	-1.312013	1.030780	1.907008	H	4.552302	4.591088	-0.346099
H	-0.868022	1.603287	2.555708	H	3.722897	2.304490	0.009001
O	0.756623	-1.432089	1.742608	B	-1.247708	-0.688601	-0.828399
C	1.639421	-1.276776	2.856708	C	-0.027714	-3.305203	0.761801
H	2.394333	-2.073265	2.861108	C	-0.252105	1.298098	0.061301
H	2.150907	-0.310168	2.789308	O	-0.773207	0.041999	0.253601
C	0.781122	-1.340189	4.111308	C	-5.749608	-0.389392	2.263101
H	0.356637	-2.351695	4.207908	C	-5.573308	-0.428692	0.878601
H	1.405719	-1.154179	4.991508	C	-4.479809	-1.093894	0.326501
H	-0.745390	-0.502511	3.286408	C	-3.537510	-1.730596	1.149101
O	-0.238793	-0.356704	4.100408	C	-3.725410	-1.687696	2.535501
C	3.054910	-0.547555	-1.063892	C	-4.821109	-1.020694	3.088501
O	2.455016	-0.914664	0.189108	H	-6.601807	0.128610	2.693001
				H	-6.290807	0.057709	0.223601
B3LYP/6-31G** Energy =				H	-4.343409	-1.102494	-0.750399
B3LYP/6-31G** Free Energy =				H	-3.020011	-2.170997	3.202901
M06-2X/LACVP** Derived Free Energy =				H	-4.943809	-0.995893	4.167501
M06-2X/LACVP** Derived Solution Free Energy =				C	0.921586	-3.769905	0.177201
Number of Imaginary Frequencies =				H	1.778785	-4.089106	-0.371499
				C	-2.920915	-3.868697	-0.006099
B3LYP/6-31G** Geometry				H	-3.324216	-4.451496	0.826801
				H	-3.719914	-3.709996	-0.733999
C	2.434692	-0.471808	-0.691599	H	-2.112716	-4.431699	-0.479799
C	3.417390	-1.475710	-0.453999	C	-1.184512	-2.735001	1.448401
C	4.001990	-1.632311	0.773301	H	-0.903911	-1.781901	1.906901
C	2.064794	0.377993	0.345801	H	-1.496814	-3.405600	2.257001
Br	3.893088	-2.657611	-1.874399	O	1.933592	-0.396507	-1.946399
H	4.745488	-2.407712	0.923001	H	1.088693	0.087195	-1.955999
C	3.625391	-0.803510	1.860601	O	-0.931607	-0.208601	-2.076599
C	2.636893	0.210692	1.649501	C	-1.424909	-0.823400	-3.279399
C	2.266995	1.022293	2.757301	H	-0.564809	-0.997402	-3.935199
C	2.844495	0.840991	3.994801	H	-1.893011	-1.780499	-3.039099
C	3.823893	-0.159210	4.196501	C	-2.426907	0.108402	-3.946599
C	4.203291	-0.964111	3.147101	H	-1.930705	1.056101	-4.204699
H	1.515196	1.791394	2.619801	H	-2.765008	-0.353498	-4.881099
H	2.542696	1.472092	4.825701	H	-3.327405	0.903504	-2.415799

O	-3.581006	0.327604	-3.152799	C	4.145107	-1.005091	-0.598101
C	-2.394612	-2.515298	0.496101	C	4.886907	-0.607089	-1.708101
O	-1.960011	-1.830899	-0.697899	H	5.094207	-0.709789	-3.854101
				H	3.085710	-2.150394	-4.138301
B3LYP/6-31G** Energy =			-6817.816728	H	1.769912	-2.844597	-2.192901
B3LYP/6-31G** Free Energy =			-6817.837327	H	4.441207	-0.663890	0.388999
M06-2X/LACVP** Derived Free Energy =			-1700.443188	H	5.758205	0.026813	-1.570601
M06-2X/LACVP** Derived Solution Free Energy =			-1700.465904	C	-0.577887	-3.382403	2.380899
Number of Imaginary Frequencies =			0	H	-1.166386	-3.573904	3.247899
				C	3.115413	-3.310493	1.273899
B3LYP/6-31G** Geometry				H	3.311015	-4.180493	0.641199
				H	4.077112	-2.875891	1.557799
C	-2.056693	-0.808406	-0.965701	H	2.590714	-3.635595	2.175799
C	-2.854790	-1.949708	-0.683301	C	0.868512	-2.886799	0.193399
C	-3.658690	-1.992210	0.424299	H	0.317810	-2.214900	-0.469901
C	-2.067896	0.282094	-0.103801	H	1.015314	-3.821799	-0.359501
Br	-2.764386	-3.447108	-1.856901	O	-1.290893	-0.857004	-2.085801
H	-4.260688	-2.872912	0.619899	H	-0.774995	-0.037903	-2.140801
C	-3.694693	-0.903010	1.331899	O	1.272203	0.898202	2.243799
C	-2.878996	0.246992	1.076199	C	1.941503	0.826404	3.509299
C	-2.901698	1.307692	2.023199	H	1.478101	1.599902	4.128999
C	-3.697798	1.239390	3.145099	H	1.763305	-0.148697	3.978799
C	-4.514495	0.109688	3.385199	C	3.440902	1.086007	3.395499
C	-4.508193	-0.939412	2.495099	H	3.583900	1.916808	2.687299
H	-2.274000	2.175793	1.857099	H	3.815102	1.410408	4.374799
H	-3.696500	2.061290	3.855199	H	3.613807	-0.628192	2.495099
H	-5.139295	0.071486	4.272399	O	4.198705	-0.052991	3.012999
H	-5.124291	-1.817414	2.670399	C	2.265011	-2.285396	0.509599
C	0.423896	3.709200	-0.985101	O	2.112408	-1.173996	1.438399
C	-1.222399	1.472996	-0.432301				
C	0.976199	2.527601	-0.565301	B3LYP/6-31G** Energy =			-6817.825910
H	1.062594	4.560901	-1.193201	B3LYP/6-31G** Free Energy =			-6817.844046
Br	2.866299	2.380206	-0.384701	M06-2X/LACVP** Derived Free Energy =			-1700.449198
C	-1.814802	2.694394	-0.903401	M06-2X/LACVP** Derived Solution Free Energy =			-1700.469727
C	-0.977704	3.825596	-1.168301	Number of Imaginary Frequencies =			0
C	-1.561707	5.036895	-1.625601				
C	-2.919608	5.131792	-1.823101	B3LYP/6-31G** Geometry			
C	-3.748605	4.012990	-1.573901				
C	-3.212502	2.825991	-1.126001	C	2.198191	0.237500	-0.370299
H	-0.912910	5.886497	-1.820101	C	3.270794	-0.533695	0.167601
H	-3.357110	6.061491	-2.173901	C	3.555494	-0.541494	1.507601
H	-4.819005	4.090687	-1.739401	C	1.431487	1.020696	0.487501
H	-3.856000	1.973989	-0.940201	Br	4.341299	-1.565990	-1.031899
B	1.381905	-0.028998	1.260199	H	4.377797	-1.139990	1.884601
C	0.077913	-3.160301	1.391499	C	2.783191	0.236803	2.406401
C	0.157402	1.397399	-0.280201	C	1.705387	1.030898	1.891901
O	0.730204	0.203101	0.058599	C	0.932783	1.787794	2.817101
C	4.514908	-1.018890	-2.989001	C	1.218083	1.767795	4.164001
C	3.390810	-1.826593	-3.147401	C	2.290787	0.992100	4.665101
C	2.644111	-2.222995	-2.035201	C	3.054191	0.242104	3.800901
C	3.011510	-1.819594	-0.745901	H	0.106280	2.383390	2.446301

H	0.613181	2.353592	4.850001	H	1.080205	-2.771905	-2.293199
H	2.506387	0.989401	5.729301	O	1.420202	-2.110504	-2.917999
H	3.878193	-0.361692	4.172101	C	-1.531094	-2.920218	0.554901
C	-1.824524	3.365581	-1.131199	O	-1.465697	-2.362418	-0.774399
C	0.319083	1.840891	-0.086299				
C	-1.962518	2.019080	-0.916299	B3LYP/6-31G** Energy =			-6817.822073
H	-2.656927	3.941277	-1.520999	B3LYP/6-31G** Free Energy =			-6817.842364
Br	-3.638014	1.180872	-1.280399	M06-2X/LACVP** Derived Free Energy =			-1700.437481
C	0.489076	3.245592	-0.311099	M06-2X/LACVP** Derived Solution Free Energy =			-1700.461312
C	-0.597727	4.012987	-0.841799	Number of Imaginary Frequencies =			0
C	-0.427934	5.405987	-1.063999				
C	0.767863	6.023293	-0.780999	B3LYP/6-31G** Geometry			
C	1.846967	5.267598	-0.263899				
C	1.712173	3.916798	-0.034899	C	-1.973608	0.182371	1.123413
H	-1.262937	5.974083	-1.465299	C	-3.013995	-0.785143	1.184613
H	0.888358	7.088194	-0.956099	C	-3.871992	-1.001555	0.140613
H	2.791464	5.758503	-0.048499	C	-1.804718	0.930673	-0.034387
H	2.546276	3.345802	0.356501	Br	-3.172881	-1.825645	2.790913
B	-1.209203	-1.062616	-1.122199	H	-4.656782	-1.745666	0.220713
C	0.935108	-3.426306	0.377701	C	-3.723802	-0.259553	-1.057087
C	-0.888114	1.239785	-0.406699	C	-2.672315	0.711361	-1.151487
O	-1.069708	-0.094116	-0.149399	C	-2.531325	1.421363	-2.376987
C	-4.693203	-1.042333	2.877701	C	-3.382922	1.190552	-3.433487
C	-3.483702	-1.359627	3.492201	C	-4.425209	0.238538	-3.330487
C	-2.449299	-1.942022	2.756101	C	-4.588099	-0.471065	-2.164287
C	-2.606898	-2.217423	1.392901	H	-1.735935	2.151374	-2.472087
C	-3.830899	-1.898329	0.787601	H	-3.252629	1.744353	-4.358587
C	-4.861402	-1.312534	1.518701	H	-5.089307	0.069029	-4.172387
H	-5.495405	-0.585237	3.449401	H	-5.379789	-1.209875	-2.071787
H	-3.335903	-1.150426	4.547701	C	1.386642	3.833016	-0.369287
H	-1.518498	-2.169018	3.263601	C	-0.707432	1.945188	-0.101987
H	-3.968698	-2.096329	-0.270199	C	1.634361	2.489320	-0.458587
H	-5.796503	-1.064438	1.025101	H	2.194633	4.545827	-0.492587
C	1.829710	-3.922202	-0.267899	Br	3.407769	1.889144	-0.851087
H	2.662712	-4.316798	-0.802399	C	-0.993151	3.345384	0.008613
C	-1.928287	-4.389920	0.346301	C	0.070436	4.296799	-0.119887
H	-2.022285	-4.898220	1.310001	C	-0.212483	5.683995	-0.005187
H	-2.890887	-4.446924	-0.166999	C	-1.493389	6.123677	0.233813
H	-1.174285	-4.904616	-0.254899	C	-2.546176	5.187763	0.368413
C	-0.119695	-2.829411	1.196501	C	-2.304258	3.836966	0.257513
H	0.118700	-1.778810	1.391901	H	0.605908	6.391606	-0.106887
H	-0.134592	-3.343011	2.164001	H	-1.699403	7.185975	0.322513
O	1.930390	0.271599	-1.692499	H	-3.554881	5.539549	0.563513
H	1.998795	-0.621801	-2.102199	H	-3.117448	3.128555	0.366813
O	-1.072105	-0.735216	-2.437699	B	1.680901	-0.491580	0.486213
C	-0.967200	-1.733015	-3.443499	C	4.488935	-2.999041	-0.816087
H	-1.309995	-2.701017	-3.060799	C	0.600274	1.526606	-0.296387
H	-1.615701	-1.447918	-4.280299	O	0.877192	0.195010	-0.416487
C	0.467500	-1.836208	-3.945699	C	-1.723640	-4.856226	-0.936487
H	0.511204	-2.605908	-4.730899	C	-1.408951	-4.032621	0.142313
H	0.777196	-0.884007	-4.384999	C	-0.222461	-3.296005	0.145813

C	0.666040	-3.361393	-0.932287	H	1.437282	-1.135614	-2.969695
C	0.336951	-4.192798	-2.014387	H	0.490172	-1.977103	-5.073095
C	-0.843039	-4.934314	-2.016887	H	-1.533545	-3.432279	-5.060795
H	-2.645532	-5.430538	-0.938787	H	-2.609551	-4.026367	-2.910795
H	-2.086552	-3.942731	0.985613	C	4.043506	0.867456	-0.480795
H	0.008431	-2.666802	0.996913	C	1.739886	-0.778617	-0.429695
H	1.003452	-4.264189	-2.868887	C	2.794212	1.413570	-0.349495
H	-1.075430	-5.570217	-2.866387	H	4.917613	1.508745	-0.510395
C	5.596529	-2.517026	-0.841787	Br	2.604134	3.311572	-0.240295
H	6.575423	-2.096913	-0.864387	C	3.037680	-1.374633	-0.558095
C	2.150718	-1.746373	-2.221587	C	4.200189	-0.538046	-0.580495
H	2.326427	-2.403371	-3.077687	C	5.485682	-1.129061	-0.707295
H	1.260410	-1.149385	-2.415487	C	5.626366	-2.493763	-0.803795
H	3.009309	-1.078461	-2.123387	C	4.481357	-3.324449	-0.776095
C	3.156843	-3.600459	-0.791887	C	3.221763	-2.781035	-0.657495
H	3.009351	-4.134561	0.153713	H	6.357090	-0.480071	-0.724395
H	3.075553	-4.346461	-1.590287	H	6.613261	-2.936174	-0.898795
O	-1.132311	0.394282	2.163713	H	4.598144	-4.401751	-0.847495
H	-1.373303	-0.202621	2.890713	H	2.351356	-3.426925	-0.634595
O	2.025393	0.120725	1.650213	B	-0.034583	1.801103	0.952605
C	2.875501	-0.491363	2.626613	C	-2.025355	4.212127	-2.246595
H	2.583895	-0.065567	3.591513	C	1.629003	0.597684	-0.306895
H	2.719516	-1.575965	2.647813	O	0.394509	1.183698	-0.214695
C	4.341497	-0.179743	2.350113	C	-4.719411	-0.533042	-0.781095
H	4.950703	-0.646935	3.132813	C	-4.524399	0.423856	-1.777095
H	4.631803	-0.632139	1.390113	C	-3.666987	1.503546	-1.562195
H	4.166073	1.599454	1.625913	C	-2.990185	1.648038	-0.343095
O	4.620778	1.208660	2.386413	C	-3.200396	0.684840	0.652605
C	1.985829	-2.579475	-0.940287	C	-4.051709	-0.398650	0.436005
O	2.088318	-1.767974	0.238913	H	-5.383420	-1.375334	-0.952795
B3LYP/6-31G** Energy =				H	-5.036401	0.330562	-2.730595
B3LYP/6-31G** Free Energy =				H	-3.534078	2.237844	-2.349095
M06-2X/LACVP** Derived Free Energy =				H	-2.692095	0.781234	1.605405
M06-2X/LACVP** Derived Solution Free Energy =				H	-4.168818	-1.146348	1.214605
Number of Imaginary Frequencies =				C	-2.590947	4.927333	-3.039595
				H	-3.093239	5.559539	-3.734595
				C	-2.956458	4.004038	0.526005
B3LYP/6-31G** Geometry				H	-3.738054	4.300247	-0.175295
				H	-3.422462	3.666043	1.454705
C	-0.117627	-1.971496	0.736005	H	-2.328547	4.873730	0.743105
C	-1.287637	-2.779082	0.706705	C	-1.299065	3.357918	-1.308795
C	-1.814442	-3.250776	-0.464895	H	-0.432959	3.911908	-0.928695
C	0.507877	-1.627803	-0.454895	H	-0.894975	2.489213	-1.835695
Br	-2.146442	-3.177072	2.374405	O	0.412678	-1.534002	1.906105
H	-2.707850	-3.865265	-0.454095	H	-0.174825	-1.760295	2.647005
C	-1.197739	-2.926183	-1.698295	O	0.702315	1.624095	2.084205
C	-0.028229	-2.097097	-1.696295	C	0.253520	2.049600	3.372305
C	0.557975	-1.769204	-2.950595	H	0.338132	3.139399	3.467405
C	0.024469	-2.241797	-4.128395	H	-0.796884	1.771712	3.512905
C	-1.125240	-3.066984	-4.123495	C	1.132511	1.341990	4.393305
C	-1.722844	-3.398477	-2.930495	H	2.163816	1.717778	4.303605

