Supplementary Material (ESI) for PCCP

Supporting Information

Quantum Mechanics/Molecular Mechanics methods can be more accurate than full Quantum Mechanics in systems involving dispersion correlations

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Cartesian coordinates (Å) of the optimised structures

B3LYP/TZVP:UFF

S	1.69318	8.75923	8.66126
S	1.26318	5.57923	6.29126
O	-3.22682	6.08923	11.62126
O	-3.26682	4.30923	10.17126
C	-2.56682	5.54923	10.46126
C	-2.80682	6.51923	9.28126
H	-3.89682	6.61923	9.26126
C	-2.25682	7.91923	9.54126
H	-2.70682	8.60923	8.79126
H	-2.57682	8.28923	10.53126
C	-0.74682	8.00923	9.46126
C	-0.10682	8.83923	8.56126
H	-0.62682	9.46923	7.85126
C	1.45318	7.56923	9.98126
H	2.28318	7.09923	10.50126
C	0.12318	7.29923	10.26126
C	-0.28682	6.31923	11.33126
H	-0.84682	6.86923	12.12126
H	0.62318	5.89923	11.83126
C	-1.12682	5.13923	10.81126
H	-1.25682	4.46923	11.66126
C	-0.41682	4.27923	9.73126
H	0.50318	3.87923	10.17126
H	-1.06682	3.40923	9.56126
C	-0.07682	4.88923	8.40126
C	1.16318	4.78923	7.84126
H	2.03318	4.29923	8.25126
C	-0.39682	6.06923	6.41126
H	-0.84682	6.65923	5.62126
C	-0.98682	5.63923	7.57126
C	-2.43682	5.92923	7.89126
H	-3.00682	4.99923	7.79126

H	-2.82682	6.59923	7.13126
C	-4.03682	5.06923	12.19126
H	-4.86682	5.54923	12.71126
H	-3.46682	4.46923	12.91126
C	-4.43682	4.24923	10.98126
H	-4.65682	3.20923	11.20126
H	-5.29682	4.69923	10.46126

B3LYP/def2-TZVP:UFF

S	1.66330	8.84020	8.71160
S	1.21800	5.65260	6.35430
O	-3.26280	6.16820	11.66100
O	-3.30800	4.40020	10.21420
C	-2.60660	5.62880	10.50620
C	-2.83610	6.59790	9.32930
H	-3.92570	6.70560	9.30680
C	-2.28480	8.00500	9.58980
H	-2.73440	8.69780	8.84450
H	-2.61390	8.36950	10.58620
C	-0.78270	8.09550	9.51810
C	-0.13280	8.91920	8.61680
H	-0.65150	9.54870	7.90580
C	1.42000	7.64480	10.03570
H	2.24470	7.17200	10.55240
C	0.09250	7.37690	10.31790
C	-0.32340	6.39580	11.38290
H	-0.88260	6.94440	12.17090
H	0.58170	5.98110	11.87940
C	-1.16100	5.22360	10.85840
H	-1.29320	4.54760	11.71030
C	-0.44850	4.36160	9.78350
H	0.47350	3.96970	10.21870
H	-1.09260	3.49300	9.61760
C	-0.11430	4.97490	8.44790
C	1.12560	4.87260	7.87980
H	1.99230	4.37910	8.29040
C	-0.42180	6.14570	6.46480
H	-0.86690	6.73090	5.67580
C	-1.02130	5.72130	7.61850
C	-2.46390	6.01720	7.93940
H	-3.03930	5.09240	7.83550
H	-2.85030	6.69590	7.17580
C	-4.06830	5.15270	12.24210
H	-4.90370	5.63000	12.75350
H	-3.49640	4.55770	12.96380
C	-4.46880	4.32890	11.03250
H	-4.67020	3.28090	11.25480
H	-5.33650	4.76210	10.52170

B3LYP/6-31G(d):UFF

S	1.67000	8.82940	8.69700
S	1.22860	5.65080	6.33920
O	-3.26610	6.17260	11.66410

O	-3.29670	4.39900	10.21040
C	-2.60480	5.63360	10.51070
C	-2.83780	6.60550	9.33190
H	-3.93010	6.71670	9.31540
C	-2.27930	8.01200	9.58790
H	-2.72840	8.70470	8.84220
H	-2.60430	8.37880	10.58480
C	-0.77700	8.09610	9.51200
C	-0.12620	8.91300	8.60500
H	-0.64420	9.54020	7.89150
C	1.42560	7.64220	10.02830
H	2.24990	7.16990	10.54630
C	0.09800	7.37950	10.31420
C	-0.31810	6.40580	11.38560
H	-0.87830	6.95910	12.16940
H	0.58660	5.99370	11.88480
C	-1.15630	5.22970	10.86780
H	-1.28970	4.55580	11.72480
C	-0.44560	4.36020	9.79110
H	0.47690	3.96170	10.22710
H	-1.10010	3.49490	9.62930
C	-0.11070	4.97260	8.45020
C	1.13170	4.86900	7.88330
H	2.00210	4.37660	8.29500
C	-0.42860	6.14520	6.45770
H	-0.87590	6.72990	5.66550
C	-1.02450	5.72030	7.61520
C	-2.47100	6.01540	7.94000
H	-3.04600	5.08530	7.85220
H	-2.86590	6.68740	7.17040
C	-4.06800	5.14860	12.23930
H	-4.90690	5.61940	12.75850
H	-3.49500	4.54420	12.95800
C	-4.46640	4.32940	11.01880
H	-4.67810	3.27830	11.23370
H	-5.33270	4.77230	10.50620

B3LYP/def2-TZVPP:UFF

S	1.66310	8.84050	8.71400
S	1.21910	5.65280	6.35540
O	-3.26390	6.16890	11.65990
O	-3.30980	4.40080	10.21320
C	-2.60770	5.62920	10.50520
C	-2.83660	6.59830	9.32820
H	-3.92540	6.70590	9.30520
C	-2.28570	8.00490	9.58880
H	-2.73480	8.69740	8.84300
H	-2.61570	8.36950	10.58500
C	-0.78350	8.09540	9.51850
C	-0.13300	8.91950	8.61800
H	-0.65130	9.54950	7.90710
C	1.41890	7.64450	10.03740
H	2.24330	7.17140	10.55440

C	0.09130	7.37650	10.31860
C	-0.32510	6.39510	11.38300
H	-0.88450	6.94350	12.17080
H	0.57970	5.98030	11.87990
C	-1.16230	5.22360	10.85810
H	-1.29490	4.54810	11.70930
C	-0.44940	4.36130	9.78340
H	0.47140	3.96900	10.21850
H	-1.09330	3.49370	9.61720
C	-0.11450	4.97470	8.44800
C	1.12580	4.87240	7.88070
H	1.99140	4.37900	8.29150
C	-0.42070	6.14610	6.46500
H	-0.86520	6.73130	5.67660
C	-1.02090	5.72140	7.61830
C	-2.46370	6.01750	7.93840
H	-3.03850	5.09340	7.83430
H	-2.84950	6.69530	7.17500
C	-4.06690	5.15240	12.24270
H	-4.90090	5.62830	12.75570
H	-3.49290	4.55860	12.96240
C	-4.46880	4.32830	11.03380
H	-4.66890	3.28100	11.25600
H	-5.33700	4.76060	10.52500

B3LYP/QZVP:UFF

S	1.68420	8.82820	8.70190
S	1.29340	5.67630	6.30690
O	-3.27950	6.19930	11.67310
O	-3.32830	4.38350	10.20050
C	-2.59550	5.64610	10.49040
C	-2.83160	6.60940	9.31580
H	-3.92110	6.72200	9.29300
C	-2.27010	8.01280	9.57120
H	-2.71380	8.70500	8.82190
H	-2.59890	8.38310	10.56560
C	-0.76710	8.09380	9.50270
C	-0.11120	8.91400	8.60240
H	-0.62550	9.54560	7.89000
C	1.43270	7.63520	10.02660
H	2.25440	7.16030	10.54630
C	0.10370	7.37240	10.30580
C	-0.31720	6.39570	11.37320
H	-0.87390	6.94890	12.15970
H	0.58570	5.97730	11.87040
C	-1.16070	5.22670	10.85350
H	-1.29700	4.55140	11.70620
C	-0.45470	4.35250	9.77170
H	0.45660	3.94300	10.21480
H	-1.11650	3.49850	9.59810
C	-0.09570	4.97160	8.43830
C	1.15130	4.86240	7.90050
H	2.01510	4.37040	8.31260

C	-0.42630	6.17140	6.44680
H	-0.86440	6.75930	5.65910
C	-1.00970	5.72990	7.59610
C	-2.45990	6.01340	7.92290
H	-3.02860	5.08270	7.83390
H	-2.85720	6.68450	7.15750
C	-4.08860	5.14120	12.27830
H	-4.91470	5.62450	12.79360
H	-3.49530	4.56010	12.98870
C	-4.50390	4.30960	11.07090
H	-4.67900	3.25960	11.29350
H	-5.37590	4.73410	10.56780

B3LYP/6-31++G(d,p):UFF

S	1.66050	8.83870	8.70310
S	1.23550	5.65690	6.33650
O	-3.26580	6.17070	11.66840
O	-3.30760	4.39440	10.21860
C	-2.60680	5.62880	10.51010
C	-2.84050	6.59920	9.33050
H	-3.93340	6.70680	9.30910
C	-2.28660	8.00730	9.58970
H	-2.73710	8.69990	8.84490
H	-2.61350	8.37200	10.58680
C	-0.78450	8.09590	9.51500
C	-0.13570	8.91760	8.61100
H	-0.65540	9.54600	7.89970
C	1.41920	7.64640	10.03030
H	2.24480	7.17530	10.54710
C	0.09220	7.37900	10.31510
C	-0.32120	6.40140	11.38430
H	-0.88130	6.95180	12.17020
H	0.58460	5.98990	11.88180
C	-1.15790	5.22440	10.86430
H	-1.28910	4.54780	11.72010
C	-0.44360	4.35810	9.78640
H	0.48090	3.96530	10.22400
H	-1.09100	3.48790	9.61980
C	-0.10680	4.97390	8.44690
C	1.13820	4.87190	7.87850
H	2.00870	4.37790	8.28940
C	-0.42150	6.15060	6.45450
H	-0.86870	6.73650	5.66230
C	-1.02030	5.72280	7.61290
C	-2.46830	6.01470	7.93660
H	-3.04220	5.08470	7.83630
H	-2.85940	6.69350	7.17060
C	-4.07450	5.15040	12.24980
H	-4.90850	5.63240	12.76580
H	-3.49850	4.55090	12.96940
C	-4.47830	4.33010	11.03210
H	-4.68740	3.27880	11.24740
H	-5.34060	4.77420	10.51450

B3LYP/cc-pVDZ:UFF

S	1.67840	8.82880	8.69900
S	1.23640	5.65580	6.33800
O	-3.26610	6.17530	11.66230
O	-3.30100	4.40130	10.20610
C	-2.60580	5.63520	10.50940
C	-2.83460	6.60740	9.33050
H	-3.93310	6.72280	9.31480
C	-2.27180	8.01680	9.58770
H	-2.71980	8.71010	8.84210
H	-2.59630	8.38330	10.58480
C	-0.76970	8.09790	9.51180
C	-0.11750	8.91490	8.60600
H	-0.63450	9.54390	7.89350
C	1.43170	7.64060	10.02910
H	2.25500	7.16710	10.54740
C	0.10360	7.37950	10.31400
C	-0.31490	6.40680	11.38540
H	-0.87500	6.96090	12.16860
H	0.58850	5.99250	11.88480
C	-1.15770	5.22920	10.86520
H	-1.29230	4.55150	11.72770
C	-0.45110	4.35870	9.78900
H	0.47330	3.94930	10.22630
H	-1.11630	3.49420	9.62100
C	-0.11090	4.97210	8.44970
C	1.13570	4.86930	7.88310
H	2.01040	4.37160	8.29800
C	-0.42400	6.15080	6.45550
H	-0.87340	6.74060	5.65850
C	-1.02380	5.72230	7.61400
C	-2.47040	6.01640	7.94010
H	-3.04550	5.07820	7.85490
H	-2.86970	6.68880	7.16440
C	-4.06910	5.15340	12.23900
H	-4.91660	5.62990	12.75290
H	-3.49520	4.55260	12.97100
C	-4.46300	4.32350	11.02470
H	-4.66060	3.26470	11.24940
H	-5.34380	4.75370	10.51040

B3LYP/aug-cc-pVDZ:UFF

S	3.20400	-1.89270	-0.03580
S	3.14510	1.94760	-0.09970
O	-3.10610	-1.10800	0.19700
O	-2.96090	1.17280	0.10330
C	-2.15580	-0.03270	0.10570
C	-1.32120	-0.01470	1.40010
H	-2.08960	0.02370	2.18980
C	-0.52940	-1.31330	1.62840
H	-0.20170	-1.33190	2.69120
H	-1.19890	-2.19080	1.50150

C	0.66680	-1.49840	0.73500
C	1.94580	-1.67060	1.23290
H	2.17780	-1.66870	2.28980
C	1.85950	-1.73810	-1.22330
H	2.01680	-1.79390	-2.29230
C	0.61820	-1.53610	-0.64700
C	-0.63700	-1.38930	-1.46270
H	-1.30170	-2.25190	-1.24280
H	-0.38480	-1.46490	-2.54350
C	-1.40120	-0.07350	-1.24450
H	-2.20610	-0.06060	-1.99910
C	-0.56930	1.20390	-1.55320
H	-0.29130	1.18020	-2.61600
H	-1.26060	2.05160	-1.43340
C	0.67530	1.47460	-0.74060
C	1.91590	1.67740	-1.29540
H	2.16940	1.67500	-2.35440
C	1.98450	1.73990	1.17560
H	2.29690	1.79020	2.21740
C	0.71500	1.51220	0.70140
C	-0.47960	1.27850	1.59660
H	-1.17950	2.12070	1.48520
H	-0.13860	1.29900	2.64100
C	-4.32960	-0.65010	-0.36950
H	-5.14400	-1.23250	0.07890
H	-4.34070	-0.79450	-1.46210
C	-4.34460	0.82900	0.01870
H	-4.83060	1.46950	-0.73140
H	-4.82360	0.99030	0.99750

BLYP/TZVP:UFF

S	-3.15310	1.91880	-0.17660
S	-3.23020	-2.00090	-0.10830
O	3.24190	1.09860	0.34480
O	2.92320	-1.29800	0.35300
C	2.19300	0.02120	0.22310
C	1.27790	0.12060	1.52830
H	2.01610	0.10420	2.36420
C	0.52740	1.46360	1.63850
H	0.16930	1.57090	2.68600
H	1.22960	2.30540	1.46090
C	-0.63660	1.59790	0.69300
C	-1.93400	1.77400	1.14000
H	-2.20160	1.81380	2.18780
C	-1.76860	1.73480	-1.31260
H	-1.89320	1.74040	-2.38740
C	-0.54320	1.57580	-0.69020
C	0.73650	1.41170	-1.46610
H	1.41540	2.25530	-1.21840
H	0.52370	1.48810	-2.55510
C	1.45840	0.07390	-1.21380
H	2.28820	0.02690	-1.95580
C	0.58750	-1.22600	-1.51140

H	0.32370	-1.22830	-2.59200
H	1.27990	-2.08500	-1.34010
C	-0.70480	-1.46700	-0.69110
C	-1.93150	-1.74880	-1.28120
H	-2.14440	-1.81980	-2.35920
C	-2.09600	-1.70730	1.21590
H	-2.44880	-1.74200	2.25840
C	-0.80170	-1.44270	0.78290
C	0.36970	-1.16770	1.75990
H	1.07250	-2.03420	1.73280
H	-0.04020	-1.11480	2.79250
C	4.41400	0.52730	-0.38890
H	5.33730	0.85480	0.14930
H	4.47120	0.90170	-1.44620
C	4.21660	-1.05490	-0.36110
H	4.20230	-1.47120	-1.40400
H	5.02300	-1.57550	0.21240

PBEPBE/TZVP:UFF

S	1.53890	9.19920	9.22800
S	1.27710	5.66280	6.37420
O	-3.23460	6.15620	11.65280
O	-3.34450	4.33870	10.22320
C	-2.61070	5.56300	10.48460
C	-2.82840	6.54370	9.31330
H	-3.92820	6.64950	9.28390
C	-2.30280	7.96950	9.58960
H	-2.72550	8.63380	8.81870
H	-2.74330	8.29440	10.54770
C	-0.81240	8.17960	9.63250
C	-0.17120	9.16700	8.92280
H	-0.60820	9.87880	8.22670
C	1.39390	7.86270	10.32870
H	2.28060	7.47240	10.82240
C	0.09780	7.42070	10.45020
C	-0.31120	6.31580	11.38850
H	-0.87440	6.75240	12.23120
H	0.59990	5.87590	11.82510
C	-1.16510	5.15300	10.83610
H	-1.30600	4.47060	11.69390
C	-0.48270	4.28870	9.75300
H	0.42250	3.84870	10.20190
H	-1.16030	3.44400	9.54170
C	-0.09650	4.95100	8.45700
C	1.15650	4.84400	7.90180
H	2.02510	4.33280	8.30970
C	-0.38450	6.15950	6.47980
H	-0.81920	6.76000	5.68440
C	-0.99300	5.71630	7.63020
C	-2.44820	5.95460	7.93680
H	-2.99570	5.00170	7.83570
H	-2.85980	6.62670	7.16660
C	-4.09420	5.16770	12.23160

H	-4.90820	5.68830	12.75410
H	-3.54570	4.52990	12.94970
C	-4.53800	4.37390	11.01420
H	-4.83290	3.33840	11.23160
H	-5.35950	4.88490	10.47830

PBE1PBE/TZVP:UFF

S	3.17450	-1.90540	-0.17170
S	3.13410	2.02660	-0.11320
O	-3.17130	-1.10210	0.33640
O	-2.90000	1.23750	0.33850
C	-2.16310	-0.03580	0.22090
C	-1.26710	-0.10990	1.50780
H	-2.00540	-0.09590	2.32820
C	-0.50480	-1.43570	1.64290
H	-0.14400	-1.51990	2.69170
H	-1.19730	-2.28960	1.48420
C	0.65920	-1.58090	0.69900
C	1.95690	-1.75400	1.14580
H	2.22550	-1.78730	2.19350
C	1.78890	-1.72660	-1.30710
H	1.91200	-1.73590	-2.38200
C	0.56450	-1.56540	-0.68370
C	-0.71660	-1.39920	-1.45660
H	-1.38730	-2.25280	-1.22010
H	-0.50330	-1.46270	-2.54650
C	-1.44770	-0.07700	-1.19060
H	-2.27480	-0.04070	-1.91860
C	-0.61340	1.21160	-1.48680
H	-0.35660	1.22050	-2.55720
H	-1.30710	2.05370	-1.31430
C	0.65940	1.46640	-0.68530
C	1.86300	1.75810	-1.26570
H	2.06920	1.82670	-2.33400
C	2.02650	1.73020	1.19120
H	2.37250	1.77410	2.22410
C	0.75600	1.45010	0.76930
C	-0.39730	1.17080	1.72850
H	-1.10390	2.01840	1.68910
H	0.00480	1.13820	2.75250
C	-4.32910	-0.57130	-0.37910
H	-5.23980	-0.90160	0.15470
H	-4.38290	-0.95130	-1.42090
C	-4.15790	0.98520	-0.36150
H	-4.14430	1.39260	-1.39430
H	-4.96900	1.49030	0.19620

mPW1PW91/TZVP:UFF

S	3.16980	-1.91320	-0.16910
S	3.14400	2.02370	-0.11340
O	-3.17230	-1.10100	0.33420
O	-2.90560	1.24250	0.33530
C	-2.16530	-0.03080	0.21880

C	-1.26810	-0.10400	1.50730
H	-2.00580	-0.08750	2.32820
C	-0.50830	-1.43130	1.64390
H	-0.14800	-1.51540	2.69280
H	-1.20260	-2.28400	1.48610
C	0.65520	-1.58020	0.70010
C	1.95210	-1.75680	1.14770
H	2.21990	-1.79040	2.19560
C	1.78510	-1.73170	-1.30520
H	1.90860	-1.74270	-2.38010
C	0.56090	-1.56630	-0.68260
C	-0.71960	-1.39820	-1.45660
H	-1.39250	-2.24980	-1.21980
H	-0.50530	-1.46360	-2.54620
C	-1.44710	-0.07340	-1.19320
H	-2.27290	-0.03530	-1.92270
C	-0.60630	1.21270	-1.49180
H	-0.34670	1.21520	-2.56160
H	-1.29630	2.05910	-1.32670
C	0.66700	1.46650	-0.68780
C	1.87200	1.75540	-1.26750
H	2.07960	1.82240	-2.33570
C	2.03320	1.73020	1.19130
H	2.37840	1.77490	2.22440
C	0.76220	1.45170	0.76830
C	-0.39320	1.17530	1.72820
H	-1.09600	2.02600	1.69130
H	0.00930	1.13950	2.75210
C	-4.33580	-0.57140	-0.37610
H	-5.24320	-0.90470	0.16160
H	-4.39340	-0.95100	-1.41790
C	-4.16880	0.98650	-0.35740
H	-4.16350	1.39620	-1.38920
H	-4.97760	1.48800	0.20690

X3LYP/TZVP:UFF

S	1.66030	8.84410	8.70590
S	1.23050	5.66250	6.34610
O	-3.26100	6.17020	11.66250
O	-3.30280	4.39590	10.21700
C	-2.60290	5.62870	10.50690
C	-2.83610	6.59460	9.32980
H	-3.92600	6.70120	9.30890
C	-2.28610	8.00280	9.58600
H	-2.73700	8.69280	8.83890
H	-2.61540	8.36960	10.58140
C	-0.78420	8.09540	9.51370
C	-0.13610	8.91990	8.61180
H	-0.65610	9.54820	7.90080
C	1.41950	7.64900	10.03080
H	2.24520	7.17790	10.54760
C	0.09280	7.37890	10.31360
C	-0.32050	6.39810	11.37990

H	-0.87880	6.94700	12.16810
H	0.58560	5.98450	11.87530
C	-1.15830	5.22490	10.85860
H	-1.28920	4.54990	11.71170
C	-0.45000	4.36020	9.78310
H	0.46990	3.96330	10.21850
H	-1.09920	3.49590	9.61530
C	-0.11150	4.97470	8.44900
C	1.12830	4.87460	7.88860
H	1.99610	4.38350	8.29990
C	-0.43000	6.15080	6.46640
H	-0.87690	6.73550	5.67800
C	-1.02240	5.72080	7.61770
C	-2.46610	6.00830	7.94180
H	-3.03500	5.07890	7.84570
H	-2.85940	6.68070	7.17610
C	-4.06730	5.15160	12.24160
H	-4.90000	5.62810	12.75730
H	-3.49360	4.55110	12.95690
C	-4.47100	4.33510	11.02770
H	-4.68490	3.28890	11.24480
H	-5.32970	4.78120	10.51320