H	0.779514	1.571394	5.404405	C	-4.167652	0.892400	0.683605
H	1.352893	-0.241213	3.320105	C	-3.367902	-0.134339	1.208705
O	1.084595	-0.065010	4.235405	C	-3.093602	-0.127252	2.580905
C	-2.104471	2.868528	-0.060195	C	-3.604352	0.878872	3.404005
O	-1.165975	2.555017	0.991505	H	-4.785964	2.679530	3.511805
B3LYP/6-31G** Energy =				H	-5.283664	2.687655	1.072405
B3LYP/6-31G** Free Energy =				H	-4.384651	0.910911	-0.379795
M06-2X/LACVP** Derived Free Energy =				H	-2.489240	-0.910182	3.023305
M06-2X/LACVP** Derived Solution Free Energy =				H	-3.376653	0.865561	4.465905
Number of Imaginary Frequencies =				C	-2.411686	-3.903386	2.689105
B3LYP/6-31G** Geometry				H	-2.682321	-4.623973	3.425605
C	1.545740	-1.318079	-0.764295	C	-4.035099	-2.121906	-0.183295
C	1.633472	-2.707983	-0.470395	H	-4.487023	-2.616184	0.678305
C	2.134050	-3.166308	0.719405	H	-4.797269	-1.518569	-0.681895
C	1.928986	-0.390398	0.201405	H	-3.683636	-2.891024	-0.879295
Br	0.945412	-3.950350	-1.751195	C	-1.714198	-2.106920	0.840905
H	2.186198	-4.232210	0.912705	H	-1.274225	-2.649541	-0.004495
C	2.562495	-2.250129	1.711205	H	-0.930566	-1.451958	1.233205
C	2.436064	-0.842722	1.463005	O	1.100363	-0.850357	-1.948295
C	2.801707	0.049160	2.511505	H	0.531032	-1.482929	-2.439495
C	3.287284	-0.422464	3.710205	O	-1.269147	0.986258	-2.288195
C	3.434716	-1.811471	3.937905	C	-1.999266	0.596594	-3.441495
C	3.073373	-2.703954	2.956805	H	-3.008882	0.267643	-3.163795
H	2.691259	1.115665	2.357805	H	-2.094423	1.477299	-4.085595
H	3.558518	0.280723	4.492205	C	-1.282320	-0.506441	-4.210095
H	3.822799	-2.167290	4.887405	H	-1.869632	-0.748512	-5.108595
H	3.164720	-3.774458	3.120505	H	-0.296103	-0.157689	-4.530095
C	1.255292	3.842935	-0.384495	H	-1.773381	-1.760617	-2.778295
C	1.724557	1.067512	-0.067595	O	-1.057578	-1.683952	-3.428795
C	0.207350	2.966586	-0.266695	C	-2.866456	-1.234164	0.265305
H	1.065444	4.906544	-0.479195	O	-2.377026	-0.629287	-0.965595
Br	-1.577918	3.633774	-0.224595	B3LYP/6-31G** Energy =			
C	2.832801	1.963058	-0.224195	B3LYP/6-31G** Free Energy =			
C	2.589469	3.365770	-0.385895	M06-2X/LACVP** Derived Free Energy =			
C	3.688812	4.253116	-0.539595	M06-2X/LACVP** Derived Solution Free Energy =			
C	4.979989	3.780353	-0.547995	Number of Imaginary Frequencies =			
C	5.224322	2.393541	-0.405195	B3LYP/6-31G** Geometry			
C	4.180978	1.509692	-0.245895	C	1.123971	1.726721	-0.639598
H	3.487064	5.314626	-0.655495	C	1.041740	3.128619	-0.403998
H	5.812823	4.466513	-0.669295	C	1.671827	3.709833	0.664102
H	6.245104	2.023491	-0.424595	C	1.870888	0.927937	0.217502
H	4.378027	0.448883	-0.143295	Br	0.015417	4.206597	-1.597398
B	-1.426078	0.358766	-1.088795	H	1.589204	4.779531	0.823602
C	-2.108646	-3.082101	1.856305	C	2.419845	2.920949	1.575002
C	0.431681	1.569775	-0.139495	C	2.521376	1.509452	1.353202
O	-0.630661	0.709627	-0.017095	C	3.277492	0.738568	2.278002
C	-4.393703	1.895711	2.870505	C	3.894279	1.331482	3.357402
C	-4.672403	1.899625	1.502905	C	3.791049	2.725779	3.573102

C	3.067832	3.501764	2.697102	H	-4.145248	-1.997494	2.996002
H	3.362016	-0.331630	2.125602	H	-3.498463	-1.318480	4.501302
H	4.464693	0.721894	4.052102	H	-4.214897	0.264704	2.278702
H	4.281839	3.179090	4.428902	O	-4.233093	0.078404	3.229702
H	2.979109	4.573962	2.850902	C	-2.692176	-0.695562	-1.490298
C	2.366281	-3.307452	-0.541798	O	-1.410574	-0.792634	-0.794398
C	2.030520	-0.530859	-0.081498				
C	1.275671	-2.838476	0.140602	B3LYP/6-31G** Energy =			-6817.816915
H	2.490504	-4.372849	-0.702898	B3LYP/6-31G** Free Energy =			-6817.837703
Br	-0.021603	-4.052604	0.828202	M06-2X/LACVP** Derived Free Energy =			-1700.436803
C	3.179130	-0.999934	-0.805298	M06-2X/LACVP** Derived Solution Free Energy =			-1700.460082
C	3.340661	-2.403931	-1.039298	Number of Imaginary Frequencies =			0
C	4.475171	-2.866506	-1.757598				
C	5.415852	-1.982085	-2.232198	B3LYP/6-31G** Geometry			
C	5.258522	-0.594889	-2.005098				
C	4.170511	-0.115712	-1.309698	C	-2.004090	0.228712	-1.080096
H	4.584495	-3.934403	-1.926098	C	-3.047101	-0.738276	-1.066296
H	6.278960	-2.345466	-2.781598	C	-3.772404	-1.011669	0.061204
H	6.002806	0.099028	-2.384098	C	-1.699683	0.919609	0.085304
H	4.056888	0.949185	-1.141798	Br	-3.407711	-1.688873	-2.694396
B	-1.271471	-0.932831	0.561302	H	-4.561012	-1.755660	0.037904
C	-2.713521	-3.208463	-1.762198	C	-3.484596	-0.327572	1.268104
C	1.089540	-1.444880	0.364002	C	-2.430086	0.644017	1.284604
O	0.006131	-1.036503	1.091502	C	-2.147379	1.298314	2.516604
C	-4.824653	2.797491	0.001702	C	-2.869682	1.014122	3.653504
C	-3.512755	2.894320	-0.464598	C	-3.915592	0.060933	3.628704
C	-2.852130	1.764234	-0.940998	C	-4.212699	-0.595764	2.457704
C	-3.480803	0.510320	-0.957098	H	-1.347071	2.028405	2.551904
C	-4.800601	0.425392	-0.494598	H	-2.632976	1.526019	4.581604
C	-5.466726	1.559477	-0.019298	H	-4.476894	-0.150961	4.533504
H	-5.342072	3.675480	0.376502	H	-5.009607	-1.333955	2.423804
H	-2.987175	3.844631	-0.461298	C	1.494449	3.834374	0.193304
H	-1.833932	1.864756	-1.298498	C	-0.605572	1.939197	0.073604
H	-5.328880	-0.521520	-0.492398	C	1.760634	2.490872	0.217004
H	-6.488924	1.468555	0.336502	H	2.305557	4.551166	0.261304
C	-2.109100	-4.192850	-2.113298	Br	3.566428	1.896852	0.424104
H	-1.566481	-5.059738	-2.410498	C	-0.908757	3.339600	0.036904
C	-2.329381	-0.487454	-2.966098	C	0.157554	4.294789	0.088404
H	-3.239983	-0.398374	-3.565198	C	-0.143231	5.682492	0.047804
H	-1.745801	0.425858	-3.096098	C	-1.444327	6.118106	-0.045896
H	-1.749162	-1.338442	-3.331398	C	-2.500437	5.178218	-0.103296
C	-3.458147	-2.034179	-1.313498	C	-2.240951	3.826615	-0.061796
H	-3.722344	-2.154985	-0.258398	H	0.677076	6.393983	0.090104
H	-4.396948	-1.967600	-1.875898	H	-1.663915	7.181009	-0.078296
O	0.469281	1.238507	-1.725698	H	-3.525733	5.527329	-0.182396
H	0.227002	0.307501	-1.575298	H	-3.056759	3.114524	-0.110196
O	-2.332871	-0.938255	1.407002	B	1.777603	-0.438629	-0.784196
C	-2.176566	-1.158051	2.819402	C	2.907180	-2.485241	3.077304
H	-1.663245	-2.111040	2.991302	C	0.716224	1.527883	0.127104
H	-1.576484	-0.349538	3.249702	O	1.011109	0.192380	0.183704
C	-3.571366	-1.156782	3.420402	C	-1.814238	-4.239390	0.543704

C	-1.198136	-3.970796	1.764804	C	-2.933987	-0.865995	4.275999
C	0.073971	-3.397110	1.804504	C	-3.560190	-1.476392	3.213799
C	0.753874	-3.087618	0.620104	H	-0.965577	1.349497	2.588799
C	0.127571	-3.370211	-0.602896	H	-1.485881	0.630499	4.879199
C	-1.146035	-3.935497	-0.643196	H	-3.158688	-1.171194	5.293499
H	-2.805643	-4.682379	0.515804	H	-4.285093	-2.269389	3.379099
H	-1.708338	-4.200891	2.695704	C	0.637432	3.623890	-0.686501
H	0.535873	-3.205015	2.766304	C	-1.139077	1.513998	-0.019301
H	0.642373	-3.141516	-1.530096	C	0.951527	2.322389	-0.975001
H	-1.622637	-4.119392	-1.601096	H	1.320236	4.422787	-0.954301
C	3.227674	-3.104444	4.064104	Br	2.574525	1.914482	-1.891401
H	3.511668	-3.655147	4.930704	C	-1.505971	2.873299	0.260999
C	3.191768	-3.655444	0.403004	C	-0.595466	3.932895	-0.059201
H	3.111560	-4.397743	1.198604	C	-0.953661	5.276897	0.230899
H	2.997263	-4.141442	-0.555796	C	-2.168059	5.574502	0.802899
H	4.213572	-3.262155	0.396904	C	-3.078964	4.534206	1.102199
C	2.531489	-1.699937	1.903104	C	-2.758469	3.221405	0.838299
H	3.364996	-1.039746	1.636704	H	-0.249157	6.066794	-0.015001
H	1.692296	-1.043528	2.147804	H	-2.433255	6.605003	1.018799
O	-1.296487	0.501405	-2.202496	H	-4.042563	4.774310	1.541699
H	-1.607494	-0.079092	-2.916196	H	-3.467973	2.435408	1.067699
O	1.965109	0.177069	-1.977296	B	1.397613	-0.807113	-0.386601
C	2.760404	-0.329339	-3.054896	C	0.982805	-2.836311	2.325099
H	2.532492	-1.386437	-3.239196	C	0.079422	1.256193	-0.627701
H	2.464010	0.251264	-3.934196	O	0.418917	-0.018909	-0.997501
C	4.257206	-0.166755	-2.804896	C	6.758014	-0.657636	-0.003101
H	4.779405	-0.196061	-3.768596	C	5.848918	0.400868	0.043999
H	4.417816	0.829043	-2.362596	C	4.573718	0.208473	0.570799
H	4.186392	-1.393355	-1.302596	C	4.170612	-1.047525	1.048299
O	4.820394	-1.193662	-2.007596	C	5.090108	-2.101929	0.993599
C	2.178880	-2.522933	0.624104	C	6.372209	-1.908934	0.473099
O	2.352289	-1.660135	-0.533096	H	7.754215	-0.508540	-0.409301
B3LYP/6-31G** Energy =				H	6.132423	1.381567	-0.327701
B3LYP/6-31G** Free Energy =				H	3.870421	1.032576	0.580199
M06-2X/LACVP** Derived Free Energy =				H	4.821504	-3.089228	1.351899
M06-2X/LACVP** Derived Solution Free Energy =				H	7.066705	-2.743537	0.439799
Number of Imaginary Frequencies =				C	-0.146196	-2.983106	2.727299
B3LYP/6-31G** Geometry				H	-1.147096	-3.070602	3.082399
C	-2.706484	-0.259996	-0.766701	C	2.741615	-0.472019	3.031299
C	-3.613989	-1.322892	-0.500601	H	3.473713	-0.915922	3.711999
C	-3.900791	-1.721690	0.777499	H	2.985919	0.585180	2.904799
C	-2.073382	0.387002	0.289199	H	1.744814	-0.555715	3.471399
Br	-4.444993	-2.194888	-1.987301	C	2.349405	-2.671617	1.837999
H	-4.603594	-2.529287	0.951499	H	2.460603	-3.183418	0.877699
C	-3.277488	-1.082193	1.877699	H	3.038503	-3.147520	2.545199
C	-2.339783	-0.025097	1.633699	O	-2.454883	0.164303	-2.028901
C	-1.698381	0.569000	2.756799	H	-2.716485	-0.526195	-2.662301
C	-1.988983	0.161201	4.039099	O	1.868209	-1.890315	-1.058701
				C	1.726508	-2.102914	-2.472201
				H	1.923212	-1.168615	-3.011101
				H	2.505405	-2.826218	-2.732401

C	0.361205	-2.653309	-2.880201	C	-6.535197	-1.216572	-0.612897
H	0.477803	-3.189509	-3.829901	C	-6.159000	-1.925974	0.526803
H	0.046402	-3.390707	-2.123901	C	-5.011698	-1.562479	1.238003
H	-0.507487	-0.967805	-2.426401	C	-4.218794	-0.486982	0.818603
O	-0.624590	-1.660004	-3.096601	C	-4.610490	0.221719	-0.327297
C	2.774412	-1.185219	1.671399	C	-5.753892	-0.140075	-1.037097
O	1.798315	-0.478715	0.869899	H	-7.423198	-1.503068	-1.168197
B3LYP/6-31G** Energy =				H	-6.754204	-2.768771	0.866103
B3LYP/6-31G** Free Energy =				H	-4.739101	-2.134080	2.118103
M06-2X/LACVP** Derived Free Energy =				H	-3.993587	1.038817	-0.686297
M06-2X/LACVP** Derived Solution Free Energy =				H	-6.031390	0.415826	-1.927997
Number of Imaginary Frequencies =				C	-1.434980	2.460605	3.779503
B3LYP/6-31G** Geometry				H	-0.694778	2.950402	4.368903
C	2.993305	-0.746215	-0.647997	C	-2.462696	-1.054590	2.609903
C	3.678600	-1.906118	-0.190797	H	-3.186897	-1.210087	3.414603
C	3.616698	-2.321517	1.112703	H	-2.262800	-2.011791	2.124403
C	2.228408	-0.008411	0.248603	H	-1.537295	-0.684294	3.054003
Br	4.719196	-2.893022	-1.467597	C	-3.333486	1.314514	2.293203
H	4.155894	-3.207220	1.430703	H	-3.640682	2.023815	1.517003
C	2.844801	-1.591814	2.050403	H	-4.214386	1.139918	2.922603
C	2.134307	-0.424911	1.611903	O	3.068807	-0.330915	-1.934897
C	1.350910	0.280693	2.567503	H	3.635104	-0.946517	-2.428597
C	1.288408	-0.139807	3.877503	O	-1.836400	-1.800893	-0.443297
C	2.001803	-1.284210	4.308903	C	-1.337803	-2.652995	-1.483697
C	2.761000	-1.995614	3.409903	H	-1.423101	-2.142895	-2.449097
H	0.782814	1.148095	2.250903	H	-0.282304	-2.891800	-1.306097
H	0.674010	0.409896	4.583903	C	-2.193009	-3.909091	-1.470397
H	1.942801	-1.600010	5.346003	H	-1.849012	-4.589693	-2.256897
H	3.308396	-2.880216	3.724503	H	-2.059511	-4.421592	-0.503197
C	0.280224	3.491798	-1.374897	H	-3.831305	-2.965084	-1.081797
C	1.541714	1.221592	-0.256297	O	-3.554808	-3.629585	-1.730197
C	-0.301981	2.254200	-1.458297	C	-2.973392	-0.030688	1.592803
H	-0.204272	4.351600	-1.824597	O	-1.898790	0.302407	0.685203
Br	-1.930382	2.043607	-2.429697	B3LYP/6-31G** Energy =			
C	2.173520	2.503189	-0.158297	B3LYP/6-31G** Free Energy =			
C	1.522825	3.652792	-0.712097	M06-2X/LACVP** Derived Free Energy =			
C	2.144531	4.925689	-0.607497	M06-2X/LACVP** Derived Solution Free Energy =			
C	3.361831	5.065484	0.017103	Number of Imaginary Frequencies =			
C	4.010126	3.931581	0.561603	B3LYP/6-31G** Geometry			
C	3.433321	2.684283	0.475003	C	-1.847278	-0.712662	1.032401
H	1.638634	5.788191	-1.032997	C	-2.432732	-2.010683	1.065501
H	3.828536	6.043082	0.092203	C	-3.227516	-2.463211	0.047901
H	4.972427	4.047277	1.051603	C	-2.083407	0.121629	-0.056299
H	3.937317	1.820981	0.895103	Br	-2.066892	-3.145170	2.555001
B	-1.360594	-0.540895	-0.242197	H	-3.660081	-3.456526	0.100201
C	-2.272783	1.919009	3.097703	C	-3.474245	-1.649620	-1.087099
C	0.307913	1.110297	-0.876397	C	-2.885691	-0.345099	-1.149899
O	-0.279292	-0.118900	-0.999397	C	-3.122418	0.436093	-2.314499

C	-3.904001	-0.040435	-3.343899	H	2.841509	-0.328497	2.740601
C	-4.493456	-1.323855	-3.270499	C	3.503437	1.727626	2.723301
C	-4.277928	-2.110548	-2.162699	H	3.049003	2.690810	2.443401
H	-2.674053	1.420109	-2.389099	H	3.913533	1.831240	3.734301
H	-4.066923	0.575660	-4.223399	H	4.302552	1.277054	0.983501
H	-5.108243	-1.685877	-4.088899	O	4.600748	1.395164	1.896401
H	-4.716394	-3.102563	-2.094599	C	2.959147	-1.400093	-0.969299
C	-0.350047	4.090990	-0.232599	O	2.614520	-0.641005	0.206201
C	-1.497155	1.499250	-0.082899				
C	0.423293	2.973218	-0.392399	B3LYP/6-31G** Energy =			-6817.820581
H	0.096819	5.077306	-0.294099	B3LYP/6-31G** Free Energy =			-6817.840048
Br	2.298887	3.148484	-0.716699	M06-2X/LACVP** Derived Free Energy =			-1700.440332
C	-2.323396	2.659421	0.111201	M06-2X/LACVP** Derived Solution Free Energy =			-1700.461906
C	-1.739442	3.964941	0.028401	Number of Imaginary Frequencies =			0
C	-2.556282	5.111113	0.218701				
C	-3.898178	4.980866	0.491701	B3LYP/6-31G** Geometry			
C	-4.476033	3.693545	0.587801				
C	-3.711293	2.563172	0.401701	C	2.217717	-1.116887	-0.425297
H	-2.098217	6.093929	0.148901	C	2.996524	-2.221381	0.022303
H	-4.514109	5.862744	0.638301	C	3.915424	-2.096876	1.030803
H	-5.533829	3.595608	0.812601	C	2.402709	0.129215	0.163003
H	-4.164058	1.581856	0.480901	Br	2.750935	-3.925183	-0.819397
B	1.618189	0.244060	0.440101	H	4.493629	-2.957472	1.349203
C	5.276511	-0.383512	-0.908399	C	4.114815	-0.844874	1.662403
C	-0.140461	1.668598	-0.315599	C	3.347908	0.285221	1.225903
O	0.662477	0.575926	-0.510499	C	3.552700	1.525522	1.894103
C	0.933082	-5.251765	-0.936499	C	4.465399	1.638228	2.918403
C	0.669649	-4.319074	0.064301	C	5.228307	0.521633	3.336503
C	1.325806	-3.086051	0.071001	C	5.052314	-0.694268	2.719203
C	2.245394	-2.757918	-0.931199	H	2.973795	2.389318	1.588303
C	2.497728	-3.703609	-1.937599	H	4.601093	2.595529	3.413303
C	1.853671	-4.939532	-1.938299	H	5.945806	0.627438	4.144403
H	0.424216	-6.211282	-0.940399	H	5.625820	-1.562564	3.032503
H	-0.059043	-4.528199	0.841101	C	0.081987	3.587500	-1.005097
H	1.108081	-2.385258	0.868101	C	1.592402	1.293909	-0.311297
H	3.198320	-3.476785	-2.736199	C	-0.464207	2.590296	-0.240597
H	2.067596	-5.655225	-2.726999	H	-0.495119	4.476796	-1.233997
C	5.928575	0.630811	-0.989499	Br	-2.216308	2.807785	0.486003
H	6.522244	1.514132	-1.041199	C	2.181295	2.314313	-1.127697
C	2.635720	-0.641305	-2.266299	C	1.409188	3.466408	-1.487797
H	3.109438	-1.144888	-3.113299	C	1.992981	4.473612	-2.302097
H	1.560919	-0.606342	-2.440399	C	3.286382	4.352020	-2.753497
H	3.019284	0.379709	-2.213199	C	4.050589	3.212925	-2.405897
C	4.494854	-1.616339	-0.822799	C	3.514796	2.222922	-1.613197
H	4.670871	-2.099233	0.144701	H	1.394975	5.342408	-2.563497
H	4.831079	-2.316427	-1.594699	H	3.722577	5.126123	-3.377497
O	-1.083589	-0.376135	2.098701	H	5.069290	3.118632	-2.770097
H	-0.568318	0.430083	1.926601	H	4.106801	1.351726	-1.356697
O	1.480268	0.835355	1.666301	B	-1.318887	-0.412709	0.449803
C	2.400574	0.672687	2.758801	C	-1.320769	-3.254309	-1.950397
H	1.802770	0.784266	3.668801	C	0.266201	1.412401	0.075703

O	-0.306293	0.446997	0.852803	C	0.717862	1.981008	2.474299
C	-6.523890	0.022557	0.462103	C	1.033160	2.085814	3.810299
C	-6.131982	-1.312341	0.549803	C	2.266969	1.598138	4.304999
C	-4.937279	-1.737833	-0.039197	C	3.162281	1.005055	3.445899
C	-4.111885	-0.838928	-0.727797	H	-0.236345	2.342489	2.109499
C	-4.520493	0.501570	-0.806797	H	0.326951	2.547000	4.494399
C	-5.708096	0.929362	-0.216697	H	2.500668	1.690943	5.361199
H	-7.449292	0.353551	0.923403	H	4.111488	0.622374	3.811699
H	-6.750677	-2.029345	1.081203	C	-2.322656	2.893449	-1.491201
H	-4.660472	-2.780831	0.058903	C	0.073265	1.835095	-0.416001
H	-3.881298	1.227074	-1.295297	C	-2.248330	1.589450	-1.081301
H	-5.996303	1.974160	-0.288397	H	-3.248163	3.287131	-1.896901
C	-0.396466	-3.733903	-2.565497	Br	-3.795109	0.473120	-1.236201
H	0.412937	-4.160898	-3.111097	C	0.027938	3.202394	-0.844401
C	-2.820384	-0.890019	-2.894897	C	-1.186172	3.734571	-1.386101
H	-3.616781	-1.444524	-3.399997	C	-1.231199	5.090470	-1.806701
H	-3.000591	0.177080	-3.033697	C	-0.122614	5.897291	-1.698201
H	-1.862983	-1.142113	-3.354997	C	1.079396	5.376215	-1.163101
C	-2.488072	-2.757717	-1.222997	C	1.153521	4.065516	-0.747701
H	-2.378271	-2.974416	-0.156297	H	-2.160606	5.477152	-2.215801
H	-3.359169	-3.319323	-1.580797	H	-0.166134	6.932891	-2.021501
O	1.312018	-1.214392	-1.423597	H	1.951583	6.017832	-1.080201
H	1.045524	-2.136794	-1.581897	H	2.078329	3.674834	-0.338801
O	-1.883182	-1.219313	1.396303	B	-1.681784	-0.806439	0.889099
C	-1.606883	-1.056611	2.797703	C	-2.119120	-4.070147	-2.171101
H	-1.717677	-2.046012	3.250903	C	-1.053520	1.040173	-0.539001
H	-0.582885	-0.701105	2.948403	O	-1.005694	-0.285926	-0.206101
C	-2.612389	-0.090218	3.408503	C	2.907468	-3.442550	0.159799
H	-2.387390	0.034684	4.473803	C	2.185965	-3.310264	1.347599
H	-2.500996	0.892283	2.923503	C	0.796163	-3.219991	1.315799
H	-4.141785	-0.699728	2.386403	C	0.096664	-3.260104	0.099499
O	-3.941886	-0.571626	3.325303	C	0.830167	-3.391090	-1.085301
C	-2.787082	-1.241919	-1.401397	C	2.223968	-3.479163	-1.054201
O	-1.701487	-0.455212	-0.858297	H	3.991269	-3.501128	0.178099
				H	2.705164	-3.273354	2.300899
B3LYP/6-31G** Energy =				H	0.245561	-3.102701	2.243899
B3LYP/6-31G** Free Energy =				H	0.322468	-3.437500	-2.041501
M06-2X/LACVP** Derived Free Energy =				H	2.775170	-3.572352	-1.985301
M06-2X/LACVP** Derived Solution Free Energy =				C	-2.141602	-4.989348	-2.955201
Number of Imaginary Frequencies =				H	-2.161186	-5.803448	-3.642001
				C	-1.998412	-4.488145	0.758399
B3LYP/6-31G** Geometry				H	-1.720195	-5.355840	0.157499
				H	-1.605809	-4.618737	1.769099
C	2.238788	0.650337	-0.691201	H	-3.089913	-4.431566	0.812899
C	3.465397	0.161461	-0.161701	C	-2.108242	-2.939647	-1.245601
C	3.780695	0.269767	1.165999	H	-3.142348	-2.647267	-1.030001
C	1.330376	1.265720	0.160199	H	-1.640659	-2.070738	-1.716801
Br	4.696814	-0.664915	-1.379101	O	1.935890	0.551732	-2.007401
H	4.727003	-0.109214	1.536099	H	2.653399	0.074245	-2.455201
C	2.867283	0.879350	2.061999	O	-2.164001	0.065952	1.819099
C	1.622974	1.379925	1.554599	C	-2.915292	-0.360463	2.961499

H	-2.501374	-1.291055	3.366499	C	-0.354281	1.296502	0.054200
H	-2.808708	0.433139	3.706499	O	-0.850596	0.026207	0.205200
C	-4.387289	-0.549192	2.613499	C	-5.242602	-0.588744	2.890000
H	-4.488672	-1.393694	1.914599	C	-4.164810	-1.233356	3.493300
H	-4.930284	-0.812702	3.528699	C	-3.193217	-1.864867	2.713300
H	-4.576715	0.800805	1.244399	C	-3.280917	-1.861366	1.316100
O	-4.985012	0.628297	2.105799	C	-4.372809	-1.211753	0.721600
C	-1.434737	-3.204334	0.134399	C	-5.342402	-0.580642	1.497600
O	-1.857358	-2.149442	1.037799	H	-5.997197	-0.096935	3.496700
B3LYP/6-31G** Energy =				H	-4.072710	-1.246257	4.575500
B3LYP/6-31G** Free Energy =				H	-2.366522	-2.356876	3.213500
M06-2X/LACVP** Derived Free Energy =				H	-4.456809	-1.196652	-0.359900
M06-2X/LACVP** Derived Solution Free Energy =				H	-6.177897	-0.082433	1.014000
Number of Imaginary Frequencies =				C	0.954661	-3.833513	-0.482200
0				H	1.756358	-4.105422	-1.130500
B3LYP/6-31G** Geometry				C	-2.903940	-3.909070	-0.088200
C	2.387700	-0.362129	-0.678500	H	-3.179347	-4.552467	0.752000
C	3.395589	-1.348740	-0.476500	H	-3.805837	-3.693360	-0.665900
C	3.940086	-1.574947	0.758400	H	-2.191346	-4.437978	-0.726300
C	1.965909	0.413076	0.397800	C	-0.939028	-2.902292	1.150700
Br	3.976777	-2.390647	-1.965200	H	-0.575318	-1.989096	1.632100
H	4.702078	-2.336955	0.881600	H	-1.133937	-3.631290	1.945500
C	3.503095	-0.831742	1.884800	O	1.915702	-0.226524	-1.939300
C	2.499806	0.174470	1.705700	H	1.067007	0.248786	-1.943600
C	2.074914	0.905574	2.849200	O	-1.012298	-0.163991	-2.127600
C	2.613311	0.654968	4.092300	C	-1.422105	-0.795786	-3.353100
C	3.606100	-0.337743	4.263500	H	-0.727501	-0.440694	-4.118700
C	4.039092	-1.065048	3.178400	H	-1.336417	-1.883687	-3.263300
H	1.312023	1.667483	2.733200	C	-2.847400	-0.395970	-3.715600
H	2.270318	1.224872	4.951000	H	-3.094005	-0.835268	-4.689000
H	4.021698	-0.524247	5.249000	H	-3.542805	-0.823263	-2.976900
H	4.799184	-1.832956	3.294900	H	-2.909080	1.380230	-2.953300
C	-0.813055	3.665007	-0.291100	O	-3.009085	1.003831	-3.840400
C	1.006221	1.537886	0.164000	C	-2.279225	-2.602077	0.422000
C	-1.253569	2.374212	-0.182600	O	-2.019416	-1.834580	-0.777200
H	-1.518446	4.467715	-0.476300	B3LYP/6-31G** Energy =			
Br	-3.114074	1.993633	-0.381400	B3LYP/6-31G** Free Energy =			
C	1.494236	2.885481	0.045500	M06-2X/LACVP** Derived Free Energy =			
C	0.570148	3.956791	-0.175900	M06-2X/LACVP** Derived Solution Free Energy =			
C	1.052163	5.287486	-0.291000	Number of Imaginary Frequencies =			
C	2.397666	5.557371	-0.198200	0			
C	3.315355	4.501760	0.011000	B3LYP/6-31G** Geometry			
C	2.877540	3.201265	0.129600	C	-1.866690	0.353540	1.134307
H	0.336472	6.087794	-0.458000	C	-3.018210	-0.473632	1.239307
H	2.758078	6.577467	-0.289100	C	-3.964512	-0.536609	0.253107
H	4.377157	4.719149	0.076900	C	-1.675371	1.117435	-0.009693
H	3.590031	2.400057	0.286400	Br	-3.206337	-1.545027	2.822107
B	-1.314504	-0.681788	-0.895000	H	-4.833528	-1.175287	0.367207
C	0.095466	-3.419203	0.258700	C	-3.797193	0.223187	-0.930993