TPSSh/TZVP:UFF

S	1.67010	8.83200	8.70280
S	1.22970	5.64050	6.35590
O	-3.28670	6.18370	11.64800
O	-3.30250	4.40630	10.19220
C	-2.61060	5.64630	10.49690
C	-2.84130	6.61340	9.32160
H	-3.93260	6.71930	9.29960
C	-2.28410	8.01950	9.57560
H	-2.72920	8.71000	8.82560
H	-2.61420	8.38930	10.56980
C	-0.78130	8.10270	9.50750
C	-0.12550	8.91740	8.60230
H	-0.63970	9.54390	7.88530
C	1.41830	7.64710	10.03480
H	2.23960	7.17460	10.55720
C	0.08910	7.38630	10.31490
C	-0.33320	6.41420	11.38560
H	-0.89600	6.96930	12.16620
H	0.56840	6.00100	11.88930
C	-1.17110	5.24030	10.86590
H	-1.31400	4.56680	11.72040
C	-0.46110	4.36560	9.79760
H	0.45940	3.97060	10.23690
H	-1.11660	3.50340	9.63480
C	-0.12130	4.97240	8.45920
C	1.12260	4.86390	7.90030
H	1.98990	4.37090	8.31430
C	-0.42530	6.13850	6.46680
H	-0.86500	6.72110	5.67070

C	-1.02570	5.71760	7.62180
C	-2.47000	6.01790	7.93630
H	-3.04540	5.09010	7.84720
H	-2.85410	6.69090	7.16460
C	-4.04390	5.12890	12.23880
H	-4.86950	5.57980	12.78940
H	-3.42720	4.53140	12.92210
C	-4.46270	4.32690	11.02080
H	-4.66230	3.27360	11.22170
H	-5.33040	4.77830	10.52400

BHandH/TZVP:UFF

S	1.65070	8.87430	8.70820
S	1.18060	5.65620	6.41210
O	-3.24390	6.15620	11.61610
O	-3.26220	4.43080	10.19430
C	-2.59020	5.63920	10.48910
C	-2.82790	6.58420	9.32910
H	-3.91760	6.67790	9.32140
C	-2.29290	8.00000	9.56990
H	-2.74700	8.67700	8.81290
H	-2.63020	8.37550	10.55970
C	-0.79160	8.10800	9.50500
C	-0.14580	8.93760	8.60620
H	-0.66740	9.56240	7.89320
C	1.41280	7.67530	10.03010
H	2.23940	7.20860	10.54950
C	0.08670	7.39640	10.30700
C	-0.32650	6.40980	11.36790
H	-0.87950	6.95710	12.16120
H	0.57970	5.99040	11.85820
C	-1.17160	5.24300	10.84590
H	-1.32000	4.57840	11.70240
C	-0.48950	4.37640	9.79460
H	0.41900	3.95480	10.22360
H	-1.16190	3.53280	9.62380
C	-0.14530	4.97960	8.48120
C	1.08190	4.88260	7.92930
H	1.94410	4.39240	8.34880
C	-0.45310	6.13550	6.51800
H	-0.90350	6.71580	5.73050
C	-1.04410	5.71350	7.65500
C	-2.46930	5.98800	7.97280
H	-3.02330	5.04920	7.90540
H	-2.87310	6.63210	7.19220
C	-4.00630	5.14130	12.18590
H	-4.83200	5.58700	12.73290
H	-3.40830	4.52960	12.86810
C	-4.41270	4.35960	10.97590
H	-4.64380	3.31610	11.17170
H	-5.26160	4.83010	10.47140

M06/TZVP:UFF

S	1.46090	9.03020	8.56980
S	1.17790	5.97700	6.26140
O	-3.18430	6.16470	11.62300
O	-3.32060	4.33690	10.28780
C	-2.60910	5.56720	10.45660
C	-2.92270	6.48860	9.27770
H	-4.01840	6.56110	9.31690
C	-2.41920	7.92810	9.45870
H	-2.90730	8.56390	8.68720
H	-2.75910	8.32730	10.43800
C	-0.92240	8.09920	9.37940
C	-0.33620	8.98370	8.49100
H	-0.90250	9.59520	7.80090
C	1.31300	7.79120	9.86630
H	2.17480	7.37000	10.36700
C	0.01060	7.42430	10.15740
C	-0.30800	6.40150	11.21970
H	-0.82380	6.92220	12.05450
H	0.63860	6.00560	11.64970
C	-1.15210	5.20820	10.74930
H	-1.24020	4.55270	11.62680
C	-0.49230	4.34150	9.66670
H	0.45410	3.93060	10.08280
H	-1.13220	3.46110	9.44500
C	-0.20530	5.04930	8.36580
C	1.06510	5.08080	7.81770
H	1.92390	4.61400	8.28180
C	-0.58760	6.27210	6.44560
H	-1.15990	6.83670	5.72140
C	-1.14030	5.72340	7.58960
C	-2.60770	5.86540	7.91020
H	-3.07430	4.85990	7.83770
H	-3.10040	6.48430	7.12790
C	-3.96590	5.19550	12.27640
H	-4.75340	5.69960	12.83800
H	-3.36130	4.59200	12.96930
C	-4.45460	4.36480	11.11870
H	-4.72570	3.34050	11.37730
H	-5.30780	4.84640	10.61880

M062X/TZVP:UFF

S	1.53890	9.19920	9.22800
S	1.27710	5.66280	6.37420
O	-3.23460	6.15620	11.65280
O	-3.34450	4.33870	10.22320
C	-2.61070	5.56300	10.48460
C	-2.82840	6.54370	9.31330
H	-3.92820	6.64950	9.28390
C	-2.30280	7.96950	9.58960
H	-2.72550	8.63380	8.81870
H	-2.74330	8.29440	10.54770
C	-0.81240	8.17960	9.63250
C	-0.17120	9.16700	8.92280

H	-0.60820	9.87880	8.22670
C	1.39390	7.86270	10.32870
H	2.28060	7.47240	10.82240
C	0.09780	7.42070	10.45020
C	-0.31120	6.31580	11.38850
H	-0.87440	6.75240	12.23120
H	0.59990	5.87590	11.82510
C	-1.16510	5.15300	10.83610
H	-1.30600	4.47060	11.69390
C	-0.48270	4.28870	9.75300
H	0.42250	3.84870	10.20190
H	-1.16030	3.44400	9.54170
C	-0.09650	4.95100	8.45700
C	1.15650	4.84400	7.90180
H	2.02510	4.33280	8.30970
C	-0.38450	6.15950	6.47980
H	-0.81920	6.76000	5.68440
C	-0.99300	5.71630	7.63020
C	-2.44820	5.95460	7.93680
H	-2.99570	5.00170	7.83570
H	-2.85980	6.62670	7.16660
C	-4.09420	5.16770	12.23160
H	-4.90820	5.68830	12.75410
H	-3.54570	4.52990	12.94970
C	-4.53800	4.37390	11.01420
H	-4.83290	3.33840	11.23160
H	-5.35950	4.88490	10.47830

M06HF/TZVP:UFF

S	1.66340	8.84490	8.68300
S	1.21650	5.68910	6.37980
O	-3.24200	6.16250	11.65380
O	-3.28060	4.40790	10.21700
C	-2.58970	5.62910	10.50440
C	-2.83500	6.59360	9.33150
H	-3.92470	6.68590	9.32700
C	-2.27940	7.99890	9.57370
H	-2.73310	8.68390	8.82400
H	-2.60410	8.37250	10.56830
C	-0.77780	8.09050	9.49580
C	-0.13320	8.91520	8.59150
H	-0.65620	9.54200	7.88120
C	1.42800	7.65080	10.00960
H	2.25600	7.18380	10.52640
C	0.10240	7.37740	10.29540
C	-0.30570	6.40090	11.36770
H	-0.85720	6.95440	12.15750
H	0.60280	5.98690	11.85820
C	-1.14890	5.22850	10.86240
H	-1.29510	4.55750	11.71390
C	-0.46380	4.34360	9.78700
H	0.45230	3.93750	10.21380
H	-1.13990	3.50760	9.60720

C	-0.11690	4.97200	8.45660
C	1.11930	4.89100	7.90340
H	1.98690	4.40390	8.31580
C	-0.43860	6.15650	6.48550
H	-0.88790	6.73860	5.69880
C	-1.03280	5.71610	7.62310
C	-2.48480	5.98340	7.94770
H	-3.02770	5.04020	7.88590
H	-2.88370	6.64140	7.17660
C	-4.05470	5.15610	12.23240
H	-4.88600	5.63630	12.73800
H	-3.47980	4.54840	12.93120
C	-4.46050	4.34590	11.00260
H	-4.67840	3.30380	11.21220
H	-5.29340	4.81590	10.47990

BLYP/TZVP

S	-3.08180	2.38140	0.01660
S	-3.08190	-2.38090	-0.01660
O	2.99130	1.16480	0.03100
O	2.99190	-1.16440	-0.03080
C	2.10500	0.00010	0.00010
C	1.30730	0.00070	1.33260
H	2.10000	-0.00420	2.09800
C	0.52180	1.31970	1.59430
H	0.20170	1.30570	2.64640
H	1.24650	2.14370	1.50790
C	-0.68600	1.63000	0.73300
C	-1.89820	2.01410	1.25760
H	-2.17430	2.10090	2.30320
C	-1.90910	2.00310	-1.23140
H	-2.19420	2.08170	-2.27520
C	-0.69230	1.62340	-0.71420
C	0.51000	1.31290	-1.58360
H	1.23120	2.14070	-1.50120
H	0.18260	1.29800	-2.63340
C	1.30730	-0.00110	-1.33250
H	2.10010	0.00400	-2.09790
C	0.52220	-1.32030	-1.59400
H	0.20250	-1.30680	-2.64630
H	1.24710	-2.14410	-1.50700
C	-0.68580	-1.63040	-0.73300
C	-1.89810	-2.01410	-1.25760
H	-2.17420	-2.10090	-2.30320
C	-1.90900	-2.00320	1.23140
H	-2.19420	-2.08180	2.27520
C	-0.69210	-1.62380	0.71430
C	0.51030	-1.31360	1.58340
H	1.23170	-2.14120	1.50050
H	0.18320	-1.29910	2.63330
C	4.33110	0.71490	-0.27130
H	5.03360	1.38810	0.23410
H	4.51960	0.73590	-1.35780

C	4.33150	-0.71390	0.27100
H	5.03420	-1.38670	-0.23450
H	4.52030	-0.73480	1.35760

PBEPBE/TZVP

S	1.53890	9.19920	9.22800
S	1.27710	5.66280	6.37420
O	-3.23460	6.15620	11.65280
O	-3.34450	4.33870	10.22320
C	-2.61070	5.56300	10.48460
C	-2.82840	6.54370	9.31330
H	-3.92820	6.64950	9.28390
C	-2.30280	7.96950	9.58960
H	-2.72550	8.63380	8.81870
H	-2.74330	8.29440	10.54770
C	-0.81240	8.17960	9.63250
C	-0.17120	9.16700	8.92280
H	-0.60820	9.87880	8.22670
C	1.39390	7.86270	10.32870
H	2.28060	7.47240	10.82240
C	0.09780	7.42070	10.45020
C	-0.31120	6.31580	11.38850
H	-0.87440	6.75240	12.23120
H	0.59990	5.87590	11.82510
C	-1.16510	5.15300	10.83610
H	-1.30600	4.47060	11.69390
C	-0.48270	4.28870	9.75300
H	0.42250	3.84870	10.20190
H	-1.16030	3.44400	9.54170
C	-0.09650	4.95100	8.45700
C	1.15650	4.84400	7.90180
H	2.02510	4.33280	8.30970
C	-0.38450	6.15950	6.47980
H	-0.81920	6.76000	5.68440
C	-0.99300	5.71630	7.63020
C	-2.44820	5.95460	7.93680
H	-2.99570	5.00170	7.83570
H	-2.85980	6.62670	7.16660
C	-4.09420	5.16770	12.23160
H	-4.90820	5.68830	12.75410
H	-3.54570	4.52990	12.94970
C	-4.53800	4.37390	11.01420
H	-4.83290	3.33840	11.23160
H	-5.35950	4.88490	10.47830

PBE1PBE/TZVP

S	3.05490	2.24550	-0.01190
S	3.05490	-2.24490	0.01190
O	-2.95400	1.13990	-0.02000
O	-2.95470	-1.13930	0.02020
C	-2.09240	0.00000	0.00010
C	-1.30580	0.00920	-1.31550
H	-2.10130	0.00560	-2.07150

C	-0.53420	1.31020	-1.56470
H	-0.22700	1.31630	-2.61510
H	-1.24660	2.13440	-1.45040
C	0.67230	1.58380	-0.72010
C	1.88350	1.93430	-1.23580
H	2.15550	2.02040	-2.27780
C	1.90120	1.90050	1.21970
H	2.18820	1.95930	2.25950
C	0.68230	1.56400	0.71240
C	-0.51480	1.27960	1.56750
H	-1.22130	2.11180	1.47350
H	-0.19440	1.26860	2.61380
C	-1.30570	-0.00970	1.31560
H	-2.10120	-0.00590	2.07160
C	-0.53460	-1.31110	1.56450
H	-0.22790	-1.31790	2.61490
H	-1.24730	-2.13500	1.44940
C	0.67200	-1.58440	0.72010
C	1.88340	-1.93440	1.23580
H	2.15540	-2.02040	2.27780
C	1.90110	-1.90060	-1.21970
H	2.18800	-1.95930	-2.25960
C	0.68210	-1.56460	-0.71240
C	-0.51540	-1.28050	-1.56720
H	-1.22200	-2.11240	-1.47240
H	-0.19540	-1.27010	-2.61360
C	-4.26600	0.70390	0.27700
H	-4.97300	1.37710	-0.20940
H	-4.44950	0.70620	1.35920
C	-4.26640	-0.70250	-0.27720
H	-4.97390	-1.37530	0.20910
H	-4.44960	-0.70470	-1.35940

B3LYP/TZVP

S	1.53340	9.22640	9.27300
S	1.25440	5.62120	6.34740
O	-3.22520	6.14990	11.64400
O	-3.33980	4.35290	10.22240
C	-2.60570	5.56580	10.48120
C	-2.82140	6.54630	9.31190
H	-3.91100	6.65550	9.28160
C	-2.29590	7.97110	9.58860
H	-2.70950	8.62710	8.81810
H	-2.73940	8.29660	10.53430
C	-0.80700	8.18850	9.64400
C	-0.17310	9.18000	8.95450
H	-0.61040	9.88830	8.26830
C	1.38510	7.87850	10.35780
H	2.26070	7.49090	10.85490
C	0.10140	7.42960	10.46210
C	-0.30650	6.31400	11.38800
H	-0.86010	6.74010	12.23020
H	0.59940	5.87310	11.81230

C	-1.16160	5.15590	10.83010
H	-1.29800	4.47720	11.67910
C	-0.48060	4.29160	9.74760
H	0.42130	3.86230	10.19200
H	-1.14910	3.44970	9.54450
C	-0.10040	4.94240	8.44400
C	1.13710	4.82020	7.88380
H	1.99560	4.30760	8.28870
C	-0.40140	6.13100	6.46730
H	-0.83930	6.72190	5.67810
C	-0.99740	5.70660	7.61840
C	-2.44830	5.95870	7.93380
H	-2.99970	5.01930	7.82970
H	-2.85160	6.63310	7.17370
C	-4.09840	5.18310	12.22350
H	-4.91560	5.71080	12.71450
H	-3.56960	4.56780	12.96050
C	-4.52360	4.36380	11.01730
H	-4.78920	3.33280	11.24970
H	-5.35260	4.83950	10.48090

mPW1PW91/TZVP

S	3.05200	2.26540	-0.01370
S	3.05210	-2.26470	0.01360
O	-2.95310	1.13980	-0.02270
O	-2.95400	-1.13920	0.02280
C	-2.09070	-0.00000	0.00010
C	-1.30360	0.00610	-1.31540
H	-2.09710	0.00200	-2.07110
C	-0.53080	1.30660	-1.56770
H	-0.22230	1.30850	-2.61610
H	-1.24260	2.13000	-1.45870
C	0.67410	1.58610	-0.72210
C	1.88280	1.94240	-1.23770
H	2.15460	2.02760	-2.27830
C	1.89830	1.91640	1.21790
H	2.18320	1.98080	2.25650
C	0.68300	1.57080	0.71060
C	-0.51380	1.28430	1.56590
H	-1.22040	2.11430	1.47190
H	-0.19380	1.27450	2.61080
C	-1.30350	-0.00680	1.31550
H	-2.09710	-0.00250	2.07120
C	-0.53130	-1.30770	1.56740
H	-0.22330	-1.31030	2.61590
H	-1.24330	-2.13080	1.45750
C	0.67390	-1.58680	0.72210
C	1.88280	-1.94240	1.23770
H	2.15470	-2.02750	2.27830
C	1.89820	-1.91650	-1.21800
H	2.18310	-1.98080	-2.25650
C	0.68270	-1.57150	-0.71060
C	-0.51440	-1.28540	-1.56550

H	-1.22130	-2.11510	-1.47050
H	-0.19500	-1.27630	-2.61060
C	-4.26690	0.70610	0.27230
H	-4.97060	1.37550	-0.22090
H	-4.45400	0.71700	1.35210
C	-4.26730	-0.70450	-0.27240
H	-4.97160	-1.37330	0.22050
H	-4.45420	-0.71530	-1.35230

X3LYP/TZVP

S	-3.06280	2.30870	0.01460
S	-3.06210	-2.30940	-0.01550
O	2.96530	1.14570	0.02580
O	2.96560	-1.14530	-0.02370
C	2.09400	0.00030	0.00080
C	1.30310	0.00370	1.32190
H	2.09360	-0.00080	2.08020
C	0.52600	1.31110	1.57800
H	0.21220	1.30520	2.62500
H	1.24200	2.13230	1.48000
C	-0.67920	1.60550	0.72640
C	-1.88610	1.97000	1.24430
H	-2.15720	2.05390	2.28490
C	-1.89930	1.95070	-1.22210
H	-2.18140	2.01950	-2.26090
C	-0.68680	1.59400	-0.71170
C	0.51160	1.29570	-1.57210
H	1.22270	2.12260	-1.48500
H	0.18810	1.28190	-2.61620
C	1.30370	-0.00390	-1.32090
H	2.09450	0.00100	-2.07880
C	0.52770	-1.31190	-1.57700
H	0.21480	-1.30680	-2.62430
H	1.24410	-2.13260	-1.47770
C	-0.67810	-1.60630	-0.72620
C	-1.88480	-1.97040	-1.24470
H	-2.15550	-2.05410	-2.28540
C	-1.89920	-1.95100	1.22180
H	-2.18190	-2.01970	2.26040
C	-0.68630	-1.59490	0.71200
C	0.51180	-1.29650	1.57260
H	1.22340	-2.12290	1.48500
H	0.18830	-1.28350	2.61660
C	4.28940	0.71090	-0.26860
H	4.98880	1.37750	0.23470
H	4.47940	0.73350	-1.34760
C	4.29060	-0.70970	0.26590
H	4.98860	-1.37600	-0.23980
H	4.48440	-0.73220	1.34420

TPSS/TZVP

S	1.54170	9.19775	9.22634
S	1.28139	5.65819	6.37604

O	-3.24012	6.16024	11.64726
O	-3.34759	4.34179	10.21600
C	-2.61064	5.56807	10.47853
C	-2.83371	6.54899	9.30916
H	-3.92773	6.65290	9.27995
C	-2.30545	7.97774	9.59026
H	-2.72584	8.64128	8.82484
H	-2.73886	8.29362	10.54828
C	-0.81125	8.18145	9.62962
C	-0.17098	9.16606	8.92223
H	-0.60561	9.87656	8.23119
C	1.39127	7.85924	10.32745
H	2.27237	7.46996	10.82075
C	0.09765	7.42069	10.44703
C	-0.31351	6.31892	11.39244
H	-0.88044	6.75762	12.22436
H	0.59246	5.88160	11.82930
C	-1.16923	5.15221	10.83852
H	-1.31325	4.47477	11.69231
C	-0.48636	4.28356	9.75311
H	0.41292	3.84308	10.20053
H	-1.16798	3.45001	9.53882
C	-0.09641	4.95157	8.45796
C	1.15362	4.83987	7.90591
H	2.01524	4.32672	8.31279
C	-0.38092	6.15976	6.48293
H	-0.81192	6.75764	5.69045
C	-0.98963	5.71987	7.63018
C	-2.44939	5.95808	7.92948
H	-2.99200	5.00844	7.83177
H	-2.85493	6.62880	7.16231
C	-4.08941	5.16017	12.23657
H	-4.89383	5.67945	12.76289
H	-3.52701	4.53190	12.94201
C	-4.53978	4.36737	11.02005
H	-4.81789	3.33206	11.23160
H	-5.35998	4.87301	10.49077

TPSSh/TZVP

S	3.06680	2.26945	-0.01471
S	3.06684	-2.26837	0.01447
O	-2.96539	1.15090	-0.02577
O	-2.96649	-1.14979	0.02631
C	-2.09359	0.00017	0.00019
C	-1.31062	0.00531	-1.32320
H	-2.10676	0.00101	-2.07814
C	-0.53334	1.31324	-1.57689
H	-0.22309	1.31375	-2.62640
H	-1.24824	2.13566	-1.46457
C	0.67646	1.59039	-0.72525
C	1.89034	1.94474	-1.24399
H	2.16505	2.02928	-2.28513
C	1.90514	1.92141	1.22224

H	2.19223	1.98758	2.26135
C	0.68495	1.57649	0.71183
C	-0.51696	1.29327	1.57318
H	-1.22726	2.12162	1.47368
H	-0.19583	1.28428	2.61937
C	-1.31046	-0.00602	1.32347
H	-2.10652	-0.00143	2.07849
C	-0.53412	-1.31471	1.57647
H	-0.22466	-1.31647	2.62621
H	-1.24940	-2.13661	1.46278
C	0.67602	-1.59143	0.72528
C	1.89014	-1.94501	1.24392
H	2.16503	-2.02953	2.28501
C	1.90462	-1.92172	-1.22240
H	2.19164	-1.98787	-2.26153
C	0.68434	-1.57754	-0.71180
C	-0.51816	-1.29477	-1.57241
H	-1.22886	-2.12257	-1.47126
H	-0.19808	-1.28710	-2.61893
C	-4.28777	0.70505	0.28242
H	-4.99148	1.38481	-0.19875
H	-4.45872	0.70218	1.36599
C	-4.28818	-0.70275	-0.28297
H	-4.99289	-1.38186	0.19764
H	-4.45827	-0.69973	-1.36669

BhandH/TZVP

S	1.45020	9.07210	9.07190
S	1.31350	5.76300	6.56550
O	-3.19440	6.13860	11.61220
O	-3.31400	4.39030	10.21640
C	-2.59590	5.57030	10.47480
C	-2.81460	6.53450	9.32960
H	-3.90550	6.61010	9.29210
C	-2.32540	7.93730	9.62420
H	-2.77710	8.61170	8.89570
H	-2.72580	8.22070	10.59980
C	-0.85820	8.14480	9.60670
C	-0.24420	9.09180	8.87120
H	-0.70640	9.79620	8.20050
C	1.33510	7.77180	10.17110
H	2.22270	7.35530	10.61650
C	0.06230	7.37570	10.36900
C	-0.32910	6.30950	11.32630
H	-0.87280	6.76680	12.15610
H	0.58040	5.88340	11.75210
C	-1.18100	5.16170	10.82140
H	-1.33100	4.50990	11.68730
C	-0.53380	4.28680	9.76800
H	0.33680	3.80710	10.21700
H	-1.24090	3.48890	9.53200
C	-0.10490	4.95990	8.51940
C	1.14060	4.87620	8.01300

H	1.97930	4.34650	8.43220
C	-0.32020	6.25150	6.63430
H	-0.73010	6.88990	5.87010
C	-0.96000	5.75940	7.71350
C	-2.40520	5.97280	7.98250
H	-2.92730	5.02050	7.86390
H	-2.80020	6.63790	7.21330
C	-4.03720	5.18730	12.18430
H	-4.84050	5.69660	12.70930
H	-3.49260	4.54970	12.88660
C	-4.47830	4.41050	10.98220
H	-4.78000	3.38860	11.19390
H	-5.28730	4.92550	10.45620

M06/TZVP

S	1.47140	9.11770	9.05710
S	1.35490	5.74710	6.53860
O	-3.22020	6.14160	11.63870
O	-3.33960	4.36430	10.22420
C	-2.61220	5.56290	10.48550
C	-2.82740	6.53790	9.32730
H	-3.92290	6.61590	9.27860
C	-2.33700	7.95700	9.62460
H	-2.78850	8.62570	8.88350
H	-2.74970	8.25090	10.59640
C	-0.85890	8.17220	9.61480
C	-0.24820	9.13080	8.87140
H	-0.71510	9.83910	8.20210
C	1.35620	7.79300	10.16380
H	2.25210	7.37260	10.59800
C	0.07370	7.39580	10.37270
C	-0.30620	6.30810	11.33070
H	-0.82370	6.75770	12.18670
H	0.61510	5.86760	11.72870
C	-1.18020	5.15290	10.83100
H	-1.32060	4.50100	11.70500
C	-0.52630	4.26510	9.76940
H	0.35110	3.79390	10.22600
H	-1.22740	3.45440	9.54120
C	-0.09680	4.93570	8.50570
C	1.16100	4.84510	8.00170
H	1.99990	4.30960	8.42270
C	-0.29870	6.25010	6.61270
H	-0.70020	6.90020	5.84840
C	-0.95000	5.74890	7.69470
C	-2.40540	5.98420	7.96220
H	-2.94750	5.04240	7.81430
H	-2.78410	6.67640	7.20160
C	-4.07180	5.17550	12.21270
H	-4.87920	5.68640	12.73900
H	-3.52800	4.53700	12.92330
C	-4.51440	4.38950	11.00340
H	-4.81650	3.36360	11.21800

H	-5.33170	4.90110	10.47550

M06HF/TZVP

S	3.10210	1.93790	0.22050
S	3.10210	-1.93780	-0.22090
O	-2.98860	1.09110	0.31440
O	-2.98840	-1.09130	-0.31360
C	-2.12330	-0.00010	0.00030
C	-1.34040	0.38690	-1.26130
H	-2.12620	0.49460	-2.01250
C	-0.67090	1.77030	-1.15340
H	-0.46320	2.12160	-2.16410
H	-1.38120	2.45820	-0.69590
C	0.61980	1.75340	-0.38390
C	1.79990	2.19690	-0.87560
H	1.97940	2.64130	-1.84030
C	2.03290	1.22430	1.37080
H	2.41490	0.86200	2.31080
C	0.74820	1.19290	0.93830
C	-0.41850	0.73480	1.79040
H	-1.04990	1.60280	1.98650
H	-0.01820	0.39380	2.74610
C	-1.34020	-0.38690	1.26180
H	-2.12590	-0.49460	2.01310
C	-0.67060	-1.77030	1.15380
H	-0.46270	-2.12150	2.16450
H	-1.38090	-2.45820	0.69650
C	0.61990	-1.75330	0.38400
C	1.80020	-2.19680	0.87550
H	1.97980	-2.64130	1.84010
C	2.03260	-1.22420	-1.37090
H	2.41450	-0.86190	-2.31100
C	0.74800	-1.19290	-0.93820
C	-0.41880	-0.73480	-1.79010
H	-1.05020	-1.60280	-1.98610
H	-0.01870	-0.39380	-2.74590
C	-4.30960	0.59740	0.47570
H	-5.00470	1.38310	0.19860
H	-4.47780	0.27870	1.50440
C	-4.30910	-0.59740	-0.47680
H	-5.00470	-1.38300	-0.20060
H	-4.47570	-0.27870	-1.50570

M062X/TZVP

S	-3.09990	1.99210	-0.16070
S	-3.09990	-1.99190	0.16070
O	2.98150	1.11970	-0.21210
O	2.98160	-1.11960	0.21210
C	2.11800	-0.00000	-0.00000
C	1.33440	0.27390	1.28920
H	2.12540	0.34660	2.04420
C	0.63390	1.64190	1.29290
H	0.40470	1.90030	2.32930

H	1.35030	2.38400	0.93090
C	-0.63130	1.70900	0.49400
C	-1.82690	2.11010	0.99800
H	-2.03660	2.44370	2.00250
C	-1.99680	1.39940	-1.34940
H	-2.35120	1.15180	-2.33800
C	-0.72420	1.30400	-0.88050
C	0.45410	0.90840	-1.73250
H	1.11300	1.77700	-1.82800
H	0.08640	0.68250	-2.73680
C	1.33430	-0.27400	-1.28920
H	2.12530	-0.34670	-2.04420
C	0.63390	-1.64200	-1.29280
H	0.40470	-1.90050	-2.32930
H	1.35030	-2.38400	-0.93080
C	-0.63130	-1.70910	-0.49400
C	-1.82690	-2.11020	-0.99800
H	-2.03670	-2.44380	-2.00240
C	-1.99670	-1.39950	1.34940
H	-2.35120	-1.15200	2.33810
C	-0.72420	-1.30400	0.88050
C	0.45420	-0.90850	1.73240
H	1.11310	-1.77710	1.82790
H	0.08650	-0.68270	2.73680
C	4.29530	0.63220	-0.41990
H	5.00190	1.39030	-0.08750
H	4.46650	0.40470	-1.47730
C	4.29530	-0.63200	0.41990
H	5.00200	-1.39010	0.08750
H	4.46640	-0.40450	1.47730

B97D/TZVP

S	3.10530	2.12370	-0.00340
S	3.10530	-2.12350	0.00330
O	-2.99660	1.15810	-0.00640
O	-2.99680	-1.15800	0.00680
C	-2.12120	0.00000	0.00010
C	-1.33320	0.02340	-1.32420
H	-2.12720	0.02190	-2.08520
C	-0.54740	1.33320	-1.56340
H	-0.24530	1.34300	-2.61940
H	-1.25360	2.16420	-1.42900
C	0.67360	1.56930	-0.71410
C	1.90310	1.87700	-1.23780
H	2.17270	1.95750	-2.28470
C	1.92720	1.80750	1.23830
H	2.21700	1.83220	2.28260
C	0.68700	1.52960	0.72310
C	-0.52230	1.26770	1.58340
H	-1.22250	2.10920	1.48520
H	-0.20290	1.24250	2.63400
C	-1.33310	-0.02360	1.32440
H	-2.12710	-0.02210	2.08540

C	-0.54740	-1.33350	1.56340
H	-0.24540	-1.34350	2.61940
H	-1.25370	-2.16440	1.42880
C	0.67370	-1.56950	0.71410
C	1.90320	-1.87700	1.23780
H	2.17280	-1.95750	2.28470
C	1.92710	-1.80740	-1.23840
H	2.21690	-1.83210	-2.28270
C	0.68690	-1.52970	-0.72310
C	-0.52260	-1.26800	-1.58320
H	-1.22270	-2.10940	-1.48470
H	-0.20340	-1.24290	-2.63380
C	-4.31670	0.69990	0.30150
H	-5.03360	1.38940	-0.15800
H	-4.47920	0.66050	1.39170
C	-4.31670	-0.69950	-0.30180
H	-5.03400	-1.38890	0.15730
H	-4.47870	-0.66000	-1.39210

TPSS-D/TZVP

S	1.54932	9.08619	9.09559
S	1.32369	5.79078	6.46849
O	-3.24426	6.15690	11.65356
O	-3.35230	4.33823	10.22020
C	-2.61663	5.56428	10.48434
C	-2.84375	6.54410	9.31751
H	-3.93813	6.64222	9.28938
C	-2.31319	7.97067	9.59928
H	-2.74467	8.63960	8.84521
H	-2.72423	8.28119	10.56840
C	-0.81790	8.15612	9.60543
C	-0.17316	9.09918	8.84852
H	-0.61040	9.79475	8.14410
C	1.39444	7.78745	10.24333
H	2.27830	7.37917	10.71584
C	0.09335	7.39335	10.41701
C	-0.32256	6.31811	11.38837
H	-0.89328	6.77584	12.20689
H	0.57996	5.88557	11.83627
C	-1.17824	5.14733	10.84611
H	-1.32537	4.47321	11.70168
C	-0.49603	4.28217	9.75910
H	0.39604	3.82916	10.20774
H	-1.18364	3.45946	9.52488
C	-0.09151	4.97603	8.48415
C	1.17508	4.91448	7.96448
H	2.03895	4.41548	8.38394
C	-0.35439	6.24442	6.54530
H	-0.77981	6.86472	5.76721
C	-0.98165	5.74899	7.65872
C	-2.44820	5.95573	7.94118
H	-2.97047	4.99497	7.84488
H	-2.86077	6.61769	7.17055

C	-4.09248	5.15490	12.24009
H	-4.89425	5.67129	12.77315
H	-3.52722	4.51996	12.93764
C	-4.54728	4.37090	11.01907
H	-4.83639	3.33753	11.22488
H	-5.35995	4.88888	10.48954

B3LYP-D/TZVP

S	1.54793	9.09019	9.11450
S	1.30892	5.77975	6.45864
O	-3.23561	6.14758	11.64833
O	-3.35063	4.35168	10.22204
C	-2.61683	5.56377	10.48566
C	-2.83575	6.54400	9.31904
H	-3.92609	6.64609	9.29050
C	-2.30500	7.96602	9.59748
H	-2.73231	8.63003	8.84128
H	-2.72039	8.28454	10.55799
C	-0.81379	8.15874	9.61273
C	-0.17172	9.09928	8.86324
H	-0.61210	9.79004	8.16074
C	1.39005	7.79091	10.25792
H	2.26721	7.37936	10.73305
C	0.09570	7.39665	10.42570
C	-0.32116	6.31473	11.38427
H	-0.88220	6.76652	12.20779
H	0.57893	5.87892	11.82611
C	-1.17650	5.15085	10.83961
H	-1.31965	4.47646	11.69092
C	-0.49515	4.28999	9.75511
H	0.39676	3.84332	10.20267
H	-1.17274	3.46249	9.52582
C	-0.09521	4.97281	8.47642
C	1.16328	4.90965	7.95592
H	2.02289	4.41263	8.37859
C	-0.36686	6.23275	6.54067
H	-0.79824	6.85053	5.76813
C	-0.98723	5.74322	7.65178
C	-2.44723	5.95839	7.94459
H	-2.97422	5.00517	7.84206
H	-2.85855	6.62251	7.17965
C	-4.09485	5.17036	12.23096
H	-4.90623	5.68804	12.74222
H	-3.54991	4.54563	12.94893
C	-4.53273	4.36499	11.01896
H	-4.80858	3.33445	11.24198
H	-5.35720	4.85797	10.48998

UFF

S	3.21200	-1.90800	0.02700
S	3.21100	1.90900	-0.03000
O	-3.01800	-1.16100	0.02400
O	-3.01800	1.16100	-0.01700

C	-2.20500	0.00000	0.00300
C	-1.35900	0.02100	1.30700
H	-2.12300	0.03300	2.11800
C	-0.56200	-1.28200	1.57800
H	-0.25800	-1.28300	2.64900
H	-1.22500	-2.16400	1.45100
C	0.65500	-1.48200	0.71600
C	1.91500	-1.67900	1.25400
H	2.11200	-1.69200	2.31700
C	1.91200	-1.71800	-1.20300
H	2.10600	-1.76600	-2.26700
C	0.65300	-1.50400	-0.66900
C	-0.56600	-1.33300	-1.53500
H	-1.22900	-2.20900	-1.37800
H	-0.26400	-1.36700	-2.60500
C	-1.36100	-0.02100	-1.30300
H	-2.12600	-0.03300	-2.11300
C	-0.56500	1.28200	-1.57600
H	-0.26200	1.28200	-2.64700
H	-1.22800	2.16400	-1.44900
C	0.65300	1.48200	-0.71500
C	1.91200	1.67900	-1.25500
H	2.10700	1.69200	-2.31900
C	1.91300	1.71800	1.20200
H	2.10900	1.76500	2.26500
C	0.65400	1.50400	0.67000
C	-0.56400	1.33200	1.53700
H	-1.22700	2.20900	1.38200
H	-0.26000	1.36600	2.60700
C	-4.32800	-0.73000	-0.15700
H	-5.00900	-1.28200	0.52600
H	-4.63100	-0.91000	-1.21200
C	-4.33000	0.73000	0.14900
H	-5.00300	1.28200	-0.54100
H	-4.64400	0.91000	1.20000

MM3

S	3.21200	-1.90800	0.02700
S	3.21100	1.90900	-0.03000
O	-3.01800	-1.16100	0.02400
O	-3.01800	1.16100	-0.01700
C	-2.20500	0.00000	0.00300
C	-1.35900	0.02100	1.30700
H	-2.12300	0.03300	2.11800
C	-0.56200	-1.28200	1.57800
H	-0.25800	-1.28300	2.64900
H	-1.22500	-2.16400	1.45100
C	0.65500	-1.48200	0.71600
C	1.91500	-1.67900	1.25400
H	2.11200	-1.69200	2.31700
C	1.91200	-1.71800	-1.20300
H	2.10600	-1.76600	-2.26700

C	0.65300	-1.50400	-0.66900
C	-0.56600	-1.33300	-1.53500
H	-1.22900	-2.20900	-1.37800
H	-0.26400	-1.36700	-2.60500
C	-1.36100	-0.02100	-1.30300
H	-2.12600	-0.03300	-2.11300
C	-0.56500	1.28200	-1.57600
H	-0.26200	1.28200	-2.64700
H	-1.22800	2.16400	-1.44900
C	0.65300	1.48200	-0.71500
C	1.91200	1.67900	-1.25500
H	2.10700	1.69200	-2.31900
C	1.91300	1.71800	1.20200
H	2.10900	1.76500	2.26500
C	0.65400	1.50400	0.67000
C	-0.56400	1.33200	1.53700
H	-1.22700	2.20900	1.38200
H	-0.26000	1.36600	2.60700
C	-4.32800	-0.73000	-0.15700
H	-5.00900	-1.28200	0.52600
H	-4.63100	-0.91000	-1.21200
C	-4.33000	0.73000	0.14900
H	-5.00300	1.28200	-0.54100
H	-4.64400	0.91000	1.20000

AMBER94

S	1.60010	8.91980	8.82010
S	1.28860	5.84770	6.43330
O	-3.20090	6.17290	11.66160
O	-3.36750	4.35970	10.27690
C	-2.61810	5.56460	10.49840
C	-2.85420	6.51280	9.30240
H	-3.93660	6.64870	9.27040
C	-2.30640	7.9377	9.49760
H	-2.72610	8.56240	8.70880
H	-2.66640	8.33140	10.44820
C	-0.80350	8.09470	9.47430
C	-0.11710	8.96810	8.62870
H	-0.61100	9.61310	7.91770
C	1.44360	7.7178000	10.05240
H	2.29110	7.28800	10.56480
C	0.12290	7.35260	10.31920
C	-0.28390	6.31610	11.34100
H	-0.80060	6.83210	12.15030
H	0.62190	5.87890	11.76160
C	-1.16570	5.16120	10.83490
H	-1.25840	4.49930	11.69750
C	-0.48080	4.28830	9.76840
H	0.43030	3.88380	10.21000
H	-1.12710	3.44370	9.52940
C	-0.11380	4.96860	8.46970
C	1.17040	4.97750	7.92220
H	2.01440	4.48920	8.38570

C	-0.39690	6.22490	6.50320
H	-0.89990	6.80880	5.74730
C	-1.04390	5.70900	7.62750
C	-2.51120	5.90640	7.93050
H	-3.00370	4.93870	7.83430
H	-2.93140	6.56120	7.16680
C	-4.02400	5.20780	12.27130
H	-4.83470	5.66330	12.84020
H	-3.42690	4.55590	12.91020
C	-4.52870	4.43700	11.06820
H	-4.90550	3.45020	11.33780
H	-5.29730	5.01210	10.55030

OPLS_2001

S	1.61420	9.01900	8.89870
S	1.28130	5.75060	6.35520
O	-3.19050	6.17040	11.63910
O	-3.35370	4.37870	10.27380
C	-2.64340	5.55510	10.51310
C	-2.83240	6.50770	9.30720
H	-3.91230	6.65210	9.26420
C	-2.29370	7.94230	9.52630
H	-2.71250	8.59240	8.75800
H	-2.66930	8.33540	10.47120
C	-0.78730	8.12720	9.53100
C	-0.12710	9.03880	8.69440
H	-0.57610	9.70110	7.96940
C	1.44080	7.77820	10.12540
H	2.31730	7.37450	10.60980
C	0.10600	7.40900	10.34620
C	-0.30180	6.33980	11.34290
H	-0.81750	6.84200	12.16160
H	0.60410	5.92480	11.78480
C	-1.17290	5.17500	10.81450
H	-1.25290	4.51160	11.67610
C	-0.50390	4.28040	9.74280
H	0.40230	3.84780	10.16700
H	-1.14970	3.43140	9.51800
C	-0.14200	4.93100	8.42040
C	1.15130	4.89330	7.87910
H	2.02280	4.42010	8.30620
C	-0.42280	6.15140	6.45280
H	-0.88190	6.74220	5.67430
C	-1.03880	5.64770	7.60770
C	-2.50300	5.87950	7.93180
H	-3.01060	4.91960	7.83540
H	-2.92770	6.50960	7.15020
C	-4.02090	5.21960	12.26720
H	-4.82370	5.68470	12.83960
H	-3.42800	4.59170	12.93380
C	-4.51660	4.42770	11.07000
H	-4.88220	3.43450	11.33090
H	-5.30400	4.96810	10.54270

MMFFs

S	1.54450	9.05400	9.00570
S	1.19620	5.64860	6.35380
O	-3.17190	6.20640	11.65750
O	-3.34130	4.35040	10.24100
C	-2.59840	5.57330	10.48410
C	-2.82560	6.52240	9.29070
H	-3.91890	6.66280	9.25540
C	-2.29750	7.95230	9.50120
H	-2.71080	8.58290	8.70140
H	-2.70670	8.36710	10.43170
C	-0.81000	8.13250	9.53420
C	-0.14100	9.06190	8.75660
H	-0.56740	9.75140	8.04110
C	1.40990	7.81460	10.16700
H	2.30260	7.44310	10.65100
C	0.10570	7.39600	10.36690
C	-0.27220	6.32270	11.34210
H	-0.76710	6.80310	12.19610
H	0.64650	5.88230	11.75460
C	-1.14620	5.17300	10.81190
H	-1.23570	4.50270	11.68310
C	-0.47430	4.28060	9.75350
H	0.45000	3.87900	10.19220
H	-1.10130	3.40160	9.55530
C	-0.14430	4.91470	8.43620
C	1.11000	4.84700	7.85470
H	1.99300	4.362100	8.24760
C	-0.44620	6.09190	6.44810
H	-0.88680	6.66600	5.64470
C	-1.06320	5.64980	7.60570
C	-2.50620	5.90740	7.91730
H	-3.05040	4.96150	7.79740
H	-2.91910	6.57440	7.14740
C	-4.02360	5.22700	12.24820
H	-4.83340	5.70410	12.80530
H	-3.42280	4.61920	12.93300
C	-4.49900	4.42980	11.06980
H	-4.85370	3.43100	11.33550
H	-5.282500	4.95570	10.51410

Potential energy surface scans

***r*(S-S) = 3.70 Å**

ONIOM(QM/MM) structure

S	-3.17000	-1.89000	-0.04000
O	2.92000	-1.20000	-0.03000
O	3.11000	1.08000	0.07000
C	2.14000	0.02000	0.02000
C	1.36000	0.07000	-1.31000
H	2.15000	0.04000	-2.07000

C	0.50000	-1.19000	-1.60000
H	0.17000	-1.14000	-2.65000
H	1.17000	-2.04000	-1.54000
C	-0.72000	-1.45000	-0.75000
C	-1.96000	-1.66000	-1.27000
H	-2.24000	-1.68000	-2.31000
C	-1.97000	-1.70000	1.20000
H	-2.26000	-1.75000	2.24000
C	-0.72000	-1.47000	0.70000
C	0.48000	-1.24000	1.57000
H	1.16000	-2.09000	1.48000
H	0.15000	-1.23000	2.61000
C	1.35000	0.03000	1.34000
H	2.14000	-0.02000	2.10000
C	0.60980	1.37070	1.59140
C	0.62260	1.41960	-1.51870
C	4.28000	-0.88000	0.23000
H	4.91000	-1.59000	-0.31000
H	4.51000	-0.94000	1.30000
C	4.38000	0.54000	-0.28000
H	5.15000	1.14000	0.21000
H	4.54000	0.57000	-1.37000
S	-3.18000	1.81000	0.02000
H	0.32000	1.39000	2.66000
H	1.30000	2.21000	1.43000
C	-0.60000	1.55000	0.72000
C	-1.87000	1.68000	1.26000
H	-2.08000	1.67000	2.32000
C	-1.86000	1.72000	-1.20000
H	-2.05000	1.74000	-2.27000
C	-0.60000	1.57000	-0.66000
H	1.32000	2.25000	-1.32000
H	0.35000	1.48000	-2.59000