C	-2.632773	1.048959	-1.072193	C	2.952181	-0.817479	2.472207
C	-2.475355	1.771555	-2.288293	H	2.314470	-1.274663	3.240607
C	-3.417557	1.692678	-3.288693	H	3.515162	-1.607593	1.966107
C	-4.571977	0.888206	-3.136593	C	3.900706	0.185598	3.109007
C	-4.752995	0.167211	-1.980193	H	3.307526	0.999013	3.557407
H	-1.594940	2.389133	-2.422293	H	4.450394	-0.310016	3.917207
H	-3.272243	2.253074	-4.207593	H	4.393427	1.030786	1.435107
H	-5.306578	0.838124	-3.934293	O	4.868718	0.679274	2.202807
H	-5.628710	-0.463368	-1.851593	C	1.648331	-2.837747	-0.976993
C	1.819290	3.624849	-0.474293	O	1.823851	-2.030951	0.196207
C	-0.468750	1.994405	-0.118893				
C	1.906357	2.261047	-0.564293	B3LYP/6-31G** Energy =			-6817.817998
H	2.699505	4.238127	-0.632893	B3LYP/6-31G** Free Energy =			-6817.839947
Br	3.582337	1.459706	-1.015593	M06-2X/LACVP** Derived Free Energy =			-1700.441074
C	-0.584115	3.418708	-0.000693	M06-2X/LACVP** Derived Solution Free Energy =			-1700.465281
C	0.577405	4.239280	-0.175693	Number of Imaginary Frequencies =			0
C	0.463940	5.650182	-0.054393				
C	-0.745245	6.236612	0.237207	B3LYP/6-31G** Geometry			
C	-1.893165	5.430140	0.421107				
C	-1.816299	4.060438	0.303907	C	2.163594	-0.959996	-1.045605
H	1.354555	6.257161	-0.193093	C	2.707391	-2.249997	-0.795505
H	-0.821219	7.315614	0.330907	C	3.265791	-2.583999	0.409295
H	-2.844354	5.896864	0.659207	C	2.170397	-0.008496	-0.034105
H	-2.701514	3.452660	0.451807	Br	2.611088	-3.546597	-2.207405
B	1.627184	-0.702846	0.413307	H	3.675688	-3.575700	0.566395
C	4.079815	-3.520206	-0.753093	C	3.293893	-1.634499	1.460895
C	0.773936	1.425775	-0.357193	C	2.725096	-0.335797	1.243495
O	0.886203	0.069872	-0.472993	C	2.727498	0.584603	2.329195
C	-2.288414	-4.691150	-1.007993	C	3.277297	0.244401	3.544295
C	-1.895595	-3.903760	0.072507	C	3.853394	-1.032700	3.748195
C	-0.636580	-3.299891	0.085607	C	3.856392	-1.952400	2.726295
C	0.248316	-3.463812	-0.985193	H	2.279401	1.561204	2.188495
C	-0.159003	-4.256902	-2.069093	H	3.267399	0.963401	4.358195
C	-1.412618	-4.866271	-2.080693	H	4.284994	-1.284101	4.712195
H	-3.267026	-5.162226	-1.017493	H	4.285890	-2.940101	2.871195
H	-2.565791	-3.740043	0.910507	C	0.348606	3.853108	-0.704705
H	-0.345065	-2.694898	0.935607	C	1.566600	1.334205	-0.293905
H	0.504293	-4.403319	-2.916693	C	-0.414197	2.740410	-0.461605
H	-1.705533	-5.474964	-2.931393	H	-0.127292	4.816609	-0.851105
C	5.227124	-3.144335	-0.713993	Br	-2.312696	2.883315	-0.377105
H	6.237432	-2.808660	-0.671693	C	2.384003	2.479103	-0.561405
C	1.929351	-2.040854	-2.260493	C	1.761706	3.752905	-0.767805
H	2.039734	-2.719156	-3.110693	C	2.571209	4.890003	-1.032205
H	1.118268	-1.344534	-2.471593	C	3.940908	4.780800	-1.094305
H	2.858065	-1.476476	-2.151993	C	4.558705	3.523398	-0.895005
C	2.693703	-3.982472	-0.795693	C	3.801803	2.403000	-0.635205
H	2.450990	-4.504766	0.136907	H	2.085211	5.849704	-1.186505
H	2.566485	-4.709069	-1.605893	H	4.550210	5.656298	-1.297805
O	-0.940589	0.414617	2.122107	H	5.640305	3.442296	-0.949105
H	-1.221403	-0.161576	2.851707	H	4.283700	1.443099	-0.486505
O	2.125998	-0.116258	1.535207	B	-1.250203	0.056112	1.068895

C	-2.812412	-3.738184	1.762295	C	-2.614213	-1.085703	2.115408
C	0.188600	1.468509	-0.265105	C	-1.939513	0.103698	1.682708
O	-0.597702	0.359311	-0.108605	C	-1.445214	0.992198	2.678608
C	-4.867203	0.180421	-2.943605	C	-1.616614	0.719598	4.017308
C	-5.040602	0.439721	-1.583305	C	-2.286813	-0.454002	4.439308
C	-4.257304	-0.216381	-0.635205	C	-2.772513	-1.337403	3.504508
C	-3.280206	-1.143583	-1.030205	H	-0.916314	1.885398	2.367308
C	-3.115507	-1.396383	-2.397205	H	-1.233514	1.413598	4.760008
C	-3.901405	-0.739981	-3.346305	H	-2.412413	-0.654203	5.498908
H	-5.477302	0.692922	-3.681505	H	-3.286212	-2.243803	3.814008
H	-5.789000	1.155523	-1.255705	C	0.061785	3.999699	-1.150092
H	-4.402903	0.007620	0.416995	C	-1.153714	1.625298	-0.206292
H	-2.367408	-2.104185	-2.736005	C	0.791685	2.851199	-0.994492
H	-3.752106	-0.948382	-4.401805	H	0.540285	4.903099	-1.512392
C	-2.318414	-4.401985	2.641995	Br	2.651085	2.856000	-1.425992
H	-1.886015	-4.983386	3.422795	C	-1.941514	2.812198	-0.367292
C	-1.217709	-2.591388	-0.497805	C	-1.321715	4.012498	-0.842392
H	-1.485411	-3.425987	-1.151805	C	-2.102116	5.188898	-0.999892
H	-0.589508	-1.894889	-1.052105	C	-3.444616	5.187897	-0.701392
H	-0.652810	-2.999089	0.342895	C	-4.061715	4.004197	-0.232392
C	-3.424910	-2.947883	0.695795	C	-3.331415	2.848197	-0.069792
H	-4.303709	-2.421081	1.085795	H	-1.616116	6.090798	-1.362392
H	-3.792312	-3.611082	-0.096105	H	-4.032916	6.092097	-0.825092
O	1.615995	-0.635195	-2.242505	H	-5.122415	4.007996	0.000808
H	1.705193	-1.394595	-2.841805	H	-3.814014	1.946497	0.289608
O	-0.991301	0.812012	2.167295	B	1.918387	0.309599	0.512408
C	-1.637802	0.678613	3.437795	C	5.463088	-1.743299	-0.042692
H	-1.569904	-0.356187	3.795795	C	0.194586	1.649899	-0.520192
H	-1.072000	1.319012	4.121195	O	0.942187	0.504899	-0.447692
C	-3.098201	1.120917	3.404695	C	-0.333611	-4.336802	-1.102692
H	-3.406900	1.396117	4.420895	C	0.351389	-3.915901	-2.241692
H	-3.161698	2.023017	2.776095	C	1.411888	-3.014501	-2.133092
H	-3.493904	-0.462682	2.354995	C	1.803588	-2.516101	-0.884592
O	-3.993603	0.112819	2.955395	C	1.109688	-2.946301	0.256708
C	-2.477608	-1.901585	0.034195	C	0.051288	-3.846701	0.146208
O	-2.123006	-1.001986	1.123095	H	-1.164711	-5.029302	-1.187192
B3LYP/6-31G** Energy =				H	0.061889	-4.286401	-3.220992
B3LYP/6-31G** Free Energy =				H	1.926488	-2.699301	-3.034092
M06-2X/LACVP** Derived Free Energy =				H	1.385288	-2.566701	1.235708
M06-2X/LACVP** Derived Solution Free Energy =				H	-0.476211	-4.160902	1.041808
Number of Imaginary Frequencies =				C	6.484387	-1.141199	0.189008
				H	7.388087	-0.613998	0.390408
				C	3.361387	-0.783900	-1.985092
B3LYP/6-31G** Geometry				H	3.689087	-1.440000	-2.795792
				H	2.505887	-0.199500	-2.323292
C	-2.281513	-0.542702	-0.645192	H	4.182787	-0.103500	-1.752992
C	-2.950212	-1.712703	-0.189492	C	4.232888	-2.484300	-0.316992
C	-3.117212	-1.984303	1.142008	H	3.945088	-3.062300	0.569408
C	-1.789713	0.364098	0.285108	H	4.405888	-3.215400	-1.115292
Br	-3.639112	-2.922303	-1.509392	O	-2.127013	-0.273302	-1.963092
H	-3.637112	-2.883203	1.455308	H	-2.480313	-1.019103	-2.475092

O	1.943886	1.133899	1.595808	B	1.506307	-0.398609	-0.997499
C	2.963886	1.048700	2.590708	C	4.959607	-0.730400	-0.607299
H	3.926786	0.811900	2.120008	C	0.641002	1.519289	0.219501
H	3.043686	2.040300	3.049008	O	1.204505	0.267290	0.174901
C	2.642587	0.021800	3.668008	C	0.417414	-3.484312	3.318601
H	3.409887	0.118400	4.454808	C	1.631513	-2.868009	3.611601
H	1.670987	0.254399	4.118908	C	2.457112	-2.409406	2.582501
H	3.099687	-1.354500	2.372608	C	2.082312	-2.558107	1.242201
O	2.576487	-1.311900	3.186008	C	0.857014	-3.180210	0.961501
C	3.019287	-1.595800	-0.732292	C	0.032015	-3.636913	1.985701
O	2.834787	-0.702400	0.391108	H	-0.228085	-3.834313	4.118101
B3LYP/6-31G** Energy =				H	1.942213	-2.736908	4.644101
B3LYP/6-31G** Free Energy =				H	3.393510	-1.930604	2.845701
M06-2X/LACVP** Derived Free Energy =				H	0.546014	-3.298011	-0.071599
M06-2X/LACVP** Derived Solution Free Energy =				H	-0.916284	-4.106415	1.743301
Number of Imaginary Frequencies =				C	5.679406	-0.359898	-1.503999
				H	6.312306	-0.029797	-2.294899
B3LYP/6-31G** Geometry				C	3.607814	-3.418204	-0.547099
C	-2.169595	0.053382	-0.779099	H	4.203116	-3.952802	0.198401
C	-3.039292	-1.077720	-0.761799	H	2.820816	-4.088106	-0.901099
C	-3.378990	-1.723121	0.398501	H	4.250114	-3.146402	-1.388399
C	-1.631496	0.495183	0.427501	C	4.106109	-1.165902	0.496701
Br	-3.818190	-1.684422	-2.410899	H	3.653806	-0.287003	0.967001
H	-4.055488	-2.570923	0.373701	H	4.732910	-1.654201	1.251101
C	-2.871891	-1.266220	1.640801	O	-1.924596	0.759882	-1.903399
C	-1.979994	-0.144818	1.657201	H	-1.590495	0.193883	-2.637299
C	-1.481695	0.295984	2.914401	O	1.045605	0.106090	-2.177599
C	-1.858094	-0.326017	4.083101	C	1.324807	-0.520309	-3.423799
C	-2.750991	-1.424420	4.062901	H	1.343305	0.270891	-4.179799
C	-3.242790	-1.885721	2.864201	H	2.300008	-1.017807	-3.402099
H	-0.799297	1.138185	2.940001	C	0.256709	-1.537112	-3.782699
H	-1.468694	0.030684	5.032101	H	0.544411	-2.040711	-4.717099
H	-3.045690	-1.899020	4.994201	H	0.191211	-2.294712	-2.990699
H	-3.929188	-2.728123	2.834301	H	-1.711491	-1.504617	-3.945199
C	0.999396	3.928490	0.284601	O	-0.990892	-0.857315	-3.950199
C	-0.722399	1.683986	0.402501	C	2.986811	-2.155505	0.071201
C	1.492099	2.657091	0.153901	O	2.211110	-1.569907	-0.996599
H	1.669194	4.779792	0.229301	Minima of Compound 4			
Br	3.355300	2.388296	-0.149999	B3LYP/6-31G** Energy =			-6587.611455
C	-1.261802	3.004584	0.543301	B3LYP/6-31G** Free Energy =			-6587.632184
C	-0.387205	4.136886	0.489201	M06-2X/LACVP** Derived Free Energy =			-1470.254361
C	-0.924008	5.444085	0.634801	M06-2X/LACVP** Derived Solution Free Energy =			-1470.272522
C	-2.272709	5.633582	0.825301	Number of Imaginary Frequencies =			0
C	-3.141506	4.517879	0.875801	B3LYP/6-31G** Geometry			
C	-2.650503	3.238981	0.737501	C	-0.441098	-1.381405	-0.941004
H	-0.246210	6.292487	0.591001	C	-0.042504	-2.744207	-0.965504
H	-2.673711	6.636781	0.935001	C	-0.729609	-3.688303	-0.248704
H	-4.206306	4.672977	1.022701				
H	-3.325300	2.391479	0.774901				