QM part

S	-3.17000	-1.89000	-0.04000
O	2.92000	-1.20000	-0.03000
O	3.11000	1.08000	0.07000
C	2.14000	0.02000	0.02000
C	1.36000	0.07000	-1.31000
H	2.15000	0.04000	-2.07000
C	0.50000	-1.19000	-1.60000
H	0.17000	-1.14000	-2.65000
H	1.17000	-2.04000	-1.54000
C	-0.72000	-1.45000	-0.75000
C	-1.96000	-1.66000	-1.27000
H	-2.24000	-1.68000	-2.31000
C	-1.97000	-1.70000	1.20000
H	-2.26000	-1.75000	2.24000
C	-0.72000	-1.47000	0.70000
C	0.48000	-1.24000	1.57000
H	1.16000	-2.09000	1.48000
H	0.15000	-1.23000	2.61000

C	1.35000	0.03000	1.34000
H	2.14000	-0.02000	2.10000
H	0.82000	0.99000	1.52000
H	0.83000	1.04000	-1.46000
C	4.28000	-0.88000	0.23000
H	4.91000	-1.59000	-0.31000
H	4.51000	-0.94000	1.30000
C	4.38000	0.54000	-0.28000
H	5.15000	1.14000	0.21000
H	4.54000	0.57000	-1.37000

***r*(S-S) = 3.75 Å**
ONIOM(QM/MM) structure

S	-3.16600	-1.91400	-0.04300
S	-3.17500	1.83600	0.02000
O	2.91600	-1.20400	-0.02600
O	3.11000	1.07700	0.06600
C	2.14000	0.01800	0.01600
C	1.36000	0.07200	-1.31300
H	2.15200	0.04300	-2.06900
C	0.49300	-1.18400	-1.60500
H	0.16800	-1.13600	-2.64700
H	1.17000	-2.04100	-1.54100
C	-0.71700	-1.45200	-0.74500
C	-1.95800	-1.67400	-1.26800
H	-2.23900	-1.69600	-2.30900
C	-1.97000	-1.71000	1.20000
H	-2.26000	-1.76100	2.23800
C	-0.72400	-1.47200	0.69600
C	0.47700	-1.23200	1.57600
H	1.15500	-2.08600	1.48800
H	0.14200	-1.22000	2.61500
C	1.34800	0.03400	1.33900
H	2.13400	-0.01800	2.10100
C	0.61500	1.35900	1.58700
H	0.32000	1.39700	2.65900
H	1.30300	2.21600	1.42600
C	-0.60400	1.55200	0.72300
C	-1.87300	1.69300	1.25500
H	-2.07600	1.68400	2.31700
C	-1.86000	1.73000	-1.20500
H	-2.05200	1.75300	-2.26900
C	-0.59700	1.57300	-0.66400
C	0.63100	1.40600	-1.52100
H	1.32000	2.25500	-1.32300
H	0.34800	1.48200	-2.59400
C	4.28100	-0.88400	0.23000
H	4.90700	-1.59700	-0.30800
H	4.50500	-0.94300	1.30100
C	4.38300	0.54200	-0.28100
H	5.14900	1.14000	0.21100
H	4.54200	0.57000	-1.36600

QM part

S	-3.16563	-1.91355	-0.04272
O	2.91644	-1.20440	-0.02564
O	3.11027	1.07721	0.06615
C	2.13985	0.01760	0.01619
C	1.35960	0.07239	-1.31280
H	2.15182	0.04299	-2.06922
C	0.49307	-1.18420	-1.60500
H	0.16794	-1.13625	-2.64690
H	1.17032	-2.04090	-1.54086
C	-0.71688	-1.45175	-0.74538
C	-1.95835	-1.67447	-1.26765
H	-2.23856	-1.69551	-2.30918
C	-1.97038	-1.70992	1.20002
H	-2.26050	-1.76118	2.23777
C	-0.72403	-1.47211	0.69639
C	0.47727	-1.23200	1.57570
H	1.15485	-2.08638	1.48751
H	0.14231	-1.22036	2.61548
C	1.34803	0.03361	1.33916
H	2.13387	-0.01840	2.10053
H	0.81755	0.99271	1.51837
H	0.83237	1.03775	-1.46362
C	4.28108	-0.88446	0.22954
H	4.90702	-1.59659	-0.30803
H	4.50463	-0.94283	1.30116
C	4.38290	0.54196	-0.28143
H	5.14939	1.13967	0.21075
H	4.54187	0.57037	-1.36576

***r*(S-S) = 3.80 Å**
ONIOM(QM/MM) structure

S	-3.16200	-1.93900	-0.04200
S	-3.17300	1.86000	0.01900
O	2.91300	-1.20500	-0.02500
O	3.11000	1.07600	0.06500
C	2.13800	0.01800	0.01600
C	1.35800	0.07300	-1.31300
H	2.15100	0.04300	-2.06900
C	0.49100	-1.18300	-1.60500
H	0.16400	-1.13400	-2.64700
H	1.16800	-2.04000	-1.54300
C	-0.71800	-1.45300	-0.74500
C	-1.95700	-1.68700	-1.26700
H	-2.23700	-1.71300	-2.30800
C	-1.96900	-1.72100	1.20100
H	-2.25900	-1.77600	2.23800
C	-0.72500	-1.47300	0.69700
C	0.47500	-1.22900	1.57700
H	1.15300	-2.08400	1.49300
H	0.13800	-1.21500	2.61700
C	1.34700	0.03600	1.33900
H	2.13300	-0.01600	2.10000

C	0.61500	1.36100	1.58600
H	0.32000	1.40000	2.65800
H	1.30400	2.21800	1.42500
C	-0.60400	1.55600	0.72200
C	-1.87200	1.70500	1.25400
H	-2.07500	1.69900	2.31700
C	-1.85900	1.74000	-1.20500
H	-2.05100	1.76500	-2.27000
C	-0.59700	1.57600	-0.66500
C	0.63100	1.40700	-1.52200
H	1.32100	2.25500	-1.32500
H	0.34800	1.48300	-2.59500
C	4.27800	-0.88700	0.23000
H	4.90300	-1.60000	-0.30700
H	4.50200	-0.94500	1.30200
C	4.38200	0.53900	-0.28200
H	5.14900	1.13600	0.21100
H	4.54100	0.56700	-1.36600

QM part

S	-3.16186	-1.93928	-0.04209
O	2.91339	-1.20522	-0.02494
O	3.11002	1.07617	0.06546
C	2.13831	0.01779	0.01617
C	1.35818	0.07276	-1.31289
H	2.15052	0.04257	-2.06916
C	0.49096	-1.18289	-1.60522
H	0.16432	-1.13372	-2.64661
H	1.16820	-2.03981	-1.54327
C	-0.71767	-1.45342	-0.74457
C	-1.95709	-1.68748	-1.26687
H	-2.23666	-1.71288	-2.30848
C	-1.96924	-1.72135	1.20070
H	-2.25883	-1.77565	2.23846
C	-0.72489	-1.47286	0.69717
C	0.47504	-1.22875	1.57739
H	1.15252	-2.08360	1.49253
H	0.13847	-1.21454	2.61665
C	1.34660	0.03556	1.33918
H	2.13256	-0.01637	2.10044
H	0.81706	0.99516	1.51780
H	0.83179	1.03836	-1.46427
C	4.27839	-0.88693	0.22998
H	4.90344	-1.59996	-0.30745
H	4.50207	-0.94525	1.30158
C	4.38208	0.53922	-0.28153
H	5.14918	1.13612	0.21067
H	4.54144	0.56703	-1.36582

***r*(S-S) = 3.85 Å**
ONIOM(QM/MM) structure

S	-3.15800	-1.96500	-0.04100
S	-3.17000	1.88400	0.01900

O	2.91000	-1.20600	-0.02500
O	3.11000	1.07500	0.06500
C	2.13700	0.01800	0.01600
C	1.35700	0.07300	-1.31300
H	2.14900	0.04200	-2.06900
C	0.48900	-1.18100	-1.60600
H	0.16000	-1.13000	-2.64700
H	1.16600	-2.03800	-1.54600
C	-0.71900	-1.45500	-0.74400
C	-1.95600	-1.70100	-1.26600
H	-2.23500	-1.73000	-2.30800
C	-1.96800	-1.73300	1.20100
H	-2.25700	-1.79000	2.23900
C	-0.72600	-1.47400	0.69800
C	0.47300	-1.22500	1.57900
H	1.15000	-2.08100	1.49800
H	0.13500	-1.20800	2.61800
C	1.34500	0.03700	1.33900
H	2.13100	-0.01500	2.10000
C	0.61500	1.36400	1.58500
H	0.32000	1.40400	2.65700
H	1.30500	2.22000	1.42400
C	-0.60300	1.55900	0.72100
C	-1.87000	1.71600	1.25300
H	-2.07300	1.71400	2.31600
C	-1.85800	1.75100	-1.20600
H	-2.05000	1.77800	-2.27100
C	-0.59600	1.57900	-0.66600
C	0.63100	1.40800	-1.52300
H	1.32100	2.25500	-1.32600
H	0.34700	1.48300	-2.59600
C	4.27500	-0.89000	0.23100
H	4.90000	-1.60400	-0.30500
H	4.49800	-0.94700	1.30300
C	4.38100	0.53600	-0.28200
H	5.14900	1.13200	0.21000
H	4.54100	0.56300	-1.36600

QM part

S	-3.15795	-1.96522	-0.04145
O	2.90999	-1.20617	-0.02462
O	3.10980	1.07507	0.06469
C	2.13661	0.01784	0.01597
C	1.35666	0.07329	-1.31309
H	2.14914	0.04233	-2.06920
C	0.48853	-1.18129	-1.60579
H	0.16026	-1.13049	-2.64660
H	1.16572	-2.03847	-1.54649
C	-0.71858	-1.45487	-0.74394
C	-1.95575	-1.70054	-1.26611
H	-2.23468	-1.73016	-2.30777
C	-1.96788	-1.73305	1.20128
H	-2.25680	-1.79046	2.23904

C	-0.72578	-1.47354	0.69786
C	0.47267	-1.22549	1.57906
H	1.15000	-2.08085	1.49780
H	0.13450	-1.20847	2.61776
C	1.34522	0.03745	1.33906
H	2.13138	-0.01451	2.10013
H	0.81669	0.99755	1.51719
H	0.83122	1.03921	-1.46488
C	4.27538	-0.88954	0.23097
H	4.89969	-1.60397	-0.30543
H	4.49816	-0.94725	1.30277
C	4.38117	0.53600	-0.28165
H	5.14905	1.13225	0.21011
H	4.54070	0.56263	-1.36595

***r*(S-S) = 3.90 Å**
ONIOM(QM/MM) structure

S	-3.15400	-1.99100	-0.04100
S	-3.16800	1.90800	0.01800
O	2.90700	-1.20700	-0.02400
O	3.10900	1.07400	0.06400
C	2.13500	0.01800	0.01600
C	1.35500	0.07400	-1.31300
H	2.14800	0.04200	-2.06900
C	0.48600	-1.18000	-1.60600
H	0.15700	-1.12800	-2.64600
H	1.16400	-2.03700	-1.54900
C	-0.71900	-1.45700	-0.74300
C	-1.95400	-1.71400	-1.26500
H	-2.23200	-1.74800	-2.30700
C	-1.96700	-1.74500	1.20200
H	-2.25500	-1.80500	2.24000
C	-0.72700	-1.47400	0.69900
C	0.47000	-1.22200	1.58100
H	1.14800	-2.07800	1.50300
H	0.13000	-1.20300	2.61900
C	1.34400	0.03900	1.33900
H	2.13000	-0.01300	2.10000
C	0.61500	1.36600	1.58500
H	0.32000	1.40700	2.65600
H	1.30500	2.22100	1.42200
C	-0.60300	1.56300	0.72000
C	-1.86900	1.72800	1.25200
H	-2.07200	1.73000	2.31500
C	-1.85700	1.76100	-1.20700
H	-2.04900	1.79100	-2.27100
C	-0.59600	1.58200	-0.66600
C	0.63100	1.40900	-1.52300
H	1.32200	2.25600	-1.32700
H	0.34700	1.48400	-2.59700
C	4.27300	-0.89200	0.23100
H	4.89600	-1.60700	-0.30500
H	4.49600	-0.95000	1.30300

C	4.38000	0.53300	-0.28200
H	5.14900	1.12900	0.20900
H	4.53900	0.55900	-1.36600

QM part

S	-3.15376	-1.99113	-0.04097
O	2.90668	-1.20703	-0.02383
O	3.10943	1.07401	0.06433
C	2.13489	0.01802	0.01610
C	1.35517	0.07381	-1.31304
H	2.14782	0.04210	-2.06896
C	0.48632	-1.17977	-1.60611
H	0.15652	-1.12752	-2.64639
H	1.16353	-2.03715	-1.54924
C	-0.71940	-1.45654	-0.74324
C	-1.95422	-1.71377	-1.26544
H	-2.23239	-1.74766	-2.30718
C	-1.96656	-1.74492	1.20181
H	-2.25490	-1.80546	2.23956
C	-0.72672	-1.47443	0.69857
C	0.47022	-1.22231	1.58078
H	1.14750	-2.07807	1.50300
H	0.13037	-1.20267	2.61890
C	1.34360	0.03935	1.33918
H	2.12986	-0.01263	2.10015
H	0.81602	0.99994	1.51678
H	0.83065	1.04003	-1.46532
C	4.27254	-0.89204	0.23119
H	4.89579	-1.60747	-0.30512
H	4.49559	-0.94962	1.30294
C	4.38002	0.53317	-0.28204
H	5.14876	1.12865	0.20934
H	4.53941	0.55917	-1.36638

***r*(S-S) = 3.95 Å**
ONIOM(QM/MM) structure

S	-3.14900	-2.01700	-0.04000
S	-3.16500	1.93300	0.01800
O	2.90300	-1.20800	-0.02300
O	3.10900	1.07300	0.06400
C	2.13300	0.01800	0.01600
C	1.35400	0.07400	-1.31300
H	2.14600	0.04200	-2.06900
C	0.48400	-1.17800	-1.60700
H	0.15300	-1.12500	-2.64600
H	1.16100	-2.03600	-1.55200
C	-0.72000	-1.45800	-0.74300
C	-1.95300	-1.72700	-1.26500
H	-2.23000	-1.76500	-2.30700
C	-1.96500	-1.75700	1.20200
H	-2.25300	-1.82100	2.24000
C	-0.72800	-1.47600	0.69900
C	0.46800	-1.21900	1.58200

H	1.14500	-2.07500	1.50800
H	0.12600	-1.19700	2.62000
C	1.34200	0.04100	1.33900
H	2.12800	-0.01100	2.10000
C	0.61500	1.36900	1.58400
H	0.32000	1.41100	2.65600
H	1.30600	2.22300	1.42100
C	-0.60300	1.56700	0.71900
C	-1.86800	1.74000	1.25200
H	-2.07000	1.74500	2.31500
C	-1.85600	1.77200	-1.20700
H	-2.04700	1.80400	-2.27200
C	-0.59600	1.58400	-0.66700
C	0.63000	1.40900	-1.52400
H	1.32300	2.25600	-1.32800
H	0.34700	1.48500	-2.59700
C	4.27000	-0.89400	0.23200
H	4.89200	-1.61100	-0.30400
H	4.49300	-0.95200	1.30400
C	4.37900	0.53100	-0.28200
H	5.14800	1.12500	0.21000
H	4.53900	0.55600	-1.36600

QM part

S	-3.14940	-2.01692	-0.04037
O	2.90347	-1.20781	-0.02338
O	3.10883	1.07304	0.06365
C	2.13310	0.01818	0.01599
C	1.35350	0.07427	-1.31317
H	2.14627	0.04181	-2.06895
C	0.48396	-1.17836	-1.60653
H	0.15257	-1.12471	-2.64624
H	1.16123	-2.03589	-1.55207
C	-0.72032	-1.45837	-0.74258
C	-1.95274	-1.72714	-1.26474
H	-2.23019	-1.76531	-2.30653
C	-1.96513	-1.75696	1.20237
H	-2.25278	-1.82069	2.24013
C	-0.72766	-1.47550	0.69919
C	0.46784	-1.21929	1.58231
H	1.14510	-2.07542	1.50787
H	0.12637	-1.19713	2.61987
C	1.34198	0.04112	1.33912
H	2.12840	-0.01089	2.09995
H	0.81540	1.00219	1.51626
H	0.82990	1.04077	-1.46590
C	4.26959	-0.89437	0.23172
H	4.89211	-1.61064	-0.30432
H	4.49253	-0.95191	1.30351
C	4.37891	0.53059	-0.28198
H	5.14815	1.12530	0.20955
H	4.53882	0.55604	-1.36625

***r*(S-S) = 4.00 Å**

ONIOM(QM/MM) structure

S	-3.14500	-2.04300	-0.04000
S	-3.16200	1.95700	0.01700
O	2.90000	-1.20900	-0.02300
O	3.10800	1.07200	0.06300
C	2.13100	0.01800	0.01600
C	1.35200	0.07500	-1.31300
H	2.14500	0.04200	-2.06900
C	0.48200	-1.17700	-1.60700
H	0.14900	-1.12100	-2.64600
H	1.15900	-2.03400	-1.55500
C	-0.72100	-1.46000	-0.74200
C	-1.95100	-1.74100	-1.26400
H	-2.22800	-1.78300	-2.30600
C	-1.96400	-1.76900	1.20300
H	-2.25100	-1.83600	2.24100
C	-0.72900	-1.47700	0.70000
C	0.46500	-1.21600	1.58400
H	1.14300	-2.07300	1.51300
H	0.12200	-1.19100	2.62100
C	1.34000	0.04300	1.33900
H	2.12700	-0.00900	2.10000
C	0.61400	1.37100	1.58300
H	0.31900	1.41400	2.65500
H	1.30700	2.22500	1.42000
C	-0.60300	1.57100	0.71900
C	-1.86700	1.75200	1.25100
H	-2.06900	1.76000	2.31400
C	-1.85500	1.78200	-1.20800
H	-2.04600	1.81700	-2.27300
C	-0.59600	1.58800	-0.66800
C	0.63000	1.41100	-1.52500
H	1.32300	2.25600	-1.32900
H	0.34700	1.48600	-2.59800
C	4.26700	-0.89700	0.23200
H	4.88800	-1.61400	-0.30400
H	4.49000	-0.95500	1.30300
C	4.37800	0.52800	-0.28200
H	5.14800	1.12200	0.20900
H	4.53700	0.55300	-1.36700

QM part

S	-3.14462	-2.04301	-0.03996
O	2.89993	-1.20858	-0.02261
O	3.10831	1.07202	0.06337
C	2.13120	0.01850	0.01616
C	1.35184	0.07501	-1.31311
H	2.14483	0.04188	-2.06865
C	0.48171	-1.17668	-1.60697
H	0.14865	-1.12144	-2.64606
H	1.15912	-2.03428	-1.55514
C	-0.72107	-1.46026	-0.74193

C	-1.95093	-1.74063	-1.26411
H	-2.22755	-1.78288	-2.30595
C	-1.96354	-1.76925	1.20280
H	-2.25057	-1.83606	2.24053
C	-0.72853	-1.47670	0.69980
C	0.46532	-1.21614	1.58404
H	1.14266	-2.07253	1.51321
H	0.12200	-1.19135	2.62093
C	1.34017	0.04308	1.33928
H	2.12671	-0.00893	2.09999
H	0.81452	1.00464	1.51594
H	0.82917	1.04183	-1.46627
C	4.26655	-0.89691	0.23176
H	4.88793	-1.61407	-0.30443
H	4.48996	-0.95457	1.30346
C	4.37763	0.52783	-0.28230
H	5.14772	1.12162	0.20900
H	4.53746	0.55284	-1.36659

r(S-S) = 4.05 Å
ONIOM(QM/MM) structure

S	-3.14000	-2.06900	-0.04000
S	-3.15900	1.98000	0.01700
O	2.89600	-1.20900	-0.02200
O	3.10800	1.07100	0.06300
C	2.12900	0.01900	0.01600
C	1.35000	0.07600	-1.31300
H	2.14300	0.04200	-2.06800
C	0.47900	-1.17500	-1.60800
H	0.14400	-1.11800	-2.64600
H	1.15700	-2.03300	-1.55900
C	-0.72200	-1.46200	-0.74100
C	-1.94900	-1.75400	-1.26400
H	-2.22500	-1.80000	-2.30500
C	-1.96200	-1.78200	1.20300
H	-2.24800	-1.85200	2.24100
C	-0.73000	-1.47800	0.70000
C	0.46300	-1.21300	1.58600
H	1.14000	-2.07000	1.51900
H	0.11800	-1.18500	2.62200
C	1.33800	0.04500	1.33900
H	2.12500	-0.00700	2.10000
C	0.61400	1.37400	1.58300
H	0.31900	1.41800	2.65500
H	1.30700	2.22600	1.42000
C	-0.60400	1.57500	0.71800
C	-1.86600	1.76400	1.25000
H	-2.06700	1.77600	2.31300
C	-1.85400	1.79400	-1.20900
H	-2.04400	1.83100	-2.27300
C	-0.59700	1.59100	-0.66800
C	0.62900	1.41200	-1.52500
H	1.32400	2.25700	-1.33000

H	0.34600	1.48700	-2.59800
C	4.26300	-0.89900	0.23200
H	4.88400	-1.61800	-0.30300
H	4.48600	-0.95700	1.30400
C	4.37600	0.52500	-0.28300
H	5.14700	1.11800	0.20800
H	4.53600	0.54900	-1.36700

QM part

S	-3.13981	-2.06914	-0.03951
O	2.89622	-1.20946	-0.02210
O	3.10784	1.07096	0.06300
C	2.12921	0.01866	0.01619
C	1.35012	0.07577	-1.31312
H	2.14324	0.04192	-2.06849
C	0.47913	-1.17488	-1.60759
H	0.14441	-1.11780	-2.64608
H	1.15662	-2.03263	-1.55867
C	-0.72199	-1.46201	-0.74142
C	-1.94911	-1.75418	-1.26353
H	-2.22486	-1.80048	-2.30545
C	-1.96185	-1.78166	1.20325
H	-2.24811	-1.85160	2.24100
C	-0.72952	-1.47781	0.70042
C	0.46261	-1.21297	1.58574
H	1.13995	-2.06971	1.51868
H	0.11755	-1.18537	2.62201
C	1.33839	0.04497	1.33931
H	2.12505	-0.00715	2.09989
H	0.81376	1.00703	1.51556
H	0.82844	1.04294	-1.46667
C	4.26333	-0.89946	0.23231
H	4.88372	-1.61794	-0.30325
H	4.48635	-0.95666	1.30409
C	4.37629	0.52473	-0.28269
H	5.14735	1.11781	0.20795
H	4.53581	0.54876	-1.36705

***r*(S-S) = 4.10 Å**
ONIOM(QM/MM) structure

S	-3.13500	-2.09500	-0.03900
S	-3.15600	2.00400	0.01600
O	2.89300	-1.21000	-0.02100
O	3.10700	1.07000	0.06300
C	2.12700	0.01900	0.01600
C	1.34800	0.07600	-1.31300
H	2.14200	0.04200	-2.06800
C	0.47700	-1.17300	-1.60800
H	0.14000	-1.11500	-2.64600
H	1.15400	-2.03100	-1.56200
C	-0.72300	-1.46400	-0.74100
C	-1.94700	-1.76800	-1.26300
H	-2.22200	-1.81800	-2.30500

C	-1.96000	-1.79400	1.20400
H	-2.24600	-1.86700	2.24100
C	-0.73100	-1.47900	0.70100
C	0.46000	-1.21000	1.58700
H	1.13700	-2.06700	1.52400
H	0.11300	-1.18000	2.62300
C	1.33600	0.04700	1.33900
H	2.12300	-0.00500	2.10000
C	0.61300	1.37600	1.58200
H	0.31800	1.42100	2.65400
H	1.30800	2.22800	1.41900
C	-0.60400	1.57900	0.71800
C	-1.86500	1.77600	1.25000
H	-2.06600	1.79100	2.31300
C	-1.85200	1.80400	-1.20900
H	-2.04300	1.84400	-2.27400
C	-0.59700	1.59400	-0.66900
C	0.62900	1.41300	-1.52600
H	1.32500	2.25700	-1.33100
H	0.34600	1.48800	-2.59900
C	4.26000	-0.90200	0.23200
H	4.88000	-1.62100	-0.30400
H	4.48400	-0.95900	1.30400
C	4.37500	0.52200	-0.28300
H	5.14700	1.11500	0.20700
H	4.53400	0.54600	-1.36800

QM part

S	-3.13472	-2.09510	-0.03915
O	2.89271	-1.21020	-0.02128
O	3.10703	1.07003	0.06287
C	2.12719	0.01890	0.01642
C	1.34836	0.07642	-1.31298
H	2.14167	0.04188	-2.06814
C	0.47675	-1.17328	-1.60801
H	0.14041	-1.11457	-2.64590
H	1.15440	-2.03110	-1.56176
C	-0.72284	-1.46405	-0.74082
C	-1.94716	-1.76785	-1.26297
H	-2.22198	-1.81822	-2.30495
C	-1.96018	-1.79419	1.20365
H	-2.24574	-1.86725	2.24138
C	-0.73052	-1.47919	0.70100
C	0.45991	-1.20998	1.58742
H	1.13734	-2.06697	1.52397
H	0.11301	-1.17978	2.62302
C	1.33642	0.04677	1.33948
H	2.12317	-0.00541	2.09998
H	0.81279	1.00932	1.51527
H	0.82766	1.04392	-1.46698
C	4.26029	-0.90173	0.23226
H	4.87958	-1.62102	-0.30351
H	4.48389	-0.95898	1.30392

C	4.37472	0.52225	-0.28312
H	5.14662	1.11454	0.20715
H	4.53394	0.54587	-1.36753

_r_(S-S) = 4.15 Å
ONIOM(QM/MM) structure

S	-3.12900	-2.12100	-0.03900
S	-3.15300	2.02800	0.01600
O	2.88900	-1.21100	-0.02100
O	3.10600	1.06900	0.06200
C	2.12500	0.01900	0.01600
C	1.34600	0.07700	-1.31300
H	2.14000	0.04200	-2.06800
C	0.47400	-1.17100	-1.60900
H	0.13600	-1.11100	-2.64600
H	1.15200	-2.02900	-1.56500
C	-0.72400	-1.46600	-0.74000
C	-1.94500	-1.78200	-1.26200
H	-2.21900	-1.83600	-2.30400
C	-1.95800	-1.80700	1.20400
H	-2.24300	-1.88300	2.24200
C	-0.73100	-1.48100	0.70100
C	0.45700	-1.20700	1.58900
H	1.13500	-2.06400	1.52900
H	0.10900	-1.17400	2.62400
C	1.33400	0.04900	1.33900
H	2.12100	-0.00300	2.10000
C	0.61200	1.37900	1.58200
H	0.31800	1.42400	2.65400
H	1.30800	2.22900	1.41800
C	-0.60400	1.58300	0.71700
C	-1.86400	1.78900	1.24900
H	-2.06400	1.80700	2.31200
C	-1.85200	1.81600	-1.21000
H	-2.04100	1.85800	-2.27400
C	-0.59700	1.59800	-0.66900
C	0.62800	1.41400	-1.52600
H	1.32500	2.25800	-1.33200
H	0.34600	1.48900	-2.60000
C	4.25700	-0.90400	0.23300
H	4.87500	-1.62400	-0.30300
H	4.48000	-0.96100	1.30500
C	4.37300	0.51900	-0.28300
H	5.14600	1.11100	0.20700
H	4.53300	0.54200	-1.36800

QM part

S	-3.12922	-2.12140	-0.03867
O	2.88891	-1.21082	-0.02095
O	3.10632	1.06916	0.06236
C	2.12504	0.01931	0.01634
C	1.34638	0.07738	-1.31307
H	2.13986	0.04224	-2.06804

C	0.47424	-1.17146	-1.60871
H	0.13609	-1.11098	-2.64593
H	1.15216	-2.02925	-1.56540
C	-0.72362	-1.46618	-0.74032
C	-1.94504	-1.78175	-1.26239
H	-2.21896	-1.83605	-2.30440
C	-1.95809	-1.80709	1.20405
H	-2.24279	-1.88326	2.24179
C	-0.73132	-1.48076	0.70149
C	0.45738	-1.20694	1.58899
H	1.13500	-2.06407	1.52920
H	0.10865	-1.17411	2.62390
C	1.33447	0.04872	1.33944
H	2.12140	-0.00349	2.09977
H	0.81178	1.01175	1.51489
H	0.82660	1.04520	-1.46743
C	4.25685	-0.90413	0.23278
H	4.87527	-1.62446	-0.30257
H	4.48015	-0.96129	1.30452
C	4.37332	0.51949	-0.28312
H	5.14595	1.11091	0.20706
H	4.53281	0.54244	-1.36752

***r*(S-S) = 4.20 Å**
ONIOM(QM/MM) structure

S	3.12300	2.14800	-0.03800
S	3.15000	-2.05200	0.01500
O	-2.88500	1.21100	-0.02000
O	-3.10600	-1.06800	0.06200
C	-2.12300	-0.02000	0.01600
C	-1.34400	-0.07800	-1.31300
H	-2.13800	-0.04300	-2.06800
C	-0.47200	1.17000	-1.60900
H	-0.13200	1.10700	-2.64600
H	-1.15000	2.02700	-1.56900
C	0.72400	1.46800	-0.74000
C	1.94300	1.79600	-1.26200
H	2.21600	1.85400	-2.30400
C	1.95600	1.82000	1.20400
H	2.24000	1.90000	2.24200
C	0.73200	1.48200	0.70200
C	-0.45500	1.20400	1.59100
H	-1.13300	2.06100	1.53500
H	-0.10400	1.16800	2.62500
C	-1.33200	-0.05100	1.34000
H	-2.12000	0.00200	2.10000
C	-0.61200	-1.38200	1.58100
H	-0.31700	-1.42800	2.65300
H	-1.30800	-2.23100	1.41700
C	0.60400	-1.58700	0.71600
C	1.86300	-1.80100	1.24900
H	2.06300	-1.82300	2.31200
C	1.85100	-1.82700	-1.21000

H	2.04000	-1.87200	-2.27500
C	0.59700	-1.60100	-0.67000
C	-0.62800	-1.41600	-1.52700
H	-1.32500	-2.25900	-1.33300
H	-0.34500	-1.49100	-2.60000
C	-4.25300	0.90700	0.23300
H	-4.87100	1.62800	-0.30200
H	-4.47700	0.96400	1.30500
C	-4.37200	-0.51700	-0.28300
H	-5.14500	-1.10700	0.20700
H	-4.53200	-0.53900	-1.36800

QM part

S	3.12344	2.14777	-0.03825
O	-2.88508	1.21142	-0.02044
O	-3.10550	-1.06830	0.06202
C	-2.12285	-0.01974	0.01639
C	-1.34441	-0.07837	-1.31311
H	-2.13811	-0.04267	-2.06786
C	-0.47172	1.16953	-1.60940
H	-0.13172	1.10731	-2.64591
H	-1.14986	2.02731	-1.56898
C	0.72444	1.46815	-0.73980
C	1.94278	1.79563	-1.26185
H	2.21562	1.85411	-2.30393
C	1.95595	1.82001	1.20442
H	2.23966	1.89957	2.24219
C	0.73220	1.48218	0.70195
C	-0.45473	1.20383	1.59062
H	-1.13250	2.06111	1.53450
H	-0.10405	1.16841	2.62480
C	-1.33244	-0.05069	1.33951
H	-2.11955	0.00153	2.09967
H	-0.81067	-1.01416	1.51458
H	-0.82552	-1.04651	-1.46779
C	-4.25343	0.90655	0.23298
H	-4.87085	1.62773	-0.30240
H	-4.47691	0.96389	1.30468
C	-4.37179	-0.51688	-0.28319
H	-5.14516	-1.10733	0.20700
H	-4.53151	-0.53945	-1.36756

***r*(S-S) = 4.25 Å**
ONIOM(QM/MM) structure

S	3.11800	2.17400	-0.03800
S	3.14700	-2.07600	0.01500
O	-2.88100	1.21200	-0.02000
O	-3.10400	-1.06700	0.06200
C	-2.12100	-0.02000	0.01600
C	-1.34200	-0.07900	-1.31300
H	-2.13600	-0.04300	-2.06800
C	-0.46900	1.16800	-1.61000
H	-0.12700	1.10400	-2.64600

H	-1.14700	2.02600	-1.57300
C	0.72500	1.47100	-0.73900
C	1.94100	1.81000	-1.26100
H	2.21300	1.87200	-2.30300
C	1.95400	1.83300	1.20500
H	2.23700	1.91600	2.24300
C	0.73300	1.48400	0.70200
C	-0.45200	1.20100	1.59200
H	-1.13000	2.05800	1.54000
H	-0.09900	1.16300	2.62600
C	-1.33000	-0.05200	1.33900
H	-2.11800	0.00000	2.10000
C	-0.61100	-1.38400	1.58100
H	-0.31600	-1.43100	2.65300
H	-1.30900	-2.23300	1.41700
C	0.60500	-1.59100	0.71600
C	1.86200	-1.81300	1.24800
H	2.06100	-1.83800	2.31100
C	1.84900	-1.83900	-1.21100
H	2.03800	-1.88600	-2.27500
C	0.59800	-1.60500	-0.67000
C	-0.62700	-1.41700	-1.52700
H	-1.32600	-2.25900	-1.33400
H	-0.34400	-1.49200	-2.60100
C	-4.25000	0.90900	0.23300
H	-4.86700	1.63100	-0.30200
H	-4.47300	0.96600	1.30500
C	-4.37000	-0.51400	-0.28300
H	-5.14400	-1.10400	0.20700
H	-4.53000	-0.53600	-1.36800

QM part

S	3.11769	2.17392	-0.03784
O	-2.88133	1.21204	-0.02007
O	-3.10447	-1.06745	0.06164
C	-2.12055	-0.02001	0.01638
C	-1.34230	-0.07919	-1.31312
H	-2.13614	-0.04286	-2.06770
C	-0.46902	1.16782	-1.61009
H	-0.12722	1.10369	-2.64592
H	-1.14746	2.02554	-1.57277
C	0.72533	1.47056	-0.73935
C	1.94057	1.80966	-1.26131
H	2.21251	1.87183	-2.30341
C	1.95385	1.83309	1.20476
H	2.23674	1.91557	2.24253
C	0.73314	1.48406	0.70243
C	-0.45193	1.20099	1.59216
H	-1.12993	2.05837	1.53983
H	-0.09941	1.16287	2.62564
C	-1.33031	-0.05245	1.33949
H	-2.11754	-0.00010	2.09953
H	-0.80958	-1.01643	1.51427

H	-0.82444	-1.04771	-1.46817
C	-4.25005	0.90868	0.23340
H	-4.86664	1.63083	-0.30163
H	-4.47331	0.96587	1.30515
C	-4.37013	-0.51438	-0.28330
H	-5.14418	-1.10411	0.20667
H	-4.52989	-0.53631	-1.36768

***r*(S-S) = 4.30 Å**
ONIOM(QM/MM) structure

S	3.11000	2.20000	-0.04000
O	-2.88000	1.21000	-0.02000
O	-3.10000	-1.07000	0.06000
C	-2.12000	-0.02000	0.02000
C	-1.34000	-0.08000	-1.31000
H	-2.13000	-0.04000	-2.07000
C	-0.47000	1.17000	-1.61000
H	-0.12000	1.10000	-2.65000
H	-1.15000	2.02000	-1.58000
C	0.73000	1.47000	-0.74000
C	1.94000	1.82000	-1.26000
H	2.21000	1.89000	-2.30000
C	1.95000	1.85000	1.21000
H	2.23000	1.93000	2.24000
C	0.73000	1.49000	0.70000
C	-0.45000	1.20000	1.59000
H	-1.13000	2.06000	1.55000
H	-0.09000	1.16000	2.63000
C	-1.33000	-0.05000	1.34000
H	-2.12000	0.00000	2.10000
C	-0.60620	-1.40010	1.57660
C	-0.61530	-1.43190	-1.53300
C	-4.25000	0.91000	0.23000
H	-4.86000	1.63000	-0.30000
H	-4.47000	0.97000	1.31000
C	-4.37000	-0.51000	-0.28000
H	-5.14000	-1.10000	0.21000
H	-4.53000	-0.53000	-1.37000
S	3.14000	-2.10000	0.01000
H	-0.32000	-1.43000	2.65000
H	-1.31000	-2.23000	1.42000
C	0.61000	-1.60000	0.72000
C	1.86000	-1.83000	1.25000
H	2.06000	-1.85000	2.31000
C	1.85000	-1.85000	-1.21000
H	2.04000	-1.90000	-2.28000
C	0.60000	-1.61000	-0.67000
H	-1.33000	-2.26000	-1.33000
H	-0.34000	-1.49000	-2.60000

QM part

S	3.11000	2.20000	-0.04000
O	-2.88000	1.21000	-0.02000

O	-3.10000	-1.07000	0.06000
C	-2.12000	-0.02000	0.02000
C	-1.34000	-0.08000	-1.31000
H	-2.13000	-0.04000	-2.07000
C	-0.47000	1.17000	-1.61000
H	-0.12000	1.10000	-2.65000
H	-1.15000	2.02000	-1.58000
C	0.73000	1.47000	-0.74000
C	1.94000	1.82000	-1.26000
H	2.21000	1.89000	-2.30000
C	1.95000	1.85000	1.21000
H	2.23000	1.93000	2.24000
C	0.73000	1.49000	0.70000
C	-0.45000	1.20000	1.59000
H	-1.13000	2.06000	1.55000
H	-0.09000	1.16000	2.63000
C	-1.33000	-0.05000	1.34000
H	-2.12000	0.00000	2.10000
H	-0.81000	-1.02000	1.51000
H	-0.82000	-1.05000	-1.47000
C	-4.25000	0.91000	0.23000
H	-4.86000	1.63000	-0.30000
H	-4.47000	0.97000	1.31000
C	-4.37000	-0.51000	-0.28000
H	-5.14000	-1.10000	0.21000
H	-4.53000	-0.53000	-1.37000

r(S-S) = 4.35 Å
ONIOM(QM/MM) structure

S	3.11000	2.23000	-0.04000
O	-2.87000	1.21000	-0.02000
O	-3.10000	-1.07000	0.06000
C	-2.12000	-0.02000	0.02000
C	-1.34000	-0.08000	-1.31000
H	-2.13000	-0.04000	-2.07000
C	-0.46000	1.16000	-1.61000
H	-0.12000	1.10000	-2.65000
H	-1.14000	2.02000	-1.58000
C	0.73000	1.48000	-0.74000
C	1.94000	1.84000	-1.26000
H	2.21000	1.91000	-2.30000
C	1.95000	1.86000	1.21000
H	2.23000	1.95000	2.24000
C	0.73000	1.49000	0.70000
C	-0.45000	1.20000	1.60000
H	-1.13000	2.05000	1.55000
H	-0.09000	1.15000	2.63000
C	-1.33000	-0.06000	1.34000
H	-2.11000	0.00000	2.10000
C	-0.60060	-1.40670	1.57850
C	-0.61530	-1.43190	-1.53300
C	-4.24000	0.91000	0.23000
H	-4.86000	1.64000	-0.30000

H	-4.47000	0.97000	1.31000
C	-4.37000	-0.51000	-0.28000
H	-5.14000	-1.10000	0.21000
H	-4.53000	-0.53000	-1.37000
S	3.14000	-2.12000	0.01000
H	-0.31000	-1.44000	2.65000
H	-1.31000	-2.24000	1.42000
C	0.61000	-1.60000	0.71000
C	1.86000	-1.84000	1.25000
H	2.06000	-1.87000	2.31000
C	1.85000	-1.86000	-1.21000
H	2.03000	-1.91000	-2.28000
C	0.60000	-1.61000	-0.67000
H	-1.33000	-2.26000	-1.34000
H	-0.34000	-1.49000	-2.60000

QM part

S	3.11000	2.23000	-0.04000
O	-2.87000	1.21000	-0.02000
O	-3.10000	-1.07000	0.06000
C	-2.12000	-0.02000	0.02000
C	-1.34000	-0.08000	-1.31000
H	-2.13000	-0.04000	-2.07000
C	-0.46000	1.16000	-1.61000
H	-0.12000	1.10000	-2.65000
H	-1.14000	2.02000	-1.58000
C	0.73000	1.48000	-0.74000
C	1.94000	1.84000	-1.26000
H	2.21000	1.91000	-2.30000
C	1.95000	1.86000	1.21000
H	2.23000	1.95000	2.24000
C	0.73000	1.49000	0.70000
C	-0.45000	1.20000	1.60000
H	-1.13000	2.05000	1.55000
H	-0.09000	1.15000	2.63000
C	-1.33000	-0.06000	1.34000
H	-2.11000	0.00000	2.10000
H	-0.81000	-1.02000	1.51000
H	-0.82000	-1.05000	-1.47000
C	-4.24000	0.91000	0.23000
H	-4.86000	1.64000	-0.30000
H	-4.47000	0.97000	1.31000
C	-4.37000	-0.51000	-0.28000
H	-5.14000	-1.10000	0.21000
H	-4.53000	-0.53000	-1.37000

***r*(S-S) = 4.40 Å**

ONIOM(QM/MM) structure

S	3.10000	2.25000	-0.04000
O	-2.87000	1.21000	-0.02000
O	-3.10000	-1.07000	0.06000
C	-2.11000	-0.02000	0.02000
C	-1.34000	-0.08000	-1.31000

H	-2.13000	-0.04000	-2.07000
C	-0.46000	1.16000	-1.61000
H	-0.11000	1.09000	-2.65000
H	-1.14000	2.02000	-1.58000
C	0.73000	1.48000	-0.74000
C	1.93000	1.85000	-1.26000
H	2.20000	1.93000	-2.30000
C	1.95000	1.87000	1.21000
H	2.23000	1.97000	2.24000
C	0.74000	1.49000	0.70000
C	-0.44000	1.19000	1.60000
H	-1.12000	2.05000	1.56000
H	-0.09000	1.15000	2.63000
C	-1.32000	-0.06000	1.34000
H	-2.11000	-0.01000	2.10000
C	-0.60150	-1.41240	1.57950
C	-0.61530	-1.43190	-1.53300
C	-4.24000	0.91000	0.23000
H	-4.85000	1.64000	-0.30000
H	-4.46000	0.97000	1.31000
C	-4.36000	-0.51000	-0.28000
H	-5.14000	-1.09000	0.21000
H	-4.53000	-0.53000	-1.37000
S	3.14000	-2.15000	0.01000
H	-0.31000	-1.44000	2.65000
H	-1.31000	-2.24000	1.42000
C	0.61000	-1.60000	0.71000
C	1.86000	-1.85000	1.25000
H	2.06000	-1.89000	2.31000
C	1.85000	-1.87000	-1.21000
H	2.03000	-1.93000	-2.28000
C	0.60000	-1.62000	-0.67000
H	-1.33000	-2.26000	-1.34000
H	-0.34000	-1.50000	-2.60000

QM part

S	3.10000	2.25000	-0.04000
O	-2.87000	1.21000	-0.02000
O	-3.10000	-1.07000	0.06000
C	-2.11000	-0.02000	0.02000
C	-1.34000	-0.08000	-1.31000
H	-2.13000	-0.04000	-2.07000
C	-0.46000	1.16000	-1.61000
H	-0.11000	1.09000	-2.65000
H	-1.14000	2.02000	-1.58000
C	0.73000	1.48000	-0.74000
C	1.93000	1.85000	-1.26000
H	2.20000	1.93000	-2.30000
C	1.95000	1.87000	1.21000
H	2.23000	1.97000	2.24000
C	0.74000	1.49000	0.70000
C	-0.44000	1.19000	1.60000
H	-1.12000	2.05000	1.56000

H	-0.09000	1.15000	2.63000
C	-1.32000	-0.06000	1.34000
H	-2.11000	-0.01000	2.10000
H	-0.81000	-1.02000	1.51000
H	-0.82000	-1.05000	-1.47000
C	-4.24000	0.91000	0.23000
H	-4.85000	1.64000	-0.30000
H	-4.46000	0.97000	1.31000
C	-4.36000	-0.51000	-0.28000
H	-5.14000	-1.09000	0.21000
H	-4.53000	-0.53000	-1.37000