C	-1.532396	-0.968899	-0.190404	H	4.737506	-0.628630	-0.766504
Br	1.497493	-3.235914	-1.967904	O	0.303707	-0.469308	-1.648104
H	-0.423014	-4.728005	-0.285004	C	3.387014	0.906277	-0.060104
C	-1.808707	-3.304098	0.587496	O	2.369711	0.337482	-0.916204
C	-2.199800	-1.926196	0.653296				
C	-3.206498	-1.567991	1.592296	B3LYP/6-31G** Energy =			-6587.611562
C	-3.819703	-2.518688	2.377896	B3LYP/6-31G** Free Energy =			-6587.632312
C	-3.465910	-3.883490	2.270596	M06-2X/LACVP** Derived Free Energy =			-1470.256768
C	-2.475511	-4.263595	1.396296	M06-2X/LACVP** Derived Solution Free Energy =			-1470.273546
H	-3.485293	-0.527190	1.697896	Number of Imaginary Frequencies =			0
H	-4.579502	-2.214785	3.091696				
H	-3.964513	-4.623388	2.889396	B3LYP/6-31G** Geometry			
H	-2.173317	-5.304496	1.320196				
C	-2.688775	3.192606	-0.107904	C	-1.683801	-1.250311	-0.496993
C	-1.933389	0.465102	-0.248304	C	-2.447497	-2.448414	-0.510393
C	-1.381077	2.821600	0.061296	C	-3.682596	-2.498518	0.080507
H	-2.971170	4.235708	-0.018604	C	-2.187005	-0.088713	0.070807
Br	-0.086971	4.168394	0.440696	Br	-1.728091	-3.996711	-1.348893
C	-3.290187	0.850209	-0.541804	H	-4.259093	-3.416720	0.055807
C	-3.668580	2.227411	-0.445204	C	-4.191800	-1.368520	0.768907
C	-5.008878	2.612717	-0.717104	C	-3.432304	-0.153217	0.792707
C	-5.942483	1.683322	-1.109804	C	-3.931708	0.923881	1.576207
C	-5.563489	0.328620	-1.255704	C	-5.125008	0.818177	2.255807
C	-4.277291	-0.077286	-0.977604	C	-5.893104	-0.367125	2.189007
H	-5.275673	3.661919	-0.624604	C	-5.429800	-1.438624	1.462807
H	-6.962381	1.987527	-1.324204	H	-3.354011	1.836683	1.649907
H	-6.292793	-0.399576	-1.597604	H	-5.476211	1.653276	2.854407
H	-4.004596	-1.116887	-1.108604	H	-6.836303	-0.433229	2.722807
B	1.030111	0.379588	-0.808004	H	-5.995197	-2.365426	1.420207
C	4.964414	1.015069	-2.053104	C	0.058683	3.605395	-0.014993
C	-0.981884	1.460498	-0.041504	C	-1.409409	1.178090	-0.048293
O	0.359215	1.192891	0.090596	C	0.651387	2.427597	0.356907
C	3.217404	-1.058122	3.814696	H	0.617880	4.533297	0.033907
C	3.507511	0.303076	3.739196	Br	2.461787	2.421503	0.940307
C	3.547214	0.947176	2.500896	C	-2.011713	2.387288	-0.550493
C	3.297410	0.241277	1.318496	C	-1.269517	3.611790	-0.508593
C	3.011104	-1.131021	1.404296	C	-1.861821	4.811488	-0.987093
C	2.968601	-1.772221	2.641396	C	-3.126721	4.807184	-1.525493
H	3.182902	-1.558322	4.778096	C	-3.846217	3.592982	-1.613893
H	3.698613	0.871475	4.644796	C	-3.307213	2.418483	-1.137693
H	3.767719	2.008175	2.466996	H	-1.285325	5.730890	-0.933593
H	2.810601	-1.699220	0.500596	H	-3.567725	5.727283	-1.896593
H	2.738495	-2.832720	2.687296	H	-4.832617	3.584378	-2.067593
C	5.177116	1.467468	-3.152404	H	-3.870110	1.497782	-1.225593
H	5.355918	1.858667	-4.127004	B	0.649299	-1.027903	-0.222193
C	3.274721	2.430477	-0.040504	C	4.059001	-1.866791	2.602407
H	4.144523	2.875073	0.451596	C	-0.066809	1.202395	0.306407
H	3.254323	2.795977	-1.069304	O	0.629795	0.062497	0.632907
H	2.369822	2.758182	0.469596	C	5.236891	1.229813	-1.952093
C	4.729711	0.465770	-0.719404	C	4.144793	0.586309	-2.532493
H	5.545213	0.758366	-0.047104	C	3.432196	-0.375893	-1.815993

C	3.789398	-0.703092	-0.500993	C	-0.971735	3.628780	-0.741201
C	4.898695	-0.062488	0.068007	C	-1.501248	4.840875	-1.260101
C	5.612792	0.896614	-0.650793	C	-2.771748	4.888862	-1.783101
H	5.790688	1.980515	-2.508093	C	-3.560536	3.715654	-1.814201
H	3.843392	0.829808	-3.547293	C	-3.082524	2.531659	-1.297701
H	2.592198	-0.877396	-2.284593	H	-0.872357	5.726881	-1.249501
H	5.209996	-0.306787	1.077507	H	-3.164557	5.817658	-2.185501
H	6.464990	1.386017	-0.187593	H	-4.552337	3.745844	-2.255301
C	4.998902	-2.153788	3.305507	H	-3.698316	1.642153	-1.342601
H	5.830403	-2.406985	3.921507	B	0.652112	-1.127103	-0.259201
C	3.638106	-3.167093	-0.015893	C	2.584214	-1.276284	2.639599
H	4.672006	-3.195689	0.332307	C	0.107289	1.182391	0.143699
H	3.069009	-3.947195	0.498707	O	0.750101	0.022398	0.495599
H	3.618507	-3.369593	-1.089193	C	5.545292	0.874446	-1.238301
C	2.892100	-1.523195	1.791507	C	4.474897	0.417235	-2.007201
H	2.622697	-0.474896	1.949207	C	3.617907	-0.560173	-1.504601
H	2.045002	-2.127398	2.138607	C	3.804212	-1.090372	-0.220401
O	-0.430400	-1.293807	-1.054493	C	4.884707	-0.629461	0.540799
C	3.017701	-1.790295	0.257207	C	5.747098	0.345548	0.035999
O	1.677402	-1.895599	-0.283193	H	6.214185	1.636253	-1.627601
B3LYP/6-31G** Energy =				H	4.305693	0.819533	-3.001701
B3LYP/6-31G** Free Energy =				H	2.798110	-0.918982	-2.119201
M06-2X/LACVP** Derived Free Energy =				H	5.055211	-1.012159	1.540599
M06-2X/LACVP** Derived Solution Free Energy =				H	6.576094	0.693256	0.645899
Number of Imaginary Frequencies =				C	2.389704	-0.334586	3.368999
B3LYP/6-31G** Geometry				H	2.198396	0.521112	3.973599
C	-1.684087	-1.195727	-0.516201	C	3.419237	-3.552675	-0.361401
C	-2.522175	-2.341635	-0.460401	H	4.454839	-3.741265	-0.066501
C	-3.747276	-2.284747	0.149999	H	2.794345	-4.390782	-0.038301
C	-2.099899	0.020369	0.005299	H	3.375436	-3.488076	-1.450501
Br	-1.915559	-3.970029	-1.235801	C	2.856725	-2.439681	1.800199
H	-4.382467	-3.163354	0.176999	H	2.096633	-3.209889	1.976699
C	-4.169688	-1.093452	0.792599	H	3.810430	-2.883772	2.110999
C	-3.332600	0.069457	0.750099	O	-0.447086	-1.339414	-1.089701
C	-3.746311	1.210053	1.492599	C	2.910623	-2.236081	0.258399
C	-4.931711	1.213641	2.193799	O	1.569122	-2.115094	-0.257801
C	-5.776900	0.080032	2.190899	(S,R) product complex			
C	-5.397288	-1.050564	1.506999	B3LYP/6-31G** Energy =			
H	-3.108620	2.084759	1.516599	B3LYP/6-31G** Free Energy =			
H	-5.216820	2.095438	2.759699	M06-2X/LACVP** Derived Free Energy =			
H	-6.713000	0.099723	2.740599	M06-2X/LACVP** Derived Solution Free Energy =			
H	-6.023080	-1.938870	1.514899	Number of Imaginary Frequencies =			
C	0.358365	3.564894	-0.257301	0			
C	-1.242911	1.225778	-0.185201	B3LYP/6-31G** Geometry			
C	0.890277	2.370299	0.151899	C	-1.635488	-1.099447	-0.588671
H	0.967556	4.462000	-0.241401	C	-2.484449	-2.236831	-0.654491
Br	2.693578	2.291117	0.745499	C	-3.745664	-2.201578	-0.120580
C	-1.782524	2.448272	-0.725701	C	-2.076964	0.089659	-0.025898

Br	-1.844078	-3.823898	-1.484416	O	-0.367321	-1.229728	-1.094565
H	-4.387174	-3.073506	-0.185827	C	2.972782	-1.967868	0.362909
C	-4.200748	-1.045131	0.561877	O	1.696621	-1.945869	-0.306892
C	-3.354771	0.109206	0.639246				
C	-3.807594	1.210417	1.417568	B3LYP/6-31G** Energy =			-6587.612327
C	-5.035565	1.186550	2.040798	B3LYP/6-31G** Free Energy =			-6587.633215
C	-5.886523	0.063785	1.919621	M06-2X/LACVP** Derived Free Energy =			-1470.256002
C	-5.471375	-1.030232	1.197868	M06-2X/LACVP** Derived Solution Free Energy =			-1470.273828
H	-3.166976	2.075633	1.533153	Number of Imaginary Frequencies =			0
H	-5.350346	2.037844	2.636986				
H	-6.855802	0.062242	2.408822	B3LYP/6-31G** Geometry			
H	-6.102132	-1.911081	1.114658				
C	0.444300	3.603067	0.033039	C	-0.622272	-1.424110	-0.954920
C	-1.203781	1.296706	-0.091430	C	-0.275264	-2.800855	-0.938325
C	0.928108	2.379162	0.413448	C	-0.932554	-3.679384	-0.118038
H	1.070995	4.484201	0.116226	C	-1.629420	-0.930271	-0.139134
Br	2.710083	2.226784	1.065443	Br	1.160818	-3.403083	-2.031230
C	-1.689741	2.553614	-0.601768	H	-0.666214	-4.730718	-0.123019
C	-0.858400	3.717117	-0.513328	C	-1.922811	-3.210380	0.782715
C	-1.337095	4.963674	-0.999096	C	-2.256447	-1.816206	0.807347
C	-2.575461	5.062427	-1.587910	C	-3.164000	-1.370012	1.807545
C	-3.381277	3.908147	-1.721587	C	-3.740575	-2.253809	2.692307
C	-2.953442	2.690630	-1.240607	C	-3.447528	-3.635670	2.628967
H	-0.694815	5.835511	-0.909622	C	-2.551525	-4.099825	1.695454
H	-2.929191	6.017620	-1.963786	H	-3.393727	-0.314530	1.880515
H	-4.346106	3.980210	-2.214603	H	-4.423443	-1.883464	3.451111
H	-3.580898	1.816941	-1.364002	H	-3.916940	-4.322167	3.326995
B	0.697772	-1.046933	-0.222872	H	-2.295128	-5.154743	1.650570
C	1.746262	-2.505393	2.504781	C	-2.616894	3.274731	-0.168411
C	0.119839	1.213685	0.320727	C	-1.979088	0.514997	-0.236778
O	0.710230	0.021357	0.661063	C	-1.314622	2.857935	-0.086320
C	5.687513	0.887542	-1.484543	H	-2.851468	4.331505	-0.105753
C	4.538568	0.470548	-2.154689	Br	0.054047	4.166035	0.132955
C	3.665374	-0.440556	-1.559104	C	-3.340332	0.942178	-0.436228
C	3.919532	-0.945800	-0.278260	C	-3.656925	2.337014	-0.379137
C	5.088684	-0.535678	0.378078	C	-4.999560	2.764947	-0.561440
C	5.961705	0.375189	-0.216179	C	-5.996854	1.857799	-0.829112
H	6.364665	1.600074	-1.946012	C	-5.683269	0.482824	-0.934681
H	4.316061	0.854194	-3.146206	C	-4.394937	0.036889	-0.741369
H	2.781615	-0.765367	-2.096607	H	-5.217966	3.827592	-0.501158
H	5.328556	-0.920635	1.363987	H	-7.018773	2.193945	-0.975802
H	6.857154	0.684273	0.315480	H	-6.465882	-0.229594	-1.177860
C	0.875718	-3.167071	3.017750	H	-4.174165	-1.018516	-0.839463
H	0.106733	-3.749615	3.469671	B	0.918002	0.280332	-1.037884
C	3.498544	-3.392247	0.130370	C	5.867356	0.596081	-0.710268
H	4.498510	-3.505511	0.558114	C	-0.976575	1.478339	-0.157947
H	2.825614	-4.118439	0.593499	O	0.360113	1.161696	-0.128121
H	3.554542	-3.594267	-0.941762	C	3.232319	-0.789441	3.538507
C	2.794878	-1.696101	1.888600	C	3.585325	0.539800	3.314352
H	3.746627	-1.912113	2.386191	C	3.611597	1.052861	2.015958
H	2.586251	-0.633775	2.041940	C	3.285518	0.244697	0.922135

C	2.938487	-1.095684	1.156798	C	4.183913	3.755883	-0.491558
C	2.908975	-1.605591	2.453188	C	5.369135	3.109032	-0.749051
H	3.207905	-1.187108	4.548904	C	5.386957	1.699616	-0.864633
H	3.838295	1.185664	4.150271	C	4.236212	0.963531	-0.690388
H	3.886557	2.090240	1.864517	H	4.146728	4.839689	-0.424276
H	2.682100	-1.742440	0.322454	H	6.285822	3.675744	-0.880369
H	2.631093	-2.643093	2.615120	H	6.317244	1.191482	-1.100158
C	6.934044	0.942919	-0.262628	H	4.269223	-0.113431	-0.796208
H	7.874637	1.245797	0.135219	B	-0.988110	-0.031335	-1.052756
C	3.323111	2.283591	-0.657763	C	-5.121853	1.780672	-0.301635
H	4.250516	2.715101	-0.274055	C	0.570545	1.562013	-0.141904
H	3.249377	2.539317	-1.718969	O	-0.655784	0.942356	-0.125419
H	2.473860	2.724364	-0.136543	C	-2.950816	-1.759360	3.447725
C	4.581805	0.170535	-1.255508	C	-2.486733	-2.453667	2.328899
H	4.504390	-0.921765	-1.224553	C	-2.652386	-1.920125	1.052366
H	4.506970	0.461637	-2.310499	C	-3.280305	-0.676385	0.870146
O	0.093263	-0.578839	-1.768377	C	-3.741866	0.011814	1.997533
C	3.341371	0.762468	-0.517795	C	-3.578690	-0.527345	3.275821
O	2.241246	0.186118	-1.266727	H	-2.821858	-2.175013	4.442824
B3LYP/6-31G** Energy =				H	-1.992216	-3.413301	2.448783
B3LYP/6-31G** Free Energy =				H	-2.279404	-2.468374	0.191848
M06-2X/LACVP** Derived Free Energy =				H	-4.241936	0.967095	1.888952
M06-2X/LACVP** Derived Solution Free Energy =				H	-3.942118	0.024585	4.137919
Number of Imaginary Frequencies =				C	-6.236303	2.148019	-0.013738
				H	-7.220521	2.465166	0.242558
B3LYP/6-31G** Geometry				C	-4.545963	-0.964030	-1.287746
C	0.907580	-1.334191	-0.962905	H	-5.509924	-0.848035	-0.788805
C	0.894983	-2.754119	-0.967061	H	-4.639058	-0.621133	-2.322683
C	1.733156	-3.464677	-0.148591	H	-4.274120	-2.021651	-1.294843
C	1.764662	-0.628581	-0.131092	C	-3.766820	1.370183	-0.666178
Br	-0.345420	-3.660905	-2.088515	H	-3.036384	1.929461	-0.075805
H	1.722876	-4.548975	-0.169110	H	-3.590179	1.639438	-1.714739
C	2.576970	-2.788421	0.768914	O	0.020656	-0.671376	-1.776697
C	2.574037	-1.355367	0.812410	C	-3.468714	-0.151025	-0.557876
C	3.344953	-0.722139	1.826265	O	-2.253795	-0.411013	-1.308788
C	4.107710	-1.457598	2.706076	(S,S) product complex			
C	4.147304	-2.868716	2.624397	B3LYP/6-31G** Energy =			
C	3.390589	-3.517578	1.677643	B3LYP/6-31G** Free Energy =			
H	3.320195	0.356778	1.913059	M06-2X/LACVP** Derived Free Energy =			
H	4.680274	-0.947386	3.474843	M06-2X/LACVP** Derived Solution Free Energy =			
H	4.760241	-3.435318	3.318691	Number of Imaginary Frequencies =			
H	3.389079	-4.602527	1.618272				
C	1.743321	3.693035	-0.131866	B3LYP/6-31G** Geometry			
C	1.770167	0.859391	-0.213179	C	-1.569082	1.355899	-0.459579
C	0.574434	2.981759	-0.067603	C	-2.187783	2.634690	-0.481534
H	1.723196	4.775263	-0.067010	C	-3.427822	2.823068	0.069844
Br	-1.069567	3.927775	0.124067	C	-2.222817	0.255031	0.075912
C	2.995656	1.594720	-0.394961	Br	-1.265574	4.095105	-1.279103
C	2.976384	3.024812	-0.329074				