_r_(S-S) = 4.45 Å
ONIOM(QM/MM) structure

S	0.00000	0.00000	0.00000
O	6.05530	0.00000	0.00000
O	6.68310	2.19500	0.00000
C	5.52480	1.34560	-0.00600
C	4.76320	1.49520	-1.33970
H	5.54280	1.29740	-2.09570
C	3.68680	0.41860	-1.59810
H	3.35130	0.51240	-2.64090
H	4.20420	-0.54680	-1.54550
C	2.46190	0.34500	-0.72080
C	1.21020	0.15500	-1.23030
H	0.92860	0.09690	-2.26800
C	1.20490	0.22480	1.23880
H	0.91680	0.22230	2.27050
C	2.45500	0.38810	0.71860
C	3.67250	0.50660	1.61090
H	4.18970	-0.46090	1.60350
H	3.33040	0.65600	2.63740
C	4.75860	1.57140	1.30930
H	5.52990	1.40960	2.07300
C	4.30090	2.98840	1.48960
C	4.31480	2.90180	-1.60500
C	7.45580	0.05200	0.24370
H	7.92720	-0.78280	-0.25860
H	7.66710	0.00230	1.32540
C	7.82490	1.41930	-0.31640
H	8.69680	1.86940	0.15500
H	7.98060	1.36220	-1.40560
S	0.74710	4.38600	-0.10820
H	4.01270	3.15380	2.56640
H	5.13430	3.72030	1.31180
C	3.13080	3.41470	0.61880
C	1.94650	3.90060	1.14580
H	1.76020	4.01300	2.20310
C	1.95350	3.84110	-1.31370
H	1.78160	3.88410	-2.38530
C	3.13790	3.37380	-0.76060
H	5.14840	3.63840	-1.44710
H	4.03550	3.02110	-2.68230

QM part

S	3.09000	2.28000	-0.04000
O	-2.87000	1.21000	-0.02000
O	-3.10000	-1.06000	0.06000
C	-2.11000	-0.02000	0.02000
C	-1.33000	-0.08000	-1.31000
H	-2.13000	-0.05000	-2.07000
C	-0.46000	1.16000	-1.61000
H	-0.11000	1.09000	-2.65000
H	-1.14000	2.02000	-1.59000
C	0.73000	1.48000	-0.74000
C	1.93000	1.87000	-1.26000
H	2.20000	1.94000	-2.30000
C	1.94000	1.89000	1.21000
H	2.22000	1.98000	2.24000
C	0.74000	1.49000	0.70000
C	-0.44000	1.19000	1.60000
H	-1.12000	2.05000	1.56000
H	-0.08000	1.14000	2.63000
C	-1.32000	-0.06000	1.34000
H	-2.11000	-0.01000	2.10000
H	-0.80000	-1.03000	1.51000
H	-0.82000	-1.05000	-1.47000
C	-4.24000	0.92000	0.23000
H	-4.85000	1.64000	-0.30000
H	-4.46000	0.97000	1.31000
C	-4.36000	-0.51000	-0.28000
H	-5.14000	-1.09000	0.21000
H	-4.52000	-0.52000	-1.37000

Potential energy surface scan with B3LYP functional

***r*(S-S) = 4.45 Å**
ONIOM(QM/MM) structure

S	3.08194	2.22539	-0.01469
S	3.08210	-2.22451	0.01449
O	-2.97737	1.14710	-0.02362
O	-2.97822	-1.14646	0.02406
C	-2.10532	-0.00001	0.00016
C	-1.31315	0.00491	-1.32204
H	-2.10265	0.00069	-2.08146
C	-0.53414	1.31395	-1.57500
H	-0.22514	1.31329	-2.62366
H	-1.24706	2.13683	-1.46854
C	0.67706	1.59376	-0.72563
C	1.89342	1.92617	-1.24473
H	2.16742	2.00061	-2.28548
C	1.90810	1.90302	1.22351
H	2.19439	1.95923	2.26209
C	0.68543	1.58024	0.71310
C	-0.51802	1.29482	1.57217

H	-1.22597	2.12388	1.47924
H	-0.19802	1.28399	2.61748
C	-1.31302	-0.00550	1.32227
H	-2.10246	-0.00113	2.08175
C	-0.53449	-1.31495	1.57483
H	-0.22586	-1.31498	2.62359
H	-1.24761	-2.13756	1.46764
C	0.67688	-1.59447	0.72566
C	1.89340	-1.92637	1.24466
H	2.16752	-2.00082	2.28538
C	1.90784	-1.90323	-1.22362
H	2.19404	-1.95944	-2.26222
C	0.68512	-1.58095	-0.71308
C	-0.51868	-1.29583	-1.57173
H	-1.22682	-2.12462	-1.47793
H	-0.19925	-1.28567	-2.61722
C	-4.30371	0.71167	0.26691
H	-5.00138	1.37838	-0.23921
H	-4.49748	0.73525	1.34543
C	-4.30405	-0.71011	-0.26737
H	-5.00251	-1.37633	0.23830
H	-4.49713	-0.73356	-1.34602

***r*(S-S) = 4.50 Å**
ONIOM(QM/MM) structure

S	3.07704	2.25045	-0.01518
S	3.07729	-2.24945	0.01498
O	-2.97471	1.14709	-0.02444
O	-2.97564	-1.14645	0.02489
C	-2.10270	-0.00004	0.00017
C	-1.31063	0.00392	-1.32205
H	-2.10033	-0.00052	-2.08129
C	-0.53179	1.31258	-1.57651
H	-0.22124	1.30972	-2.62471
H	-1.24555	2.13518	-1.47321
C	0.67778	1.59717	-0.72631
C	1.89173	1.93871	-1.24528
H	2.16521	2.01530	-2.28602
C	1.90578	1.91812	1.22290
H	2.19099	1.97859	2.26154
C	0.68581	1.58510	0.71245
C	-0.51635	1.29605	1.57216
H	-1.22535	2.12441	1.48072
H	-0.19536	1.28474	2.61717
C	-1.31050	-0.00460	1.32229
H	-2.10013	-0.00001	2.08160
C	-0.53212	-1.31367	1.57633
H	-0.22197	-1.31153	2.62465
H	-1.24606	-2.13600	1.47226
C	0.67764	-1.59791	0.72634
C	1.89177	-1.93889	1.24520
H	2.16537	-2.01549	2.28591
C	1.90556	-1.91832	-1.22302

H	2.19069	-1.97878	-2.26168
C	0.68552	-1.58584	-0.71243
C	-0.51700	-1.29714	-1.57169
H	-1.22618	-2.12524	-1.47933
H	-0.19662	-1.28653	-2.61688
C	-4.30107	0.71191	0.26637
H	-4.99870	1.37826	-0.24026
H	-4.49487	0.73629	1.34487
C	-4.30145	-0.71027	-0.26685
H	-4.99993	-1.37608	0.23932
H	-4.49454	-0.73452	-1.34548

_r_(S-S) = 4.55 Å
ONIOM(QM/MM) structure

S	3.07202	2.27547	-0.01561
S	3.07231	-2.27442	0.01535
O	-2.97200	1.14709	-0.02510
O	-2.97296	-1.14644	0.02564
C	-2.09999	-0.00004	0.00021
C	-1.30805	0.00311	-1.32204
H	-2.09796	-0.00152	-2.08109
C	-0.52943	1.31144	-1.57789
H	-0.21737	1.30650	-2.62564
H	-1.24406	2.13370	-1.47765
C	0.67851	1.60077	-0.72687
C	1.88998	1.95144	-1.24574
H	2.16286	2.03027	-2.28646
C	1.90349	1.93304	1.22239
H	2.18765	1.99757	2.26107
C	0.68625	1.58994	0.71191
C	-0.51456	1.29713	1.57228
H	-1.22462	2.12480	1.48247
H	-0.19254	1.28523	2.61697
C	-1.30788	-0.00381	1.32234
H	-2.09770	0.00096	2.08147
C	-0.52972	-1.31256	1.57773
H	-0.21805	-1.30836	2.62560
H	-1.24455	-2.13455	1.47671
C	0.67839	-1.60153	0.72691
C	1.89006	-1.95164	1.24564
H	2.16310	-2.03048	2.28633
C	1.90325	-1.93325	-1.22253
H	2.18729	-1.99778	-2.26124
C	0.68595	-1.59070	-0.71189
C	-0.51526	-1.29826	-1.57176
H	-1.22549	-2.12566	-1.48098
H	-0.19389	-1.28708	-2.61665
C	-4.29839	0.71209	0.26587
H	-4.99597	1.37812	-0.24125
H	-4.49228	0.73716	1.34433
C	-4.29875	-0.71042	-0.26646
H	-4.99727	-1.37591	0.24009
H	-4.49178	-0.73537	-1.34508

***r*(S-S) = 4.60 Å**
ONIOM(QM/MM) structure

S	3.06688	2.30047	-0.01583
S	3.06717	-2.29943	0.01557
O	-2.96923	1.14709	-0.02557
O	-2.97018	-1.14644	0.02613
C	-2.09721	-0.00003	0.00021
C	-1.30537	0.00256	-1.32206
H	-2.09547	-0.00218	-2.08093
C	-0.52708	1.31069	-1.57908
H	-0.21357	1.30391	-2.62639
H	-1.24266	2.13251	-1.48171
C	0.67922	1.60468	-0.72725
C	1.88810	1.96461	-1.24599
H	2.16031	2.04592	-2.28671
C	1.90121	1.94773	1.22205
H	2.18435	2.01601	2.26078
C	0.68674	1.59471	0.71156
C	-0.51265	1.29792	1.57259
H	-1.22376	2.12490	1.48464
H	-0.18953	1.28521	2.61694
C	-1.30520	-0.00326	1.32236
H	-2.09521	0.00163	2.08132
C	-0.52738	-1.31181	1.57892
H	-0.21427	-1.30578	2.62636
H	-1.24315	-2.13336	1.48075
C	0.67910	-1.60543	0.72729
C	1.88818	-1.96479	1.24590
H	2.16055	-2.04612	2.28658
C	1.90098	-1.94793	-1.22219
H	2.18399	-2.01622	-2.26095
C	0.68644	-1.59547	-0.71153
C	-0.51336	-1.29905	-1.57206
H	-1.22466	-2.12576	-1.48313
H	-0.19090	-1.28707	-2.61662
C	-4.29562	0.71219	0.26556
H	-4.99321	1.37800	-0.24186
H	-4.48954	0.73774	1.34400
C	-4.29596	-0.71055	-0.26616
H	-4.99448	-1.37582	0.24068
H	-4.48900	-0.73596	-1.34477

***r*(S-S) = 4.65 Å**
ONIOM(QM/MM) structure

S	3.06156	2.32549	-0.01597
S	3.06192	-2.32440	0.01568
O	-2.96637	1.14708	-0.02587
O	-2.96733	-1.14645	0.02650
C	-2.09435	-0.00005	0.00023
C	-1.30262	0.00215	-1.32206
H	-2.09291	-0.00267	-2.08074
C	-0.52476	1.31018	-1.58013

H	-0.20984	1.30172	-2.62702
H	-1.24134	2.13148	-1.48550
C	0.67989	1.60881	-0.72751
C	1.88607	1.97809	-1.24614
H	2.15753	2.06202	-2.28685
C	1.89893	1.96230	1.22181
H	2.18107	2.03411	2.26058
C	0.68727	1.59946	0.71133
C	-0.51062	1.29850	1.57305
H	-1.22283	2.12479	1.48713
H	-0.18635	1.28484	2.61703
C	-1.30243	-0.00289	1.32240
H	-2.09262	0.00206	2.08117
C	-0.52503	-1.31133	1.57998
H	-0.21050	-1.30363	2.62699
H	-1.24179	-2.13237	1.48455
C	0.67981	-1.60957	0.72755
C	1.88622	-1.97825	1.24603
H	2.15785	-2.06218	2.28670
C	1.89871	-1.96248	-1.22196
H	2.18072	-2.03429	-2.26077
C	0.68699	-1.60023	-0.71129
C	-0.51134	-1.29966	-1.57249
H	-1.22372	-2.12569	-1.48557
H	-0.18776	-1.28674	-2.61669
C	-4.29277	0.71227	0.26531
H	-4.99033	1.37793	-0.24234
H	-4.48675	0.73813	1.34374
C	-4.29310	-0.71063	-0.26599
H	-4.99165	-1.37574	0.24101
H	-4.48608	-0.73635	-1.34460

***r*(S-S) = 4.70 Å**
ONIOM(QM/MM) structure

S	3.05611	2.35050	-0.01602
S	3.05651	-2.34939	0.01572
O	-2.96343	1.14708	-0.02610
O	-2.96439	-1.14647	0.02675
C	-2.09140	-0.00006	0.00024
C	-1.29977	0.00187	-1.32208
H	-2.09026	-0.00301	-2.08057
C	-0.52242	1.30985	-1.58110
H	-0.20611	1.29983	-2.62756
H	-1.24006	2.13057	-1.48914
C	0.68057	1.61314	-0.72768
C	1.88396	1.99181	-1.24620
H	2.15462	2.07841	-2.28691
C	1.89662	1.97682	1.22165
H	2.17777	2.05197	2.26045
C	0.68784	1.60425	0.71117
C	-0.50851	1.29896	1.57360
H	-1.22183	2.12455	1.48983
H	-0.18305	1.28425	2.61720

C	-1.29957	-0.00262	1.32242
H	-2.08996	0.00238	2.08101
C	-0.52267	-1.31101	1.58096
H	-0.20675	-1.30174	2.62754
H	-1.24048	-2.13148	1.48819
C	0.68051	-1.61388	0.72773
C	1.88414	-1.99195	1.24609
H	2.15497	-2.07855	2.28675
C	1.89643	-1.97697	-1.22181
H	2.17746	-2.05212	-2.26065
C	0.68758	-1.60500	-0.71114
C	-0.50922	-1.30012	-1.57303
H	-1.22270	-2.12546	-1.48825
H	-0.18445	-1.28616	-2.61685
C	-4.28984	0.71231	0.26516
H	-4.98739	1.37786	-0.24264
H	-4.48383	0.73840	1.34358
C	-4.29016	-0.71070	-0.26584
H	-4.98871	-1.37570	0.24129
H	-4.48313	-0.73665	-1.34446

***r*(S-S) = 4.75 Å**
ONIOM(QM/MM) structure

S	3.05053	2.37548	-0.01601
S	3.05093	-2.37441	0.01574
O	-2.96043	1.14707	-0.02632
O	-2.96135	-1.14648	0.02690
C	-2.08837	-0.00006	0.00021
C	-1.29682	0.00167	-1.32211
H	-2.08750	-0.00324	-2.08042
C	-0.52003	1.30967	-1.58203
H	-0.20231	1.29813	-2.62806
H	-1.23877	2.12974	-1.49271
C	0.68126	1.61763	-0.72780
C	1.88179	2.00571	-1.24620
H	2.15160	2.09501	-2.28690
C	1.89427	1.99134	1.22154
H	2.17444	2.06970	2.26038
C	0.68844	1.60910	0.71106
C	-0.50633	1.29938	1.57419
H	-1.22078	2.12424	1.49266
H	-0.17964	1.28355	2.61740
C	-1.29665	-0.00240	1.32242
H	-2.08723	0.00263	2.08082
C	-0.52029	-1.31080	1.58187
H	-0.20297	-1.30001	2.62803
H	-1.23920	-2.13063	1.49175
C	0.68120	-1.61835	0.72784
C	1.88196	-2.00583	1.24610
H	2.15193	-2.09512	2.28676
C	1.89411	-1.99147	-1.22169
H	2.17416	-2.06983	-2.26056
C	0.68819	-1.60982	-0.71104

C	-0.50701	-1.30051	-1.57365
H	-1.22162	-2.12513	-1.49114
H	-0.18099	-1.28541	-2.61707
C	-4.28681	0.71232	0.26508
H	-4.98440	1.37778	-0.24279
H	-4.48076	0.73859	1.34350
C	-4.28713	-0.71077	-0.26570
H	-4.98565	-1.37570	0.24158
H	-4.48017	-0.73690	-1.34429

***r*(S-S) = 4.80 Å**
ONIOM(QM/MM) structure

S	3.04480	2.40047	-0.01599
S	3.04522	-2.39942	0.01574
O	-2.95733	1.14705	-0.02650
O	-2.95822	-1.14650	0.02703
C	-2.08525	-0.00006	0.00019
C	-1.29379	0.00150	-1.32214
H	-2.08466	-0.00344	-2.08027
C	-0.51760	1.30953	-1.58296
H	-0.19845	1.29649	-2.62853
H	-1.23748	2.12892	-1.49630
C	0.68194	1.62226	-0.72790
C	1.87952	2.01975	-1.24618
H	2.14847	2.11171	-2.28688
C	1.89186	2.00594	1.22144
H	2.17103	2.08742	2.26031
C	0.68904	1.61404	0.71098
C	-0.50408	1.29977	1.57483
H	-1.21969	2.12387	1.49562
H	-0.17612	1.28278	2.61762
C	-1.29363	-0.00221	1.32242
H	-2.08442	0.00283	2.08063
C	-0.51786	-1.31064	1.58278
H	-0.19912	-1.29833	2.62849
H	-1.23791	-2.12979	1.49533
C	0.68189	-1.62296	0.72794
C	1.87970	-2.01985	1.24609
H	2.14879	-2.11180	2.28676
C	1.89173	-2.00605	-1.22158
H	2.17080	-2.08752	-2.26048
C	0.68881	-1.61474	-0.71095
C	-0.50472	-1.30088	-1.57431
H	-1.22050	-2.12475	-1.49414
H	-0.17742	-1.28460	-2.61732
C	-4.28369	0.71233	0.26501
H	-4.98131	1.37771	-0.24293
H	-4.47759	0.73875	1.34344
C	-4.28402	-0.71083	-0.26556
H	-4.98251	-1.37570	0.24183
H	-4.47710	-0.73712	-1.34415

***r*(S-S) = 4.85 Å**

ONIOM(QM/MM) structure

S	3.03891	2.42549	-0.01597
S	3.03937	-2.42441	0.01576
O	-2.95413	1.14706	-0.02670
O	-2.95505	-1.14651	0.02715
C	-2.08204	-0.00006	0.00016
C	-1.29066	0.00129	-1.32218
H	-2.08173	-0.00367	-2.08012
C	-0.51508	1.30939	-1.58391
H	-0.19445	1.29480	-2.62902
H	-1.23613	2.12806	-1.50000
C	0.68264	1.62696	-0.72800
C	1.87720	2.03387	-1.24616
H	2.14525	2.12844	-2.28686
C	1.88938	2.02064	1.22134
H	2.16752	2.10522	2.26025
C	0.68965	1.61907	0.71089
C	-0.50175	1.30016	1.57549
H	-1.21856	2.12347	1.49871
H	-0.17246	1.28193	2.61786
C	-1.29052	-0.00204	1.32241
H	-2.08152	0.00302	2.08043
C	-0.51538	-1.31054	1.58370
H	-0.19520	-1.29671	2.62895
H	-1.23660	-2.12897	1.49894
C	0.68259	-1.62767	0.72803
C	1.87738	-2.03393	1.24609
H	2.14558	-2.12848	2.28675
C	1.88929	-2.02072	-1.22147
H	2.16736	-2.10527	-2.26039
C	0.68944	-1.61979	-0.71087
C	-0.50238	-1.30131	-1.57499
H	-1.21936	-2.12439	-1.49721
H	-0.17375	-1.28383	-2.61756
C	-4.28047	0.71238	0.26497
H	-4.97812	1.37771	-0.24299
H	-4.47429	0.73893	1.34342
C	-4.28085	-0.71085	-0.26543
H	-4.97934	-1.37565	0.24206
H	-4.47398	-0.73725	-1.34401

***r*(S-S) = 4.90 Å**

ONIOM(QM/MM) structure

S	3.03285	2.45053	-0.01597
S	3.03340	-2.44937	0.01574
O	-2.95083	1.14705	-0.02683
O	-2.95179	-1.14653	0.02731
C	-2.07875	-0.00010	0.00017
C	-1.28747	0.00109	-1.32218
H	-2.07874	-0.00390	-2.07993
C	-0.51254	1.30927	-1.58485
H	-0.19040	1.29313	-2.62948
H	-1.23481	2.12719	-1.50373

C	0.68332	1.63178	-0.72808
C	1.87477	2.04811	-1.24613
H	2.14189	2.14527	-2.28684
C	1.88682	2.03541	1.22124
H	2.16392	2.12300	2.26018
C	0.69026	1.62419	0.71081
C	-0.49935	1.30053	1.57621
H	-1.21741	2.12302	1.50192
H	-0.16868	1.28103	2.61811
C	-1.28732	-0.00191	1.32244
H	-2.07852	0.00316	2.08026
C	-0.51281	-1.31048	1.58463
H	-0.19112	-1.29511	2.62941
H	-1.23523	-2.12818	1.50265
C	0.68331	-1.63251	0.72812
C	1.87503	-2.04813	1.24605
H	2.14230	-2.14525	2.28672
C	1.88679	-2.03544	-1.22137
H	2.16382	-2.12300	-2.26033
C	0.69009	-1.62492	-0.71079
C	-0.49997	-1.30174	-1.57567
H	-1.21817	-2.12401	-1.50037
H	-0.16998	-1.28300	-2.61781
C	-4.27718	0.71242	0.26488
H	-4.97482	1.37769	-0.24316
H	-4.47102	0.73909	1.34332
C	-4.27757	-0.71088	-0.26537
H	-4.97609	-1.37560	0.24218
H	-4.47067	-0.73739	-1.34395

Potential energy surface scan with B97D functional

***r*(S-S) = 4.00 Å**
ONIOM(QM/MM) structure

S	-3.12432	-2.00002	0.00306
S	-3.12422	1.99998	-0.00308
O	3.00653	-1.15810	0.00306
O	3.00662	1.15789	-0.00304
C	2.13101	0.00002	0.00002
C	1.34246	-0.03434	-1.32398
H	2.13563	-0.03675	-2.08574
C	0.55755	-1.34824	-1.55106
H	0.26221	-1.37277	-2.60866
H	1.26121	-2.17815	-1.39912
C	-0.66990	-1.56077	-0.70524
C	-1.90875	-1.82474	-1.22975
H	-2.17991	-1.89826	-2.27669
C	-1.93664	-1.72868	1.24543
H	-2.23127	-1.72491	2.28855
C	-0.68528	-1.50605	0.73118
C	0.52797	-1.25473	1.58901
H	1.22431	-2.09909	1.49001

H	0.21117	-1.22603	2.64026
C	1.34245	0.03439	1.32401
H	2.13561	0.03672	2.08578
C	0.55768	1.34839	1.55105
H	0.26237	1.37302	2.60866
H	1.26141	2.17822	1.39903
C	-0.66977	1.56092	0.70524
C	-1.90867	1.82472	1.22974
H	-2.17985	1.89818	2.27668
C	-1.93652	1.72871	-1.24544
H	-2.23114	1.72493	-2.28856
C	-0.68514	1.50621	-0.73118
C	0.52813	1.25489	-1.58898
H	1.22455	2.09918	-1.48987
H	0.21139	1.22629	-2.64025
C	4.32653	-0.69734	0.30732
H	5.04357	-1.39047	-0.14656
H	4.48906	-0.64912	1.39715
C	4.32660	0.69704	-0.30735
H	5.04369	1.39011	0.14654
H	4.48907	0.64885	-1.39719

***r*(S-S) = 4.05 Å**
ONIOM(QM/MM) structure

S	-3.12081	-2.02503	0.00096
S	-3.12072	2.02497	-0.00098
O	3.00475	-1.15812	0.00010
O	3.00485	1.15791	-0.00005
C	2.12926	0.00001	0.00002
C	1.34081	-0.03098	-1.32407
H	2.13414	-0.03220	-2.08569
C	0.55535	-1.34364	-1.55450
H	0.25855	-1.36437	-2.61178
H	1.25927	-2.17413	-1.40673
C	-0.67081	-1.56125	-0.70798
C	-1.90803	-1.83343	-1.23233
H	-2.17916	-1.90723	-2.27928
C	-1.93465	-1.74565	1.24320
H	-2.22817	-1.74889	2.28665
C	-0.68550	-1.51121	0.72867
C	0.52721	-1.25878	1.58690
H	1.22425	-2.10251	1.48699
H	0.21021	-1.23182	2.63815
C	1.34079	0.03103	1.32410
H	2.13411	0.03218	2.08574
C	0.55548	1.34380	1.55448
H	0.25872	1.36464	2.61177
H	1.25947	2.17422	1.40662
C	-0.67069	1.56141	0.70798
C	-1.90794	1.83344	1.23232
H	-2.17910	1.90720	2.27926
C	-1.93453	1.74569	-1.24322
H	-2.22804	1.74893	-2.28667

C	-0.68536	1.51137	-0.72867
C	0.52738	1.25895	-1.58686
H	1.22449	2.10260	-1.48682
H	0.21044	1.23210	-2.63813
C	4.32476	-0.69813	0.30554
H	5.04181	-1.39011	-0.15009
H	4.48728	-0.65267	1.39550
C	4.32483	0.69781	-0.30559
H	5.04194	1.38974	0.15002
H	4.48725	0.65238	-1.39556

***r*(S-S) = 4.10 Å**
ONIOM(QM/MM) structure

S	3.11710	-2.05006	-0.00029
S	3.11706	2.04994	0.00023
O	-3.00281	-1.15812	0.00120
O	-3.00297	1.15794	-0.00107
C	-2.12737	0.00002	0.00005
C	-1.33901	-0.02959	1.32416
H	-2.13250	-0.03024	2.08564
C	-0.55359	-1.34165	1.55631
H	-0.25564	-1.36018	2.61331
H	-1.25803	-2.17224	1.41132
C	0.67144	-1.56337	0.70914
C	1.90669	-1.84493	1.23333
H	2.17734	-1.92106	2.28024
C	1.93304	-1.76030	-1.24234
H	2.22582	-1.76845	-2.28599
C	0.68596	-1.51513	-0.72760
C	-0.52590	-1.26022	-1.58634
H	-1.22353	-2.10359	-1.48718
H	-0.20824	-1.23326	-2.63739
C	-1.33904	0.02968	-1.32409
H	-2.13254	0.03027	-2.08555
C	-0.55376	1.34184	-1.55622
H	-0.25589	1.36048	-2.61325
H	-1.25825	2.17236	-1.41111
C	0.67132	1.56353	-0.70913
C	1.90659	1.84494	-1.23335
H	2.17722	1.92105	-2.28027
C	1.93300	1.76032	1.24232
H	2.22581	1.76845	2.28596
C	0.68588	1.51530	0.72762
C	-0.52598	1.26042	1.58635
H	-1.22367	2.10372	1.48710
H	-0.20835	1.23356	2.63742
C	-4.32280	-0.69848	-0.30492
H	-5.03989	-1.39000	0.15134
H	-4.48515	-0.65417	-1.39495
C	-4.32298	0.69811	0.30475
H	-5.04006	1.38953	-0.15167
H	-4.48555	0.65381	1.39475

***r*(S-S) = 4.15 Å**
ONIOM(QM/MM) structure

S	3.11326	-2.07504	-0.00004
S	3.11322	2.07496	0.00001
O	-3.00086	-1.15812	0.00174
O	-3.00097	1.15798	-0.00171
C	-2.12540	0.00001	0.00002
C	-1.33713	-0.02892	1.32417
H	-2.13078	-0.02919	2.08550
C	-0.55202	-1.34065	1.55751
H	-0.25307	-1.35757	2.61427
H	-1.25710	-2.17112	1.41480
C	0.67196	-1.56622	0.70977
C	1.90511	-1.85750	1.23381
H	2.17507	-1.93665	2.28069
C	1.93159	-1.77430	-1.24192
H	2.22378	-1.78665	-2.28571
C	0.68655	-1.51879	-0.72706
C	-0.52430	-1.26083	-1.58637
H	-1.22253	-2.10390	-1.48862
H	-0.20575	-1.23324	-2.63715
C	-1.33715	0.02898	-1.32414
H	-2.13081	0.02921	-2.08546
C	-0.55214	1.34080	-1.55745
H	-0.25327	1.35783	-2.61423
H	-1.25728	2.17121	-1.41461
C	0.67187	1.56634	-0.70976
C	1.90502	1.85757	-1.23382
H	2.17497	1.93674	-2.28070
C	1.93156	1.77427	1.24191
H	2.22377	1.78655	2.28569
C	0.68648	1.51892	0.72707
C	-0.52439	1.26097	1.58636
H	-1.22266	2.10399	1.48854
H	-0.20587	1.23346	2.63715
C	-4.32083	-0.69857	-0.30455
H	-5.03794	-1.38988	0.15200
H	-4.48321	-0.65473	-1.39461
C	-4.32094	0.69830	0.30450
H	-5.03807	1.38955	-0.15211
H	-4.48337	0.65445	1.39454

***r*(S-S) = 4.20 Å**
ONIOM(QM/MM) structure

S	3.10926	-2.10005	0.00118
S	3.10921	2.09995	-0.00122
O	-2.99872	-1.15814	0.00362
O	-2.99887	1.15797	-0.00355
C	-2.12330	0.00000	0.00003
C	-1.33513	-0.02682	1.32423
H	-2.12894	-0.02636	2.08540
C	-0.54987	-1.33777	1.55996

H	-0.24948	-1.35172	2.61636
H	-1.25555	-2.16839	1.42086
C	0.67274	-1.56821	0.71146
C	1.90390	-1.86841	1.23533
H	2.17352	-1.94905	2.28219
C	1.92962	-1.79025	-1.24056
H	2.22079	-1.80819	-2.28457
C	0.68690	-1.52367	-0.72551
C	-0.52309	-1.26335	-1.58533
H	-1.22216	-2.10581	-1.48790
H	-0.20396	-1.23634	-2.63595
C	-1.33515	0.02690	-1.32418
H	-2.12898	0.02639	-2.08534
C	-0.55004	1.33795	-1.55988
H	-0.24975	1.35204	-2.61630
H	-1.25578	2.16850	-1.42061
C	0.67262	1.56837	-0.71144
C	1.90380	1.86845	-1.23534
H	2.17340	1.94908	-2.28221
C	1.92957	1.79025	1.24055
H	2.22077	1.80815	2.28455
C	0.68681	1.52383	0.72552
C	-0.52319	1.26354	1.58532
H	-1.22233	2.10593	1.48778
H	-0.20412	1.23664	2.63596
C	-4.31870	-0.69910	-0.30343
H	-5.03580	-1.38968	0.15424
H	-4.48108	-0.65704	-1.39356
C	-4.31884	0.69876	0.30334
H	-5.03597	1.38924	-0.15443
H	-4.48132	0.65669	1.39344

***r*(S-S) = 4.25 Å**
ONIOM(QM/MM) structure

S	-3.10511	2.12506	0.00367
S	-3.10506	-2.12493	-0.00370
O	2.99648	1.15815	0.00703
O	2.99667	-1.15795	-0.00699
C	2.12109	-0.00000	0.00002
C	1.33301	0.02296	1.32431
H	2.12701	0.02134	2.08531
C	0.54710	1.33256	1.56387
H	0.24478	1.34199	2.61978
H	1.25326	2.16368	1.42990
C	-0.67383	1.56909	0.71444
C	-1.90321	1.87712	1.23816
H	-2.17294	1.95729	2.28504
C	-1.92698	1.80877	-1.23802
H	-2.21662	1.83416	-2.28231
C	-0.68694	1.53007	-0.72273
C	0.52241	1.26831	-1.58297
H	1.22260	2.10973	-1.48445
H	0.20310	1.24339	-2.63360

C	1.33303	-0.02308	-1.32427
H	2.12704	-0.02139	-2.08527
C	0.54728	-1.33280	-1.56378
H	0.24507	-1.34238	-2.61971
H	1.25351	-2.16383	-1.42963
C	-0.67370	-1.56928	-0.71443
C	-1.90311	-1.87711	-1.23818
H	-2.17284	-1.95724	-2.28506
C	-1.92691	-1.80880	1.23801
H	-2.21658	-1.83418	2.28230
C	-0.68683	-1.53026	0.72274
C	0.52255	-1.26854	1.58294
H	1.22281	-2.10988	1.48426
H	0.20332	-1.24378	2.63359
C	4.31649	0.70003	-0.30134
H	5.03357	1.38926	0.15840
H	4.47888	0.66123	-1.39159
C	4.31664	-0.69962	0.30127
H	5.03378	-1.38873	-0.15856
H	4.47912	-0.66080	1.39149

***r*(S-S) = 4.30 Å**
ONIOM(QM/MM) structure

S	-3.10080	2.15010	0.00639
S	-3.10075	-2.14988	-0.00643
O	2.99409	1.15818	0.01071
O	2.99441	-1.15788	-0.01066
C	2.11877	0.00001	0.00003
C	1.33079	0.01881	1.32439
H	2.12497	0.01601	2.08521
C	0.54407	1.32693	1.56802
H	0.23963	1.33147	2.62336
H	1.25071	2.15857	1.43961
C	-0.67502	1.56988	0.71759
C	-1.90261	1.88557	1.24116
H	-2.17257	1.96485	2.28806
C	-1.92410	1.82796	-1.23528
H	-2.21203	1.86114	-2.27983
C	-0.68690	1.53686	-0.71978
C	0.52180	1.27365	-1.58044
H	1.22323	2.11392	-1.48069
H	0.20234	1.25102	-2.63108
C	1.33081	-0.01900	-1.32435
H	2.12500	-0.01611	-2.08516
C	0.54435	-1.32732	-1.56787
H	0.24010	-1.33212	-2.62326
H	1.25109	-2.15882	-1.43915
C	-0.67484	-1.57018	-0.71757
C	-1.90248	-1.88559	-1.24118
H	-2.17244	-1.96481	-2.28809
C	-1.92401	-1.82799	1.23527
H	-2.21198	-1.86112	2.27982
C	-0.68675	-1.53716	0.71980

C	0.52201	-1.27403	1.58037
H	1.22355	-2.11418	1.48035
H	0.20270	-1.25166	2.63106
C	4.31413	0.70112	-0.29912
H	5.03117	1.38891	0.16283
H	4.47652	0.66580	-1.38948
C	4.31437	-0.70045	0.29902
H	5.03154	-1.38804	-0.16302
H	4.47687	-0.66511	1.38936

***r*(S-S) = 4.35 Å**
ONIOM(QM/MM) structure

S	3.09634	2.17521	-0.00860
S	3.09628	-2.17475	0.00856
O	-2.99153	1.15828	-0.01364
O	-2.99213	-1.15772	0.01379
C	-2.11638	0.00002	0.00005
C	-1.32851	0.01534	-1.32441
H	-2.12290	0.01165	-2.08503
C	-0.54112	1.32216	-1.57156
H	-0.23462	1.32228	-2.62632
H	-1.24828	2.15418	-1.44832
C	0.67617	1.57120	-0.72012
C	1.90179	1.89505	-1.24356
H	2.17179	1.97413	-2.29047
C	1.92138	1.84617	1.23302
H	2.20773	1.88636	2.27778
C	0.68703	1.54310	0.71739
C	-0.52085	1.27794	1.57856
H	-1.22345	2.11720	1.47828
H	-0.20100	1.25690	2.62912
C	-1.32848	-0.01571	1.32447
H	-2.12284	-0.01184	2.08511
C	-0.54154	-1.32288	1.57137
H	-0.23534	-1.32351	2.62621
H	-1.24889	-2.15466	1.44758
C	0.67589	-1.57176	0.72012
C	1.90162	-1.89514	1.24355
H	2.17167	-1.97416	2.29046
C	1.92115	-1.84625	-1.23307
H	2.20750	-1.88634	-2.27782
C	0.68671	-1.54365	-0.71739
C	-0.52135	-1.27866	-1.57833
H	-1.22414	-2.11769	-1.47747
H	-0.20184	-1.25812	-2.62900
C	-4.31170	0.70220	0.29711
H	-5.02855	1.38881	-0.16689
H	-4.47436	0.66989	1.38752
C	-4.31202	-0.70099	-0.29723
H	-5.02929	-1.38723	0.16665
H	-4.47444	-0.66862	-1.38767

***r*(S-S) = 4.40 Å**

ONIOM(QM/MM) structure

S	-3.09169	2.20017	0.01061
S	-3.09166	-2.19978	-0.01067
O	2.98908	1.15821	0.01661
O	2.98962	-1.15776	-0.01653
C	2.11388	0.00002	0.00003
C	1.32609	0.01217	1.32451
H	2.12065	0.00760	2.08497
C	0.53819	1.31786	1.57493
H	0.22971	1.31388	2.62911
H	1.24599	2.15010	1.45659
C	-0.67727	1.57290	0.72251
C	-1.90091	1.90487	1.24576
H	-2.17096	1.98393	2.29267
C	-1.91847	1.86435	-1.23092
H	-2.20316	1.91129	-2.27586
C	-0.68704	1.54950	-0.71513
C	0.52005	1.28222	-1.57670
H	1.22391	2.12038	-1.47589
H	0.19990	1.26276	-2.62721
C	1.32612	-0.01251	-1.32445
H	2.12069	-0.00780	-2.08490
C	0.53862	-1.31850	-1.57469
H	0.23044	-1.31497	-2.62896
H	1.24656	-2.15054	-1.45582
C	-0.67702	-1.57338	-0.72249
C	-1.90075	-1.90488	-1.24579
H	-2.17081	-1.98385	-2.29270
C	-1.91835	-1.86439	1.23092
H	-2.20310	-1.91125	2.27585
C	-0.68682	-1.54998	0.71515
C	0.52040	-1.28286	1.57656
H	1.22443	-2.12083	1.47526
H	0.20051	-1.26384	2.62715
C	4.30917	0.70284	-0.29555
H	5.02614	1.38832	0.16994
H	4.47157	0.67315	-1.38607
C	4.30955	-0.70177	0.29541
H	5.02676	-1.38691	-0.17019
H	4.47211	-0.67200	1.38591

***r*(S-S) = 4.45 Å**

ONIOM(QM/MM) structure

S	3.08695	2.22538	-0.01274
S	3.08689	-2.22455	0.01264
O	-2.98620	1.15842	-0.01930
O	-2.98730	-1.15742	0.01951
C	-2.11136	0.00007	0.00008
C	-1.32366	0.00884	-1.32449
H	-2.11846	0.00359	-2.08471
C	-0.53496	1.31316	-1.57830
H	-0.22427	1.30473	-2.63183
H	-1.24325	2.14577	-1.46530

C	0.67856	1.57438	-0.72480
C	1.90005	1.91468	-1.24795
H	2.17012	1.99362	-2.29487
C	1.91562	1.88253	1.22879
H	2.19866	1.93619	2.27387
C	0.68726	1.55569	0.71293
C	-0.51885	1.28611	1.57513
H	-1.22391	2.12329	1.47422
H	-0.19814	1.26790	2.62549
C	-1.32359	-0.00954	1.32461
H	-2.11834	-0.00395	2.08488
C	-0.53574	-1.31452	1.57794
H	-0.22563	-1.30707	2.63164
H	-1.24438	-2.14668	1.46386
C	0.67807	-1.57539	0.72481
C	1.89980	-1.91474	1.24793
H	2.16999	-1.99352	2.29483
C	1.91522	-1.88263	-1.22888
H	2.19827	-1.93613	-2.27396
C	0.68669	-1.55671	-0.71294
C	-0.51981	-1.28748	-1.57464
H	-1.22523	-2.12420	-1.47256
H	-0.19979	-1.27026	-2.62522
C	-4.30655	0.70422	0.29351
H	-5.02316	1.38861	-0.17412
H	-4.46940	0.67749	1.38404
C	-4.30713	-0.70199	-0.29371
H	-5.02451	-1.38570	0.17374
H	-4.46965	-0.67516	-1.38428

***r*(S-S) = 4.50 Å**
ONIOM(QM/MM) structure

S	3.08196	2.25043	-0.01323
S	3.08199	-2.24950	0.01296
O	-2.98356	1.15841	-0.01989
O	-2.98466	-1.15742	0.02047
C	-2.10871	0.00005	0.00022
C	-1.32118	0.00795	-1.32441
H	-2.11621	0.00245	-2.08442
C	-0.53273	1.31193	-1.57971
H	-0.22062	1.30137	-2.63280
H	-1.24192	2.14422	-1.46976
C	0.67928	1.57789	-0.72543
C	1.89826	1.92763	-1.24847
H	2.16765	2.00895	-2.29539
C	1.91343	1.89761	1.22822
H	2.19544	1.95547	2.27336
C	0.68777	1.56046	0.71236
C	-0.51708	1.28724	1.57522
H	-1.22318	2.12376	1.47587
H	-0.19536	1.26852	2.62528
C	-1.32101	-0.00869	1.32472
H	-2.11593	-0.00287	2.08483

C	-0.53334	-1.31330	1.57947
H	-0.22172	-1.30371	2.63271
H	-1.24286	-2.14518	1.46852
C	0.67889	-1.57890	0.72546
C	1.89816	-1.92769	1.24838
H	2.16776	-2.00887	2.29526
C	1.91298	-1.89775	-1.22837
H	2.19490	-1.95549	-2.27354
C	0.68718	-1.56147	-0.71233
C	-0.51813	-1.28863	-1.57460
H	-1.22456	-2.12472	-1.47400
H	-0.19720	-1.27090	-2.62491
C	-4.30398	0.70437	0.29285
H	-5.02049	1.38846	-0.17538
H	-4.46711	0.67833	1.38335
C	-4.30438	-0.70220	-0.29347
H	-5.02190	-1.38562	0.17419
H	-4.46656	-0.67608	-1.38411

Optimised structures of (a)
B3LYP/TZVP:UFF

S	-3.33520	-0.00020	-0.60740
S	2.98870	-0.00000	-1.36620
N	-0.22700	2.30440	1.96090
N	-0.22680	-2.30380	1.96130
C	-2.29970	-1.46780	-1.07800
C	-2.29990	1.46740	-1.07810
C	-1.10630	1.73630	-0.20430
C	-1.25030	2.12140	1.13340
C	1.00290	2.07910	1.49100
C	1.27600	1.70550	0.17720
C	0.18680	1.57060	-0.68140
C	2.69660	1.45720	-0.26610
C	2.69670	-1.45730	-0.26610
C	1.27610	-1.70550	0.17740
C	1.00310	-2.07860	1.49140
C	-1.25010	-2.12110	1.13380
C	-1.10610	-1.73640	-0.20400
C	0.18690	-1.57090	-0.68120
H	-2.00360	-1.36430	-2.12240
H	-3.02030	-2.28570	-1.02310
H	-2.00380	1.36390	-2.12260
H	-3.02050	2.28520	-1.02320
H	-2.24020	2.26960	1.55430
H	1.81330	2.19990	2.20450
H	0.35260	1.27860	-1.71200
H	3.35640	1.38270	0.59920
H	3.06410	2.28700	-0.87520
H	3.35660	-1.38270	0.59910
H	3.06410	-2.28710	-0.87520
H	1.81350	-2.19900	2.20490
H	-2.24000	-2.26920	1.55480
H	0.35280	-1.27930	-1.71190

B3LYP/TZVP

S	-0.44439	3.29125	0.85841
S	-0.22106	-3.11102	1.08672
N	-1.29079	0.33968	-2.55804
N	2.62487	0.53118	-1.16418
C	0.85543	2.25699	1.68325
C	-1.87805	2.12468	0.71143
C	-1.70346	1.01207	-0.28552
C	-1.52191	1.27916	-1.64772
C	-1.20546	-0.92601	-2.13726
C	-1.37975	-1.31724	-0.81251
C	-1.66056	-0.31523	0.11520
C	-1.24097	-2.76545	-0.41763
C	1.48006	-2.63307	0.53958
C	1.71580	-1.16601	0.28291
C	2.39255	-0.74947	-0.86041
C	2.14934	1.45785	-0.33965
C	1.44359	1.16462	0.83323
C	1.26122	-0.17359	1.15004
H	0.44266	1.85208	2.60870
H	1.61277	2.99442	1.95653
H	-2.10742	1.72816	1.70184
H	-2.69877	2.78522	0.42457
H	-1.53945	2.30413	-2.00564
H	-0.97607	-1.66567	-2.89959
H	-1.77740	-0.57327	1.16176
H	-0.84539	-3.35103	-1.24941
H	-2.21265	-3.19206	-0.15654
H	1.74036	-3.22034	-0.34272
H	2.10892	-2.98905	1.35960
H	2.75987	-1.48128	-1.57457
H	2.30949	2.49152	-0.63108
H	0.70660	-0.45326	2.03872