H	-3.893314	3.802154	0.038722	C	3.099002	1.384940	0.541307
C	-4.087204	1.753253	0.726451	O	1.820407	1.624424	-0.096329
C	-3.475260	0.457617	0.758243				
C	-4.122149	-0.562118	1.509958	B3LYP/6-31G** Energy =			-6587.609532
C	-5.317716	-0.325557	2.151541	B3LYP/6-31G** Free Energy =			-6587.630619
C	-5.940384	0.941758	2.076293	M06-2X/LACVP** Derived Free Energy =			-1470.253695
C	-5.331489	1.959538	1.380982	M06-2X/LACVP** Derived Solution Free Energy =			-1470.272877
H	-3.656564	-1.536523	1.588608	Number of Imaginary Frequencies =			0
H	-5.783689	-1.120265	2.726419				
H	-6.887118	1.111763	2.579853	B3LYP/6-31G** Geometry			
H	-5.784257	2.946149	1.333667				
C	-0.406600	-3.668905	-0.036431	C	-0.214315	-1.441326	-0.883566
C	-1.594735	-1.092330	-0.042322	C	0.450533	-2.694842	-0.820924
C	0.303819	-2.573361	0.377911	C	-0.006407	-3.686624	0.007068
H	0.045423	-4.653992	-0.000661	C	-1.333418	-1.183236	-0.106378
Br	2.092295	-2.777401	0.993238	Br	2.025123	-2.951497	-1.853803
C	-2.315806	-2.215576	-0.586187	H	0.501412	-4.644451	0.039078
C	-1.715989	-3.516248	-0.556940	C	-1.107764	-3.448456	0.868317
C	-2.426325	-4.631535	-1.077240	C	-1.762864	-2.173125	0.847390
C	-3.669103	-4.474258	-1.643545	C	-2.781621	-1.935897	1.811094
C	-4.246073	-3.185557	-1.719262	C	-3.161685	-2.914228	2.702871
C	-3.591351	-2.089135	-1.203481	C	-2.547915	-4.187955	2.683724
H	-1.957406	-5.610702	-1.032657	C	-1.537392	-4.443596	1.787325
H	-4.200469	-5.331196	-2.046156	H	-3.256470	-0.963677	1.850172
H	-5.213702	-3.056844	-2.194934	H	-3.937415	-2.702048	3.432514
H	-4.045928	-1.109737	-1.282587	H	-2.863655	-4.953019	3.386425
B	0.706419	0.867608	-0.098275	H	-1.037101	-5.408130	1.777170
C	5.155518	2.844479	0.902863	C	-3.281714	2.668832	-0.274250
C	-0.274102	-1.275641	0.346109	C	-2.009834	0.136549	-0.251972
O	0.533923	-0.230899	0.725584	C	-1.921024	2.572343	-0.148414
C	5.249790	-1.716784	-1.613617	H	-3.760348	3.641394	-0.245168
C	5.532083	-1.472345	-0.269716	Br	-0.906703	4.171654	0.072594
C	4.836592	-0.484987	0.428545	C	-3.426454	0.226570	-0.497490
C	3.843697	0.274480	-0.204059	C	-4.064425	1.508012	-0.486762
C	3.579983	0.032515	-1.558912	C	-5.463613	1.602852	-0.715259
C	4.272104	-0.957992	-2.256115	C	-6.210398	0.480509	-0.984026
H	5.787769	-2.489609	-2.154705	C	-5.578573	-0.783453	-1.043476
H	6.295250	-2.052600	0.241131	C	-4.228133	-0.908207	-0.804654
H	5.073046	-0.311524	1.471861	H	-5.927840	2.584895	-0.689292
H	2.825800	0.620614	-2.071131	H	-7.277548	0.562670	-1.166235
H	4.044493	-1.134658	-3.303416	H	-6.163158	-1.665500	-1.287141
C	6.260164	2.931535	1.383735	H	-3.761831	-1.883278	-0.868051
H	7.239159	3.007916	1.796766	B	0.883387	0.574608	-0.979262
C	2.907330	1.105817	2.036034	C	4.967903	0.060708	-1.241773
H	3.858382	1.201138	2.564569	C	-1.264875	1.310886	-0.175711
H	2.219132	1.846312	2.454333	O	0.107419	1.321287	-0.107470
H	2.501902	0.107503	2.200973	C	3.378273	0.294381	3.683143
C	3.815908	2.756195	0.330373	C	3.507367	1.648733	3.379262
H	3.855004	2.948849	-0.747502	C	3.407695	2.084871	2.057198
H	3.173183	3.531070	0.765917	C	3.178874	1.176066	1.016436
O	-0.300407	1.258423	-0.973678	C	3.058968	-0.186686	1.331457

C	3.154071	-0.619859	2.653292	C	4.864793	-3.028882	2.008684
H	3.450463	-0.045617	4.712118	C	4.907789	-1.616166	2.055980
H	3.678678	2.372566	4.170853	C	3.969459	-0.860472	1.388497
H	3.502126	3.144737	1.847640	H	3.797350	-4.741714	1.286937
H	2.901436	-0.911038	0.540288	H	5.616091	-3.612246	2.532210
H	3.053832	-1.678031	2.876838	H	5.686008	-1.120841	2.628963
C	5.390364	-1.065944	-1.341292	H	4.013529	0.220180	1.444652
H	5.753323	-2.064407	-1.416999	B	-0.948133	0.031694	-0.199937
C	2.699095	3.100751	-0.620968	C	-2.104358	-1.369052	2.496225
H	3.480611	3.774956	-0.260000	C	0.836571	-1.401010	-0.605588
H	2.552378	3.301354	-1.686057	O	-0.228533	-0.717462	-1.135187
H	1.770314	3.321354	-0.096396	C	-7.065867	0.275712	-1.360671
C	4.484906	1.435709	-1.154081	C	-7.034055	0.477665	0.019896
H	4.392597	1.845158	-2.167822	C	-5.823260	0.421672	0.708365
H	5.222392	2.052240	-0.626483	C	-4.621424	0.160821	0.033285
O	0.301163	-0.466957	-1.704547	C	-4.664881	-0.046286	-1.349931
C	3.109335	1.635007	-0.443732	C	-5.877219	0.014133	-2.040170
O	2.198222	0.786080	-1.173972	H	-8.007883	0.321517	-1.899151
B3LYP/6-31G** Energy =			-6587.609874	H	-7.951905	0.681497	0.563800
B3LYP/6-31G** Free Energy =			-6587.631849	H	-5.823631	0.585983	1.782265
M06-2X/LACVP** Derived Free Energy =			-1470.256169	H	-3.746330	-0.257311	-1.882920
M06-2X/LACVP** Derived Solution Free Energy =			-1470.273570	H	-5.888025	-0.146240	-3.114505
Number of Imaginary Frequencies =			0	C	-1.057514	-1.556003	3.069594
B3LYP/6-31G** Geometry				H	-0.136475	-1.724307	3.578227
C	0.894191	1.536729	0.135347	C	-3.039248	1.394783	1.573988
C	0.975546	2.955548	0.096895	H	-3.889219	1.622456	2.222056
C	2.109157	3.587977	-0.340065	H	-2.142698	1.317051	2.189197
C	1.988311	0.756693	-0.221888	H	-2.907588	2.222157	0.874984
Br	-0.517221	4.001850	0.653463	C	-3.353079	-1.140075	1.773577
H	2.153893	4.671393	-0.356085	H	-4.178869	-1.005745	2.481032
C	3.209648	2.833257	-0.815936	H	-3.590177	-2.021056	1.166688
C	3.147430	1.402709	-0.784115	O	-0.296361	0.994842	0.550636
C	4.229262	0.682147	-1.362973	C	-3.302280	0.091054	0.813485
C	5.318053	1.335702	-1.895870	O	-2.267886	-0.214205	-0.134736
C	5.394309	2.747599	-1.879300	B3LYP/6-31G** Energy =			-6587.615038
C	4.355610	3.478644	-1.353729	B3LYP/6-31G** Free Energy =			-6587.635358
H	4.186023	-0.398928	-1.398180	M06-2X/LACVP** Derived Free Energy =			-1470.256157
H	6.123848	0.759062	-2.340128	M06-2X/LACVP** Derived Solution Free Energy =			-1470.274858
H	6.262579	3.249165	-2.295596	Number of Imaginary Frequencies =			0
H	4.385474	4.564788	-1.355259	B3LYP/6-31G** Geometry			
C	1.785652	-3.555773	-0.022743	C	0.622971	-1.483232	-0.605656
C	1.923325	-0.724435	-0.069179	C	0.277534	-2.858731	-0.530689
C	0.783147	-2.820496	-0.598599	C	1.064695	-3.740754	0.161387
H	1.738190	-4.639214	-0.031442	C	1.779497	-0.999965	-0.011101
Br	-0.711572	-3.693067	-1.386869	Br	-1.308810	-3.458364	-1.395294
C	2.928530	-1.474106	0.637753	H	0.797535	-4.790977	0.204445
C	2.862584	-2.906085	0.632895	C	2.204595	-3.277675	0.867092
C	3.858230	-3.657161	1.313866	C	2.559331	-1.889649	0.810533

C	3.647610	-1.451283	1.614611	B3LYP/6-31G** Energy =			-6587.610872
C	4.365382	-2.336655	2.387844	B3LYP/6-31G** Free Energy =			-6587.632531
C	4.041247	-3.712841	2.401199	M06-2X/LACVP** Derived Free Energy =			-1470.255011
C	2.977937	-4.169064	1.658600	M06-2X/LACVP** Derived Solution Free Energy =			-1470.272778
H	3.905549	-0.399785	1.628086	Number of Imaginary Frequencies =			0
H	5.185664	-1.971515	2.998577				
H	4.621048	-4.400963	3.008711	B3LYP/6-31G** Geometry			
H	2.699950	-5.219320	1.676608				
C	2.848563	3.181748	-0.332019	C	1.198967	-1.389701	-0.670585
C	2.147066	0.432557	-0.206288	C	1.617258	-2.743036	-0.561809
C	1.579090	2.798026	0.008089	C	2.687365	-3.083427	0.223093
H	3.115794	4.232576	-0.342498	C	1.881800	-0.374888	-0.017523
Br	0.284878	4.124520	0.461817	Br	0.658316	-4.085445	-1.507865
C	3.454297	0.820401	-0.672532	H	3.004632	-4.118373	0.290068
C	3.806132	2.208709	-0.712989	C	3.354248	-2.094416	0.989984
C	5.098529	2.596497	-1.158111	C	2.937262	-0.725937	0.898415
C	6.007186	1.657967	-1.586228	C	3.564986	0.215929	1.759889
C	5.649808	0.289827	-1.593521	C	4.569117	-0.164696	2.622430
C	4.412327	-0.117936	-1.147537	C	5.009504	-1.507356	2.672459
H	5.347543	3.654069	-1.167639	C	4.407643	-2.451219	1.874331
H	6.989546	1.964004	-1.932636	H	3.236136	1.247327	1.745512
H	6.356555	-0.448241	-1.960753	H	5.023411	0.574726	3.275190
H	4.154785	-1.169174	-1.172561	H	5.808489	-1.791482	3.350472
B	-0.862371	0.314846	-0.477413	H	4.716918	-3.491954	1.917647
C	-2.605549	0.428523	2.341233	C	0.715657	3.770251	-0.364430
C	1.206804	1.427157	0.036915	C	1.475147	1.041056	-0.248167
O	-0.105676	1.154083	0.325299	C	-0.212528	2.796092	-0.109286
C	-7.033151	-0.682265	-0.170120	H	0.422430	4.814231	-0.358167
C	-5.874530	-1.388230	-0.489951	Br	-2.005942	3.309724	0.286995
C	-4.625033	-0.767323	-0.435705	C	2.441380	2.040236	-0.629001
C	-4.517889	0.576936	-0.060529	C	2.052540	3.417516	-0.673131
C	-5.688025	1.277956	0.264667	C	3.002538	4.408344	-1.039494
C	-6.934584	0.656703	0.210345	C	4.285541	4.058624	-1.387975
H	-8.003141	-1.168893	-0.214605	C	4.664055	2.696067	-1.389923
H	-5.938037	-2.432222	-0.783712	C	3.771116	1.715900	-1.017627
H	-3.731055	-1.326434	-0.683690	H	2.687841	5.448228	-1.053680
H	-5.635638	2.320624	0.566198	H	5.002698	4.821301	-1.675666
H	-7.827591	1.220328	0.464975	H	5.668452	2.417867	-1.694718
C	-2.426550	-0.546368	3.030899	H	4.077142	0.677494	-1.038507
H	-2.276698	-1.408337	3.638542	B	-1.005966	-0.606154	-0.741607
C	-3.136464	2.565004	-0.821137	C	-3.871065	0.237716	-2.641257
H	-3.880987	3.282414	-0.466912	C	0.143702	1.419042	-0.106486
H	-2.153717	3.040304	-0.765573	O	-0.874474	0.515299	0.063478
H	-3.362017	2.323936	-1.862749	C	-3.470370	-0.513548	3.909936
C	-2.805655	1.609401	1.505291	C	-2.802834	-1.564005	3.276952
H	-1.906727	2.233364	1.527908	C	-2.809797	-1.661890	1.887705
H	-3.626237	2.212458	1.910867	C	-3.477104	-0.711357	1.099569
O	-0.238424	-0.646170	-1.267637	C	-4.139273	0.338597	1.744839
C	-3.157521	1.281345	0.021836	C	-4.137307	0.435459	3.138404
O	-2.200467	0.372259	-0.549087	H	-3.467240	-0.435435	4.993094
				H	-2.275468	-2.309160	3.865579

H	-2.284090	-2.480121	1.404828	H	5.589731	-3.278778	-0.751387
H	-4.660259	1.097640	1.172750	H	7.124537	-1.507038	-1.554820
H	-4.655891	1.260900	3.617438	H	6.313545	0.845541	-1.722975
C	-3.794746	0.160563	-3.843849	H	4.040203	1.433278	-1.036356
H	-3.720650	0.085751	-4.903913	B	-0.873785	-0.360545	-0.387003
C	-4.373932	-2.103407	-0.789754	C	-2.554666	-3.038148	-1.532112
H	-5.401396	-1.932427	-0.456108	C	1.251433	-1.318657	0.218879
H	-4.367993	-2.252979	-1.871981	O	-0.085702	-1.122155	0.460574
H	-4.000400	-3.008598	-0.306332	C	-6.675586	1.258852	1.056721
C	-3.963998	0.362266	-1.187955	C	-6.707245	-0.113442	1.308332
H	-5.006490	0.562475	-0.913355	C	-5.599812	-0.905568	1.009519
H	-3.378133	1.226619	-0.860973	C	-4.440567	-0.345112	0.452061
O	0.088755	-1.121978	-1.428705	C	-4.420808	1.030960	0.195292
C	-3.490964	-0.901891	-0.422046	C	-5.529619	1.823855	0.499653
O	-2.170389	-1.264614	-0.890644	H	-7.535894	1.878732	1.291629
B3LYP/6-31G** Energy =				H	-7.593137	-0.570115	1.740253
B3LYP/6-31G** Free Energy =				H	-5.647382	-1.970771	1.217399
M06-2X/LACVP** Derived Free Energy =				H	-3.542476	1.483725	-0.248116
M06-2X/LACVP** Derived Solution Free Energy =				H	-5.492265	2.890389	0.296509
Number of Imaginary Frequencies =				C	-1.639622	-3.723580	-1.921606
B3LYP/6-31G** Geometry				H	-0.826003	-4.332450	-2.239929
C	0.498050	1.505468	-0.612357	C	-2.770331	-2.018409	1.355198
C	0.067461	2.858880	-0.640893	H	-3.591572	-2.620616	1.751563
C	0.762321	3.829970	0.030973	H	-1.938082	-2.678723	1.115677
C	1.655902	1.139302	0.058384	H	-2.455119	-1.321930	2.136261
Br	-1.499442	3.308953	-1.623106	C	-3.644103	-2.193342	-1.051880
H	0.428640	4.861211	-0.005469	H	-4.484418	-2.815543	-0.723839
C	1.892600	3.485735	0.815624	H	-4.016646	-1.566972	-1.870235
C	2.338721	2.123948	0.856577	O	-0.274542	0.566466	-1.245336
C	3.416168	1.805218	1.728770	C	-3.240185	-1.243764	0.119091
C	4.037343	2.778593	2.479468	O	-2.215959	-0.387067	-0.407650
C	3.622576	4.128130	2.399760	B3LYP/6-31G** Energy =			
C	2.568035	4.469926	1.586496	B3LYP/6-31G** Free Energy =			
H	3.742345	0.776010	1.811579	M06-2X/LACVP** Derived Free Energy =			
H	4.851396	2.504892	3.144002	M06-2X/LACVP** Derived Solution Free Energy =			
H	4.126942	4.886350	2.990931	Number of Imaginary Frequencies =			
H	2.221875	5.498404	1.531334	B3LYP/6-31G** Geometry			
C	3.036246	-2.954754	-0.009457	C	-1.052795	1.434560	0.139681
C	2.127408	-0.270997	-0.046497	C	-1.168897	2.848925	0.073946
C	1.729588	-2.656946	0.275266	C	-2.334279	3.444241	-0.329208
H	3.381749	-3.981186	0.045972	C	-2.140362	0.616611	-0.140659
Br	0.549366	-4.068842	0.766751	Br	0.329066	3.925264	0.555022
C	3.474942	-0.577697	-0.454141	H	-2.408303	4.525455	-0.368184
C	3.931156	-1.934370	-0.414337	C	-3.433400	2.648975	-0.740017
C	5.262397	-2.243958	-0.802530	C	-3.336732	1.220937	-0.670308
C	6.111470	-1.260683	-1.251891	C	-4.424663	0.459241	-1.180422
C	5.652894	0.074289	-1.338448	C	-5.549401	1.072263	-1.686259
C	4.374708	0.407375	-0.948788	C	-5.657548	2.481953	-1.707881

C	-4.615776	3.251704	-1.247459	M06-2X/LACVP** Derived Solution Free Energy =			-1470.272842
H	-4.357563	-0.621298	-1.184804	Number of Imaginary Frequencies =			0
H	-6.359372	0.464999	-2.078989				
H	-6.553655	2.951402	-2.101913	B3LYP/6-31G** Geometry			
H	-4.671840	4.336312	-1.278913				
C	-1.821212	-3.678264	0.280088	C	-0.759505	1.535165	0.437489
C	-2.035707	-0.855588	0.076157	C	-0.544887	2.937667	0.368028
C	-0.860887	-2.953024	-0.374484	C	-1.470027	3.758049	-0.221612
H	-1.745578	-4.758826	0.333347	C	-1.920550	0.960933	-0.058854
Br	0.631057	-3.828209	-1.169749	Br	1.060867	3.661154	1.090565
C	-2.995138	-1.588809	0.861428	H	-1.301598	4.828664	-0.261207
C	-2.891847	-3.016998	0.934618	C	-2.628013	3.207753	-0.828253
C	-3.842543	-3.752298	1.692550	C	-2.852109	1.792507	-0.777402
C	-4.839604	-3.110416	2.388361	C	-3.970103	1.273569	-1.487392
C	-4.917167	-1.698907	2.359049	C	-4.833550	2.105573	-2.165133
C	-4.023695	-0.959588	1.615999	C	-4.634224	3.505327	-2.170724
H	-3.753817	-4.834746	1.724058	C	-3.549057	4.041043	-1.518344
H	-5.555787	-3.681165	2.971468	H	-4.135135	0.203698	-1.505378
H	-5.685961	-1.190683	2.933344	H	-5.673463	1.680055	-2.706132
H	-4.093859	0.120926	1.616030	H	-5.327612	4.150003	-2.702071
B	0.815663	-0.019644	-0.270824	H	-3.367357	5.112181	-1.533215
C	4.298860	2.861879	-0.255075	C	-2.592141	-3.305649	0.191893
C	-0.954795	-1.538691	-0.462833	C	-2.138098	-0.503727	0.122850
O	0.073125	-0.873460	-1.081380	C	-1.397703	-2.800798	-0.247726
C	6.748078	-1.984875	0.055081	H	-2.770060	-4.375193	0.176579
C	6.847733	-0.686883	0.556824	Br	-0.057366	-3.991048	-0.899864
C	5.720210	0.130529	0.623812	C	-3.356668	-1.020486	0.692520
C	4.470477	-0.330996	0.182539	C	-3.584767	-2.434782	0.706733
C	4.378370	-1.637283	-0.316283	C	-4.789871	-2.949315	1.255886
C	5.509103	-2.454436	-0.377357	C	-5.727013	-2.109226	1.808959
H	7.625695	-2.622996	0.005594	C	-5.487080	-0.716004	1.840403
H	7.805353	-0.306045	0.900432	C	-4.338689	-0.186135	1.295470
H	5.821190	1.138193	1.009865	H	-4.947189	-4.024321	1.244297
H	3.419867	-2.020336	-0.644093	H	-6.640822	-2.512068	2.234812
H	5.415230	-3.465179	-0.764588	H	-6.213352	-0.055999	2.305150
C	5.042974	3.758789	0.064030	H	-4.168671	0.882187	1.340744
H	5.709822	4.541050	0.343974	B	0.861873	-0.126161	0.134886
C	2.947271	0.977511	1.723328	C	3.491648	-2.024388	1.763965
H	3.822834	1.465409	2.155349	C	-1.143438	-1.402924	-0.244069
H	2.103459	1.666584	1.780868	O	0.111781	-1.005946	-0.632316
H	2.727530	0.083689	2.313691	C	6.967438	1.238407	-0.360726
C	3.353653	1.826089	-0.664318	C	6.924185	-0.087529	-0.793930
H	3.599032	1.469585	-1.671084	C	5.711255	-0.773015	-0.827201
H	2.359895	2.286772	-0.710171	C	4.520198	-0.151437	-0.425639
O	0.175259	0.936777	0.500244	C	4.572064	1.178628	0.006754
C	3.235799	0.578389	0.270256	C	5.787685	1.865325	0.036699
O	2.146205	-0.193448	-0.279714	H	7.911222	1.775249	-0.334122
				H	7.834615	-0.590812	-1.106622
B3LYP/6-31G** Energy =			-6587.613870	H	5.702040	-1.803885	-1.171146
B3LYP/6-31G** Free Energy =			-6587.634386	H	3.661164	1.675392	0.318120
M06-2X/LACVP** Derived Free Energy =			-1470.254123	H	5.808168	2.897326	0.375555

C	3.683089	-1.871107	2.945926	H	3.812179	-1.187548	1.527470
H	3.857201	-1.721059	3.986004	B	-0.735171	0.912031	-0.122956
C	2.849263	-1.243425	-1.963150	C	-4.058654	3.346525	0.482749
H	3.667312	-1.800430	-2.427173	C	0.161186	-1.301618	-0.357384
H	1.936154	-1.837047	-2.032964	O	-0.565650	-0.249149	-0.860677
H	2.717813	-0.313469	-2.522987	C	-5.375131	-1.568287	1.213078
C	3.243098	-2.230007	0.339245	C	-4.357403	-0.874017	1.865241
H	2.292880	-2.759144	0.201267	C	-3.617122	0.094930	1.187028
H	4.018689	-2.880685	-0.080988	C	-3.871366	0.375962	-0.160707
O	0.231542	0.768374	0.992837	C	-4.908311	-0.315170	-0.802549
C	3.194708	-0.920577	-0.500074	C	-5.652668	-1.279250	-0.123292
O	2.199589	-0.058682	0.079099	H	-5.949572	-2.324054	1.740541
B3LYP/6-31G** Energy =				H	-4.137137	-1.082036	2.908295
B3LYP/6-31G** Free Energy =				H	-2.843657	0.643928	1.711447
M06-2X/LACVP** Derived Free Energy =				H	-5.137796	-0.114050	-1.843969
M06-2X/LACVP** Derived Solution Free Energy =				H	-6.447222	-1.807698	-0.642497
Number of Imaginary Frequencies =				C	-4.274978	3.803039	1.579080
B3LYP/6-31G** Geometry				H	-4.456819	4.198890	2.551091
C	1.544149	1.320941	0.334444	C	-2.809375	1.090519	-2.377029
C	2.231133	2.564355	0.297658	H	-3.730191	1.150037	-2.963091
C	3.513458	2.642249	-0.178554	H	-2.098997	1.806182	-2.801015
C	2.168311	0.147959	-0.065473	H	-2.400343	0.084238	-2.465757
Br	1.341809	4.131407	0.905746	C	-3.815103	2.818331	-0.856522
H	4.030224	3.595603	-0.192760	H	-3.218238	3.538988	-1.429269
C	4.153103	1.489876	-0.701080	H	-4.769456	2.700765	-1.383320
C	3.472024	0.229122	-0.673687	O	0.243096	1.331450	0.769224
C	4.107476	-0.879715	-1.298532	C	-3.071846	1.448750	-0.905482
C	5.353130	-0.757184	-1.873354	O	-1.821691	1.700147	-0.230732
C	6.040774	0.478147	-1.853469	Minima of Compound 6			
C	5.446823	1.578505	-1.282061	B3LYP/6-31G** Energy =			
H	3.594075	-1.832310	-1.334992	B3LYP/6-31G** Free Energy =			
H	5.809074	-1.618611	-2.352190	M06-2X/LACVP** Derived Free Energy =			
H	7.026145	0.558016	-2.302305	M06-2X/LACVP** Derived Solution Free Energy =			
H	5.950441	2.541317	-1.279580	Number of Imaginary Frequencies =			
C	0.146656	-3.664935	0.198353	B3LYP/6-31G** Geometry			
C	1.460096	-1.152215	0.111081	B	-1.642990	-2.923993	0.843499
C	-0.476325	-2.571863	-0.344060	C	-0.403842	-1.772347	-2.028363
H	-0.349950	-4.629000	0.195703	C	-6.520028	-0.756420	0.199585
Br	-2.220824	-2.746108	-1.082432	C	-5.623737	-0.838320	1.265927
C	2.082196	-2.263156	0.786061	C	-4.251640	-0.908260	1.028326
C	1.420559	-3.533554	0.805134	C	-3.745084	-0.904343	-0.279463
C	2.034780	-4.638041	1.454725	C	-4.654399	-0.813123	-1.341334
C	3.240809	-4.495365	2.098980	C	-6.028436	-0.742164	-1.104843
C	3.875866	-3.232163	2.125247	H	-7.589027	-0.703050	0.383499
C	3.315841	-2.148814	1.485350	H	-5.991718	-0.846703	2.288062
H	1.521207	-5.595552	1.445278	H	-3.561614	-0.967815	1.863127
H	3.698171	-5.342977	2.600188	H	-4.303204	-0.798438	-2.367544
H	4.812688	-3.112506	2.661136				

H	-6.713459	-0.678022	-1.945468	O	-1.850115	-5.106907	0.711921
C	0.782671	-1.932524	-2.187243	C	-2.095845	-5.570514	2.043847
H	1.830204	-2.070227	-2.322957	H	-2.819610	-6.390824	2.020269
C	-1.682786	0.518810	-0.448214	H	-1.159260	-5.947913	2.472638
H	-2.151169	1.135227	-1.220777	C	-2.623296	-4.328204	2.803330
H	-1.901157	0.960297	0.526981	H	-3.713440	-4.347091	2.919567
H	-0.600341	0.513481	-0.599676	H	-2.170692	-4.209129	3.792241
C	-1.843370	-1.591071	-1.853015	O	-2.262864	-3.217021	1.971880
H	-2.344896	-2.560999	-1.920974	C	-1.726088	-1.576969	-0.480106
H	-2.221624	-0.969785	-2.672419	O	-1.585580	-3.010922	-0.364709
O	-2.290303	-3.869568	0.071171				
C	-2.214238	-5.117095	0.773783	B3LYP/6-31G** Energy =			-754.789394
H	-3.204913	-5.359372	1.176602	B3LYP/6-31G** Free Energy =			-754.808111
H	-1.916780	-5.910599	0.081868	M06-2X/LACVP** Derived Free Energy =			-754.723078
C	-1.172086	-4.871871	1.893248	M06-2X/LACVP** Derived Solution Free Energy =			-754.739028
H	-1.494802	-5.261459	2.863606	Number of Imaginary Frequencies =			0
H	-0.197388	-5.312359	1.650224				
O	-1.039794	-3.448875	1.965536	B3LYP/6-31G** Geometry			
C	-2.225538	-0.917338	-0.501037				
O	-1.576863	-1.593504	0.589552	B	-1.996429	-3.714871	0.773805
				C	-1.186024	0.061679	-2.324634
B3LYP/6-31G** Energy =		-754.789391		C	-5.978575	-0.474733	-0.423437
B3LYP/6-31G** Free Energy =		-754.808093		C	-5.030419	0.376448	0.141784
M06-2X/LACVP** Derived Free Energy =		-754.723076		C	-3.679112	0.024990	0.145153
M06-2X/LACVP** Derived Solution Free Energy =		-754.739021		C	-3.252731	-1.184374	-0.415042
Number of Imaginary Frequencies =		0		C	-4.214951	-2.030378	-0.986760
				C	-5.564349	-1.681817	-0.989054
B3LYP/6-31G** Geometry				H	-7.029721	-0.201322	-0.423827
				H	-5.339350	1.318639	0.585490
B	-1.895396	-3.729539	0.743808	H	-2.960343	0.703174	0.590432
C	-1.213555	0.094488	-2.327178	H	-3.902103	-2.972658	-1.425573
C	-5.930668	-0.490053	-0.258620	H	-6.292601	-2.354303	-1.433638
C	-4.965578	0.356928	0.283810	C	-1.154398	1.218581	-2.670460
C	-3.613738	0.011371	0.232253	H	-1.136087	2.237268	-2.981366
C	-3.203667	-1.187813	-0.361042	C	-0.892273	-0.879205	0.564470
C	-4.183060	-2.029571	-0.909375	H	-0.802152	0.186237	0.342008
C	-5.532960	-1.686922	-0.856845	H	-1.294514	-1.007382	1.570465
H	-6.982152	-0.221258	-0.216279	H	0.110517	-1.314903	0.527819
H	-5.261557	1.291183	0.752428	C	-1.211068	-1.337348	-1.908594
H	-2.881636	0.686110	0.660727	H	-0.197212	-1.754977	-1.937450
H	-3.883019	-2.963981	-1.373252	H	-1.813293	-1.925783	-2.609734
H	-6.274516	-2.356034	-1.284193	O	-2.407126	-3.183279	1.979845
C	-1.199440	1.256354	-2.657158	C	-2.800345	-4.280867	2.814421
H	-1.196461	2.279495	-2.953627	H	-2.381046	-4.149000	3.816325
C	-0.809839	-0.886482	0.535145	H	-3.893849	-4.293909	2.893896
H	-0.732121	0.182444	0.325042	C	-2.252509	-5.536389	2.091671
H	-1.174119	-1.030908	1.553330	H	-1.334877	-5.913266	2.560026
H	0.192582	-1.317204	0.455185	H	-2.979942	-6.352849	2.052187
C	-1.217914	-1.310466	-1.930854	O	-1.954728	-5.092649	0.763625
H	-0.204234	-1.723250	-2.003077	C	-1.773479	-1.580855	-0.473902
H	-1.843341	-1.891376	-2.617811	O	-1.643590	-3.013501	-0.332892

				C	-1.071703	-1.028280	-2.660729	
B3LYP/6-31G** Energy =				-754.788450	C	-6.129727	-0.843183	-0.282797
B3LYP/6-31G** Free Energy =				-754.807372	C	-5.420512	-0.681309	0.908899
M06-2X/LACVP** Derived Free Energy =				-754.721772	C	-4.030433	-0.775686	0.914576
M06-2X/LACVP** Derived Solution Free Energy =				-754.738411	C	-3.318903	-1.038838	-0.266838
Number of Imaginary Frequencies =				0	C	-4.039691	-1.198229	-1.455635
					C	-5.433289	-1.100657	-1.462130
B3LYP/6-31G** Geometry				H	-7.213336	-0.769349	-0.290404	
				H	-5.949638	-0.481068	1.836371	
B	-1.964146	-3.447490	0.513135	H	-3.487218	-0.656183	1.846842	
C	-0.357385	-0.742749	-2.234627	H	-3.522305	-1.389567	-2.388619	
C	-6.428279	-0.624205	-0.026821	H	-5.972536	-1.230098	-2.396256	
C	-5.549172	0.279196	0.568723	C	-1.015671	-0.408317	-3.696332	
C	-4.169126	0.102701	0.450531	H	-0.970861	0.142400	-4.607160	
C	-3.643417	-0.981073	-0.263262	C	-1.207257	0.307360	0.000736	
C	-4.537918	-1.880250	-0.863096	H	-1.613997	0.752533	0.911543	
C	-5.915965	-1.706535	-0.743991	H	-0.118541	0.253708	0.097014	
H	-7.501547	-0.487242	0.067377	H	-1.456796	0.947396	-0.847715	
H	-5.934531	1.124130	1.132328	C	-1.112239	-1.797511	-1.418344	
H	-3.506146	0.815678	0.928199	H	-0.082900	-2.012094	-1.106357	
H	-4.147156	-2.726321	-1.419323	H	-1.598442	-2.763352	-1.587832	
H	-6.589789	-2.418047	-1.212849	O	-2.313273	-4.001519	0.356599	
C	0.809969	-0.810911	-2.536553	C	-2.587486	-5.209425	1.079571	
H	1.838392	-0.883776	-2.804296	H	-3.665561	-5.274516	1.268198	
C	-1.271760	-0.487969	0.601120	H	-2.286881	-6.072989	0.478972	
H	-1.353283	0.600468	0.533320	C	-1.772388	-5.071718	2.389130	
H	-1.565559	-0.805885	1.602378	H	-2.342016	-5.368085	3.275038	
H	-0.226064	-0.752428	0.430683	H	-0.846433	-5.659252	2.360633	
C	-1.773038	-0.640890	-1.885518	O	-1.444496	-3.680563	2.470988	
H	-2.371335	-1.200662	-2.613070	C	-1.787310	-1.098643	-0.199882	
H	-2.097422	0.404689	-1.950213	O	-1.388151	-1.831845	0.983033	
O	-1.755374	-4.796217	0.319383					
C	-1.847679	-5.429144	1.599351	B3LYP/6-31G** Energy =				-754.789241
H	-2.465309	-6.329154	1.521706	B3LYP/6-31G** Free Energy =				-754.808118
H	-0.844037	-5.726056	1.927892	M06-2X/LACVP** Derived Free Energy =				-754.722432
C	-2.467828	-4.355903	2.527720	M06-2X/LACVP** Derived Solution Free Energy =				-754.738051
H	-3.535844	-4.530040	2.705412	Number of Imaginary Frequencies =				0
H	-1.962066	-4.285849	3.495387					
O	-2.309437	-3.123998	1.811366	B3LYP/6-31G** Geometry				
C	-2.134314	-1.172521	-0.464848	B	-1.987310	-0.527031	-0.019035	
O	-1.825235	-2.579168	-0.519146	C	-0.013497	1.961674	1.176648	
				C	4.305908	-0.877056	0.405607	
B3LYP/6-31G** Energy =				-754.788482	C	4.092134	0.166073	-0.496787
B3LYP/6-31G** Free Energy =				-754.806824	C	2.793950	0.533724	-0.846497
M06-2X/LACVP** Derived Free Energy =				-754.721918	C	1.684934	-0.130597	-0.302614
M06-2X/LACVP** Derived Solution Free Energy =				-754.737558	C	1.909412	-1.173051	0.602566
Number of Imaginary Frequencies =				0	C	3.209805	-1.542472	0.952228
					H	5.316630	-1.165691	0.679163
B3LYP/6-31G** Geometry				H	4.935859	0.695365	-0.930396	
B	-1.718590	-3.122273	1.241324	H	2.652161	1.349030	-1.550877	

H	1.060449	-1.690858	1.030231	H	-2.503197	-2.808770	-1.898640
H	3.362654	-2.354698	1.657403	O	-2.264009	-4.654694	2.041417
C	-0.027383	2.140534	2.370756	C	-1.143611	-5.503685	2.308322
H	-0.023896	2.289453	3.425443	H	-1.106778	-5.740456	3.375849
C	0.069029	0.147441	-2.225647	H	-1.260808	-6.440478	1.749987
H	0.761240	0.790480	-2.775374	C	0.089208	-4.696010	1.832778
H	0.255459	-0.887344	-2.524227	H	0.633274	-4.240745	2.668640
H	-0.952688	0.419865	-2.502328	H	0.791850	-5.294874	1.246171
C	-0.021261	1.756529	-0.269778	O	-0.457263	-3.654346	1.010146
H	0.727830	2.404828	-0.738445	C	-2.418583	-1.597076	-0.109775
H	-0.996206	2.049287	-0.673444	O	-2.707253	-2.749578	0.706473
O	-2.728511	-1.431335	0.708607				
C	-4.109027	-1.172176	0.437762	B3LYP/6-31G** Energy =			-754.786828
H	-4.510399	-1.976462	-0.190909	B3LYP/6-31G** Free Energy =			-754.805477
H	-4.671173	-1.154821	1.376359	M06-2X/LACVP** Derived Free Energy =			-754.720321
C	-4.122313	0.194998	-0.290542	M06-2X/LACVP** Derived Solution Free Energy =			-754.737334
H	-4.770090	0.202224	-1.172133	Number of Imaginary Frequencies =			0
H	-4.426509	1.013394	0.372381				
O	-2.760855	0.402810	-0.693782	B3LYP/6-31G** Geometry			
C	0.266115	0.287258	-0.706569				
O	-0.637039	-0.608283	-0.042401	B	-1.733235	-3.355835	0.781297
				C	-1.309727	-0.792477	-2.491442
B3LYP/6-31G** Energy =			-754.789062	C	-6.134674	-0.806572	-0.711891
B3LYP/6-31G** Free Energy =			-754.807812	C	-5.369753	-1.833529	-1.265758
M06-2X/LACVP** Derived Free Energy =			-754.722471	C	-3.997678	-1.898525	-1.025942
M06-2X/LACVP** Derived Solution Free Energy =			-754.737668	C	-3.363700	-0.942307	-0.219732
Number of Imaginary Frequencies =			0	C	-4.140498	0.088146	0.325581
				C	-5.513235	0.156083	0.082587
B3LYP/6-31G** Geometry				H	-7.203478	-0.756237	-0.898503
				H	-5.840453	-2.586865	-1.891173
B	-1.825525	-3.635063	1.224679	H	-3.408150	-2.690984	-1.472010
C	-1.347271	-1.123795	-2.390284	H	-3.682674	0.846104	0.952332
C	-6.248382	0.285255	-0.965778	H	-6.095890	0.961309	0.521029
C	-5.056429	0.956631	-1.238640	C	-1.463705	-1.202656	-3.616493
C	-3.828960	0.357603	-0.955959	H	-1.604820	-1.575020	-4.604384
C	-3.769035	-0.927368	-0.396330	C	-1.398073	-0.392179	1.335817
C	-4.971785	-1.594163	-0.128776	H	-1.537199	0.692082	1.345757
C	-6.199253	-0.992555	-0.410188	H	-1.950931	-0.827890	2.168866
H	-7.203900	0.754092	-1.182683	H	-0.332038	-0.592813	1.476229
H	-5.078019	1.952508	-1.672138	C	-1.095400	-0.264010	-1.147107
H	-2.916392	0.893700	-1.188142	H	-1.392721	0.791023	-1.117072
H	-4.941136	-2.582643	0.311841	H	-0.024037	-0.302892	-0.913987
H	-7.119148	-1.526898	-0.189544	O	-1.333583	-4.653901	0.546634
C	-0.964432	-0.305489	-3.192474	C	-1.733570	-5.432690	1.678763
H	-0.637315	0.416527	-3.904154	H	-2.197905	-6.363772	1.339969
C	-1.465281	-0.664672	0.648693	H	-0.847289	-5.684868	2.274177
H	-1.222583	0.216414	0.052287	C	-2.715123	-4.522467	2.457136
H	-1.934254	-0.337690	1.580491	H	-3.762117	-4.792912	2.275190
H	-0.533669	-1.186250	0.879462	H	-2.537638	-4.528336	3.536724
C	-1.774439	-2.137135	-1.429489	O	-2.476302	-3.207968	1.936592
H	-0.906320	-2.743473	-1.147481	C	-1.847904	-1.005592	0.000431

O	-1.384616	-2.366143	-0.078338	B	-1.679388	-3.374016	0.828767
				C	-0.775829	-1.977601	-1.979149
B3LYP/6-31G** Energy =			-754.786826	C	-6.695949	0.164961	-0.361697
B3LYP/6-31G** Free Energy =			-754.805467	C	-5.652811	0.956256	-0.844948
M06-2X/LACVP** Derived Free Energy =			-754.720321	C	-4.344488	0.475076	-0.831361
M06-2X/LACVP** Derived Solution Free Energy =			-754.737339	C	-4.051054	-0.804828	-0.337319
Number of Imaginary Frequencies =			0	C	-5.104940	-1.591741	0.140554
				C	-6.415143	-1.108763	0.130295
B3LYP/6-31G** Geometry				H	-7.715718	0.538579	-0.369698
				H	-5.855297	1.950839	-1.231957
B	-1.645191	-3.350062	0.788960	H	-3.549052	1.111676	-1.208757
C	-1.303100	-0.740622	-2.456891	H	-4.891762	-2.583559	0.518935
C	-6.102510	-0.846736	-0.613070	H	-7.218122	-1.735247	0.508486
C	-5.484176	0.115055	0.184873	C	0.340333	-2.416413	-2.124552
C	-4.107430	0.064055	0.408562	H	1.326626	-2.796849	-2.255845
C	-3.323437	-0.948305	-0.159864	C	-1.694803	-0.387300	0.474662
C	-3.954557	-1.903691	-0.969295	H	-0.659644	-0.726892	0.443085
C	-5.330559	-1.855662	-1.189848	H	-1.745922	0.628713	0.075208
H	-7.174363	-0.809617	-0.784683	H	-2.024903	-0.359688	1.516214
H	-6.072291	0.906341	0.641046	C	-2.129322	-1.451219	-1.818354
H	-3.652028	0.820860	1.038461	H	-2.841318	-2.106503	-2.332845
H	-3.359862	-2.682017	-1.433039	H	-2.200008	-0.469650	-2.300376
H	-5.798879	-2.608047	-1.818187	O	-1.878570	-4.728648	1.005961
C	-1.466566	-1.139044	-3.584825	C	-0.817558	-5.211168	1.834162
H	-1.615918	-1.501149	-4.575316	H	-1.207206	-5.416050	2.839345
C	-1.344950	-0.388875	1.375936	H	-0.421128	-6.143822	1.421184
H	-1.499418	0.693056	1.401252	C	0.224508	-4.067598	1.839400
H	-1.880161	-0.842730	2.210818	H	0.641585	-3.872817	2.831990
H	-0.274348	-0.575773	1.499552	H	1.051633	-4.261741	1.145515
C	-1.077883	-0.225849	-1.109029	O	-0.501606	-2.917890	1.388733
H	-1.389640	0.824372	-1.061693	C	-2.604211	-1.321407	-0.336289
H	-0.002988	-0.252299	-0.890910	O	-2.636030	-2.645828	0.204119
O	-2.374172	-3.227136	1.956123				
C	-2.587967	-4.551449	2.462552	B3LYP/6-31G** Energy =			-754.783722
H	-2.397334	-4.568558	3.539766	B3LYP/6-31G** Free Energy =			-754.802077
H	-3.633143	-4.834558	2.289577	M06-2X/LACVP** Derived Free Energy =			-754.717736
C	-1.603220	-5.437318	1.660680	M06-2X/LACVP** Derived Solution Free Energy =			-754.733956
H	-0.705149	-5.682341	2.241250	Number of Imaginary Frequencies =			0
H	-2.057610	-6.371607	1.317292				
O	-1.230683	-4.639343	0.532519	B3LYP/6-31G** Geometry			
C	-1.804042	-0.992292	0.039147				
O	-1.322419	-2.344921	-0.062800	B	-1.587693	-2.827613	1.009726
				C	-1.220227	-1.980858	-2.063220
B3LYP/6-31G** Energy =			-754.787589	C	-6.324111	-1.056496	-0.376080
B3LYP/6-31G** Free Energy =			-754.806493	C	-5.558201	-0.926758	-1.532465
M06-2X/LACVP** Derived Free Energy =			-754.721141	C	-4.168967	-0.804502	-1.449362
M06-2X/LACVP** Derived Solution Free Energy =			-754.736916	C	-3.523847	-0.808873	-0.208514
Number of Imaginary Frequencies =			0	C	-4.306009	-0.940185	0.948647
				C	-5.690125	-1.065557	0.868309
B3LYP/6-31G** Geometry				H	-7.403994	-1.152592	-0.441561
				H	-6.037566	-0.924752	-2.507231

H	-3.596482	-0.723575	-2.366151
H	-3.820618	-0.954389	1.919750
H	-6.275062	-1.170191	1.777713
C	-1.198113	-3.030475	-2.660267
H	-1.200316	-3.959546	-3.181308
C	-1.772565	0.817860	0.525783
H	-2.164198	1.586398	-0.146442
H	-2.275732	0.917089	1.489749
H	-0.701760	0.983506	0.677018
C	-1.199371	-0.691989	-1.374767
H	-1.533078	0.096301	-2.059874
H	-0.162735	-0.451758	-1.111883
O	-2.607327	-3.588252	0.481241
C	-2.297938	-4.957379	0.759749
H	-3.199834	-5.476354	1.098112
H	-1.944152	-5.438348	-0.160755
C	-1.193488	-4.894357	1.842199
H	-1.592469	-5.077707	2.847937
H	-0.379157	-5.602416	1.659978
O	-0.693490	-3.555681	1.769397
C	-2.015080	-0.587401	-0.055231
O	-1.422348	-1.482458	0.900913

References

- (1) Becke, A. D. *Phys. Rev. A* **1988**, 38, 3098.
- (2) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, 37, 785.
- (3) Krishnan R.; Binkley J. S.; Seeger R.; Pople J. A. *J. Chem. Phys.* **1980**, 72, 650.
- (4) Gill, P. M. W.; Johnson, B. G.; Pople, J. A.; Frisch, M. J. *Chem. Phys. Lett.* **1992**, 197, 499.
- (5) Frisch, M. J.; et al., *Gaussian 03*; Gaussian, Inc., Wallingford CT, 2004.
- (6) Zhao, Y.; Truhlar, D. *Theor. Chem. Acc.* **2008**, 120, 215.
- (7) Hay, P. J.; Wadt, W. R. *J. Chem. Phys.* **1985**, 82, 270.
- (8) Jaguar, version 7.6, Schrodinger, LLC, New York, NY, 2009.
- (9) Simón, L.; Goodman, J. M. *Org. Biomol. Chem.* **2011**, 9, 689.
- (10) Grayson, M. N.; Pellegrinet, S. C.; Goodman, J. M. *J. Am. Chem. Soc.* **2012**, 134, 2716.
- (11) Grev R. S.; Janssen C. L.; Schaefer H. F. *J. Chem. Phys.* **1991**, 95, 5128.
- (12) Kaminski, G. A.; Friesner, R. A.; Tirado-Rives, J.; Jorgensen, W. *J. Phys. Chem. B* **2001**, 105, 6474.
- (13) Jorgensen, W. L.; Maxwell, D. S.; Tirado-Rives, J. *J. Am. Chem. Soc.* **1996**, 118, 11225.
- (14) Jorgensen, W. L.; Tirado-Rives, J. *J. Am. Chem. Soc.* **1988**, 110, 1657.
- (15) Mennucci B.; Tomasi J. *J. Chem. Phys.* **1997**, 106, 5151.