TPSS/TZVP

S	-0.42005	3.28242	0.81926
S	-0.22893	-3.08864	1.07045
N	-1.51713	0.33287	-2.61440
N	2.81909	0.52179	-1.06633
C	0.87735	2.26155	1.68561
C	-1.88531	2.13628	0.70003
C	-1.75499	1.02243	-0.30693
C	-1.69171	1.27977	-1.68622
C	-1.36900	-0.93197	-2.18407
C	-1.42560	-1.31478	-0.84054
C	-1.65372	-0.30663	0.10095
C	-1.24484	-2.76432	-0.44873
C	1.49387	-2.64293	0.54091
C	1.76537	-1.17416	0.30607
C	2.53531	-0.76177	-0.78580
C	2.29530	1.45485	-0.26402
C	1.49844	1.16711	0.85620

C	1.26995	-0.17603	1.15071
H	0.44404	1.86076	2.60684
H	1.61639	3.01963	1.96363
H	-2.09880	1.74215	1.69809
H	-2.69266	2.82466	0.43068
H	-1.76767	2.30161	-2.05598
H	-1.19219	-1.67713	-2.96005
H	-1.69915	-0.56184	1.15786
H	-0.82782	-3.33888	-1.28154
H	-2.20607	-3.22133	-0.18569
H	1.75272	-3.22887	-0.34624
H	2.09724	-3.02506	1.37274
H	2.94542	-1.49835	-1.47692
H	2.50415	2.48896	-0.53538
H	0.66100	-0.45415	2.00880

B3LYP-D/TZVP

S	-0.44439	3.29125	0.85841
S	-0.22106	-3.11102	1.08672
N	-1.29079	0.33968	-2.55804
N	2.62487	0.53118	-1.16418
C	0.85543	2.25699	1.68325
C	-1.87805	2.12468	0.71143
C	-1.70346	1.01207	-0.28552
C	-1.52191	1.27916	-1.64772
C	-1.20546	-0.92601	-2.13726
C	-1.37975	-1.31724	-0.81251
C	-1.66056	-0.31523	0.11520
C	-1.24097	-2.76545	-0.41763
C	1.48006	-2.63307	0.53958
C	1.71580	-1.16601	0.28291
C	2.39255	-0.74947	-0.86041
C	2.14934	1.45785	-0.33965
C	1.44359	1.16462	0.83323
C	1.26122	-0.17359	1.15004
H	0.44266	1.85208	2.60870
H	1.61277	2.99442	1.95653
H	-2.10742	1.72816	1.70184
H	-2.69877	2.78522	0.42457
H	-1.53945	2.30413	-2.00564
H	-0.97607	-1.66567	-2.89959
H	-1.77740	-0.57327	1.16176
H	-0.84539	-3.35103	-1.24941
H	-2.21265	-3.19206	-0.15654
H	1.74036	-3.22034	-0.34272
H	2.10892	-2.98905	1.35960
H	2.75987	-1.48128	-1.57457
H	2.30949	2.49152	-0.63108
H	0.70660	-0.45326	2.03872

TPSS-D/TZVP

S	-0.45676	3.30409	0.87500
S	-0.21570	-3.10896	1.10331

N	-1.22689	0.33546	-2.55703
N	2.60710	0.54909	-1.19487
C	0.84862	2.25845	1.69338
C	-1.88722	2.12437	0.71789
C	-1.68759	1.01221	-0.27982
C	-1.46996	1.27892	-1.64176
C	-1.16697	-0.93698	-2.12695
C	-1.37339	-1.32679	-0.80146
C	-1.66427	-0.31986	0.12489
C	-1.25601	-2.77699	-0.39941
C	1.48252	-2.63423	0.52230
C	1.70545	-1.16239	0.26332
C	2.37813	-0.73902	-0.88613
C	2.12800	1.47327	-0.35591
C	1.42892	1.17255	0.82433
C	1.24804	-0.17226	1.13840
H	0.43257	1.84310	2.61638
H	1.60664	2.99859	1.96868
H	-2.11939	1.72411	1.70962
H	-2.70845	2.78481	0.42131
H	-1.46622	2.30687	-2.00102
H	-0.93007	-1.68205	-2.88647
H	-1.80601	-0.57847	1.17257
H	-0.87569	-3.37924	-1.23032
H	-2.23013	-3.18746	-0.11066
H	1.72630	-3.22347	-0.36708
H	2.12161	-2.98995	1.33852
H	2.74676	-1.47013	-1.60543
H	2.28342	2.51095	-0.64749
H	0.69664	-0.45858	2.03191

Optimised structures of (b)
B3LYP/TZVP:UFF

S	-3.33520	-0.00020	-0.60740
S	2.98870	-0.00000	-1.36620
N	-0.22700	2.30440	1.96090
N	-0.22680	-2.30380	1.96130
C	-2.29970	-1.46780	-1.07800
C	-2.29990	1.46740	-1.07810
C	-1.10630	1.73630	-0.20430
C	-1.25030	2.12140	1.13340
C	1.00290	2.07910	1.49100
C	1.27600	1.70550	0.17720
C	0.18680	1.57060	-0.68140
C	2.69660	1.45720	-0.26610
C	2.69670	-1.45730	-0.26610
C	1.27610	-1.70550	0.17740
C	1.00310	-2.07860	1.49140
C	-1.25010	-2.12110	1.13380
C	-1.10610	-1.73640	-0.20400
C	0.18690	-1.57090	-0.68120
H	-2.00360	-1.36430	-2.12240
H	-3.02030	-2.28570	-1.02310

H	-2.00380	1.36390	-2.12260
H	-3.02050	2.28520	-1.02320
H	-2.24020	2.26960	1.55430
H	1.81330	2.19990	2.20450
H	0.35260	1.27860	-1.71200
H	3.35640	1.38270	0.59920
H	3.06410	2.28700	-0.87520
H	3.35660	-1.38270	0.59910
H	3.06410	-2.28710	-0.87520
H	1.81350	-2.19900	2.20490
H	-2.24000	-2.26920	1.55480
H	0.35280	-1.27930	-1.71190

B3LYP/TZVP

Fe	1.53414	12.27973	5.55433
F	4.88844	13.42894	4.82021
F	7.35303	13.72637	5.80558
F	7.73015	14.58471	8.36754
F	5.56622	15.14625	9.93074
F	3.09127	14.87111	8.97642
F	5.00389	9.74267	4.07516
F	7.45342	9.41293	5.07258
F	7.94797	9.84536	7.72060
F	5.91493	10.64215	9.35598
F	3.45663	11.01425	8.38608
C	1.32532	13.67941	7.08700
H	1.29531	13.44384	8.13664
C	0.20649	13.74267	6.21672
H	-0.81760	13.55028	6.49389
C	0.67589	14.06950	4.91329
H	0.07060	14.17265	4.02686
C	2.08696	14.20538	4.97148
H	2.73369	14.44140	4.14365
C	2.50377	13.97937	6.32661
C	3.86967	14.11969	6.85593
C	5.01105	13.86086	6.08751
C	6.29922	14.01071	6.57855
C	6.49602	14.43994	7.88376
C	5.39233	14.71688	8.67761
C	4.11260	14.56074	8.16341
C	1.52153	10.34636	6.34333
H	1.42877	10.10077	7.38734
C	0.44987	10.50177	5.42677
H	-0.59801	10.40714	5.66385
C	0.99675	10.83163	4.15524
H	0.43719	11.03819	3.25685
C	2.40928	10.87945	4.27909
H	3.10345	11.11483	3.49117
C	2.75244	10.56461	5.63619
C	4.10980	10.40311	6.18091
C	5.18456	9.99261	5.38108
C	6.46625	9.80850	5.88104
C	6.72138	10.02193	7.22806

C	5.68293	10.42149	8.05752
C	4.41242	10.60583	7.53343

TPSS/TZVP

Fe	1.53137	12.27875	5.54867
F	4.79864	13.59699	4.60889
F	7.32125	13.89436	5.44220
F	7.86669	14.50923	8.05801
F	5.79791	14.83700	9.82225
F	3.26251	14.57780	9.01799
F	5.12104	9.89987	4.19279
F	7.51993	9.59918	5.33779
F	7.83501	9.94256	8.03531
F	5.66834	10.61567	9.57121
F	3.25881	10.95344	8.45600
C	1.37049	13.56584	7.13446
H	1.40274	13.28459	8.17610
C	0.19960	13.63369	6.32004
H	-0.80631	13.39984	6.64193
C	0.59475	14.02016	5.00017
H	-0.05875	14.13445	4.14563
C	2.01178	14.19270	4.98946
H	2.61025	14.47703	4.13679
C	2.50725	13.93107	6.32130
C	3.90002	14.06488	6.77215
C	4.99717	13.91660	5.90720
C	6.31623	14.06372	6.31876
C	6.59822	14.36949	7.64670
C	5.54450	14.52863	8.53997
C	4.23215	14.38148	8.10031
C	1.47098	10.36386	6.27729
H	1.32049	10.07933	7.30810
C	0.44698	10.55483	5.30089
H	-0.61582	10.45430	5.47619
C	1.06714	10.93578	4.06880
H	0.55673	11.18016	3.14694
C	2.47911	10.98187	4.27557
H	3.21998	11.25371	3.53898
C	2.74666	10.60774	5.64463
C	4.06926	10.45227	6.26637
C	5.21030	10.10597	5.52358
C	6.46645	9.93729	6.09879
C	6.63044	10.10408	7.46937
C	5.52576	10.43912	8.24636
C	4.28396	10.60666	7.64602

B3LYP-D/TZVP

Fe	1.50713	12.28196	5.54075
F	4.74444	13.38937	4.63014
F	7.27331	13.41507	5.49149
F	7.84757	14.00507	8.09059
F	5.81822	14.56587	9.82532
F	3.27857	14.55328	8.99642

F	5.13380	9.95554	4.21938
F	7.55358	9.88451	5.34985
F	7.86223	10.42201	8.00460
F	5.68005	11.05540	9.51381
F	3.24675	11.14622	8.41303
C	1.35196	13.61552	7.12005
H	1.37387	13.33287	8.15765
C	0.19759	13.70804	6.30044
H	-0.81326	13.50086	6.61228
C	0.61094	14.07865	4.98939
H	-0.03065	14.20625	4.13258
C	2.02313	14.21406	4.99158
H	2.63737	14.46688	4.14497
C	2.49741	13.93595	6.31779
C	3.89311	13.97968	6.77156
C	4.96840	13.71137	5.91621
C	6.28676	13.71687	6.34291
C	6.58303	14.00634	7.66832
C	5.54693	14.28304	8.54911
C	4.23350	14.26948	8.09822
C	1.49248	10.34671	6.28828
H	1.36138	10.09045	7.32518
C	0.46148	10.49440	5.32497
H	-0.59380	10.37532	5.51127
C	1.05898	10.86266	4.08663
H	0.53574	11.07944	3.16927
C	2.46257	10.94194	4.27640
H	3.19006	11.22018	3.53439
C	2.74768	10.61465	5.64398
C	4.07569	10.54761	6.26552
C	5.22391	10.23551	5.52835
C	6.49000	10.19026	6.09640
C	6.65035	10.45529	7.44895
C	5.53556	10.76678	8.21578
C	4.28218	10.80463	7.62617

TPSS-D/TZVP

Fe	1.51120	12.28137	5.54079
F	4.75629	13.43110	4.59613
F	7.29476	13.50117	5.44523
F	7.87540	14.05090	8.06358
F	5.83418	14.54143	9.82390
F	3.28528	14.49314	9.00547
F	5.14043	9.98779	4.22338
F	7.56047	9.87476	5.36893
F	7.86187	10.36777	8.04473
F	5.66782	11.00222	9.55599
F	3.23606	11.13962	8.43884
C	1.35109	13.57102	7.11585
H	1.37595	13.28791	8.15706
C	0.18880	13.65265	6.29010
H	-0.82325	13.43426	6.60316
C	0.60148	14.02565	4.97119

H	-0.04262	14.14439	4.11024
C	2.02119	14.17630	4.97216
H	2.63392	14.43830	4.12260
C	2.50019	13.90917	6.30880
C	3.89543	13.96322	6.75891
C	4.97823	13.73099	5.89537
C	6.30197	13.75810	6.31471
C	6.60166	14.02888	7.64659
C	5.56135	14.26914	8.53806
C	4.24361	14.23679	8.09130
C	1.47973	10.38598	6.30187
H	1.34569	10.12320	7.34062
C	0.44446	10.54525	5.33229
H	-0.61511	10.43494	5.52037
C	1.04755	10.91661	4.08828
H	0.52408	11.14039	3.16853
C	2.46098	10.98719	4.27940
H	3.19313	11.26558	3.53676
C	2.74478	10.64412	5.65294
C	4.07030	10.56746	6.27689
C	5.22559	10.25535	5.54301
C	6.49134	10.18751	6.11771
C	6.64827	10.42971	7.47831
C	5.52892	10.74109	8.24466
C	4.27752	10.80358	7.64529

Optimised structures of (c)
B3LYP/TZVP:UFF

C	0.75070	1.68160	-2.32300
C	1.93890	2.02340	-2.94980
C	2.18600	3.25070	-3.79560
H	3.26120	3.51890	-3.80010
H	1.66600	4.13080	-3.36890
C	1.70840	3.02450	-5.22500
H	1.90270	3.93440	-5.83070
H	0.61750	2.81450	-5.23770
H	2.25140	2.16960	-5.68140
C	2.81290	0.95860	-2.75050
C	2.13150	0.01520	-1.95790
C	2.64160	-1.21180	-1.42980
C	4.09850	-1.45110	-1.45700
C	4.69890	-2.19060	-2.50820
H	4.07980	-2.62750	-3.28180
C	6.11290	-2.30780	-2.60160
H	6.55140	-2.83920	-3.43590
C	6.95260	-1.71620	-1.63330
H	8.03090	-1.76730	-1.70130
C	6.31800	-1.08770	-0.57330
C	4.96500	-0.96920	-0.47640
C	1.79730	-2.26750	-0.97880
C	2.15910	-3.36820	-0.18270
C	3.47080	-3.62720	0.50920
H	3.75080	-2.75370	1.12580

H	4.26170	-3.84060	-0.23710
H	3.41720	-4.49850	1.18930
C	1.04620	-4.19820	-0.11500
C	0.95110	-5.51120	0.62530
H	-0.10510	-5.80470	0.78260
H	1.39210	-5.40920	1.63830
C	1.65640	-6.62200	-0.14520
H	1.57270	-7.57530	0.41760
H	2.73230	-6.38460	-0.28170
H	1.18350	-6.75440	-1.14190
C	0.05070	-3.58800	-0.86440
C	0.63390	3.66070	0.74390
C	1.81580	4.19090	0.03020
C	1.81450	5.54380	-0.68840
H	2.55380	5.52770	-1.50680
H	0.82220	5.71520	-1.14120
C	2.15520	6.73070	0.27020
H	2.13520	7.68200	-0.28380
H	3.15790	6.60020	0.70440
H	1.42690	6.79000	1.09300
C	2.84650	3.28590	0.10430
C	4.19210	3.46560	-0.60510
H	4.61750	2.50320	-0.92500
H	4.93050	3.97160	0.04070
H	4.05980	4.09240	-1.49900
C	2.41050	2.11400	0.93430
C	3.10020	1.03290	1.44790
C	4.57790	0.94430	1.29270
C	5.44110	1.93180	1.82080
H	5.02980	2.79270	2.33280
C	6.83820	1.85770	1.60320
H	7.47250	2.67700	1.91510
C	7.39920	0.76320	0.91780
H	8.43730	0.75990	0.61330
C	6.56050	-0.30750	0.63170
C	5.17870	-0.19240	0.75060
C	2.45030	-0.07880	2.18950
C	2.96550	-1.00700	3.13240
C	4.32940	-0.97490	3.82720
H	4.69470	0.05590	3.95230
H	5.09310	-1.54160	3.26530
H	4.25410	-1.42760	4.82750
C	1.97430	-2.01790	3.36300
C	2.11030	-3.23030	4.28790
H	3.17090	-3.53030	4.34490
H	1.55380	-4.08270	3.85980
C	1.57830	-2.96330	5.73400
H	1.70070	-3.86120	6.35980
H	0.51040	-2.69850	5.70840
H	2.12810	-2.13370	6.20390
C	0.82940	-1.69970	2.60470
C	-0.41180	-2.45630	2.43300
H	-0.35120	-3.52400	2.67420

C	-1.62400	-1.96280	2.03180
C	-2.89370	-2.69160	1.78780
C	-3.02110	-4.21340	1.79790
H	-2.05070	-4.68870	1.59840
H	-3.73950	-4.54970	1.03330
H	-3.37880	-4.57300	2.77870
C	-3.90080	-1.78160	1.57650
C	-5.37080	-2.07980	1.27050
H	-5.76930	-1.29120	0.60920
H	-5.43740	-3.03720	0.72530
C	-6.25690	-2.16510	2.55500
H	-7.30180	-2.37650	2.27950
H	-6.22720	-1.21650	3.11180
H	-5.90120	-2.96790	3.21830
C	-3.35000	-0.41080	1.69950
C	-4.02600	0.77940	1.76880
H	-5.12070	0.74570	1.77870
C	-3.41770	2.10480	1.83550
C	-3.97730	3.36380	2.15120
C	-5.38270	3.60490	2.70930
H	-6.03410	2.74940	2.46100
H	-5.82080	4.50110	2.23390
C	-5.39200	3.80360	4.26030
H	-6.41890	3.97940	4.61730
H	-4.77170	4.66680	4.54430
H	-4.99470	2.91060	4.76610
C	-2.98210	4.36880	1.90630
C	-3.15320	5.87320	2.10030
H	-2.46720	6.43400	1.44670
H	-2.94630	6.17580	3.14230
H	-4.18410	6.18050	1.86290
C	-1.80640	3.72810	1.45520
C	-0.56740	4.29480	0.93550
H	-0.62500	5.34760	0.63630
C	4.16020	0.81900	-3.40930
H	4.17190	-0.09290	-4.03820
H	4.96430	0.78200	-2.64890
H	4.38870	1.66390	-4.08480
N	0.88490	0.48590	-1.70670
H	0.19550	0.07470	-1.04330
N	0.51680	-2.43180	-1.38850
N	1.10950	-0.47830	1.94040
N	-1.89450	-0.54390	1.78460
H	-1.46780	0.08420	2.51540
N	-2.06110	2.33150	1.47880
N	0.96720	2.29530	1.14180
H	0.64650	2.04010	2.11120
N	-2.07060	0.72450	-2.17510
H	-1.46210	-0.03370	-2.54810
N	-2.45730	-2.12680	-1.57210
H	-1.86360	-1.49590	-0.99220
C	-1.19460	-4.16430	-1.17120
H	-1.30720	-5.22380	-1.00400

C	-2.30060	-3.46220	-1.67220
C	-3.44130	-4.02510	-2.24020
C	-3.72450	-5.47490	-2.51580
H	-2.88500	-6.13380	-2.22450
H	-3.90440	-5.61660	-3.60160
H	-4.62930	-5.78660	-1.95350
C	-4.30010	-2.97130	-2.52490
C	-5.65760	-3.07500	-3.17140
H	-5.79230	-2.24930	-3.90200
H	-5.74230	-4.02640	-3.73680
C	-6.76600	-3.02910	-2.12520
H	-7.75220	-3.12670	-2.62550
H	-6.74570	-2.06680	-1.57330
H	-6.64890	-3.86710	-1.40550
C	-3.64870	-1.81120	-2.12420
C	-4.16990	-0.51120	-2.22510
H	-5.22320	-0.40820	-2.44290
C	-3.41580	0.66420	-2.08370
C	-3.93630	1.95020	-1.98440
C	-5.38800	2.35140	-2.08280
H	-5.85520	1.84090	-2.95150
H	-5.47810	3.44320	-2.26220
C	-6.15400	2.00960	-0.81280
H	-7.22430	2.27430	-0.94190
H	-5.74820	2.59600	0.03330
H	-6.08320	0.92670	-0.58400
C	-2.84680	2.81210	-1.95390
C	-2.92340	4.31030	-1.87010
H	-1.92900	4.77140	-1.71370
H	-3.56610	4.59870	-1.01250
H	-3.36440	4.71300	-2.80530
C	-1.70790	2.01840	-2.07470
C	-0.40410	2.48580	-2.29610
H	-0.29370	3.52820	-2.54790
H	0.05630	-1.89440	-2.15430
H	0.52390	-0.08720	1.17200
H	-1.50080	1.64030	0.92870

B3LYP/TZVP

C	18.41998	6.31633	5.93668
C	19.47164	6.26007	4.93736
C	20.49874	5.16554	4.87519
H	20.88273	5.09111	3.85610
H	20.01699	4.20519	5.07801
C	21.67359	5.35893	5.84992
H	22.37789	4.52658	5.77575
H	21.32480	5.41777	6.88206
H	22.21635	6.28089	5.63043
C	19.44474	7.40177	4.19112
C	18.30491	8.21344	4.61519
C	17.82657	9.40188	4.12886
C	18.38403	10.02413	2.89749
C	18.99350	11.31266	3.02596

H	19.02805	11.75082	4.01585
C	19.53769	12.01029	1.96870
H	19.99757	12.97426	2.15280
C	19.50541	11.49169	0.65109
H	19.92316	12.04329	-0.18183
C	18.91166	10.27017	0.51942
C	18.36136	9.53077	1.60708
C	16.84156	10.22733	4.83701
C	15.95927	11.19722	4.35941
C	15.64062	11.52180	2.93103
H	15.75384	10.65204	2.28797
H	16.28506	12.31083	2.53044
H	14.60903	11.86851	2.83873
C	15.35247	11.82253	5.48323
C	14.33242	12.92398	5.43482
H	13.73399	12.91607	6.34913
H	13.62633	12.73188	4.62069
C	14.93971	14.32369	5.24148
H	14.15926	15.08848	5.20604
H	15.50967	14.38034	4.31183
H	15.62024	14.57018	6.05989
C	15.84602	11.20961	6.63544
C	17.23262	2.74729	2.13965
C	18.44666	3.00485	1.38742
C	19.45583	1.94606	1.05577
H	20.45088	2.39323	0.99396
H	19.49979	1.21916	1.87065
C	19.15906	1.21232	-0.26388
H	19.90791	0.43937	-0.45304
H	19.16764	1.90629	-1.10656
H	18.17781	0.73391	-0.23950
C	18.50366	4.33256	1.07121
C	19.66492	5.00196	0.40192
H	19.81521	6.01248	0.77621
H	19.52998	5.08506	-0.67873
H	20.58203	4.43670	0.57592
C	17.29009	4.98464	1.57188
C	16.82656	6.26914	1.41989
C	17.43336	7.16747	0.40518
C	17.43962	6.75754	-0.96390
H	16.99230	5.79906	-1.19857
C	17.96402	7.51983	-1.98906
H	17.92406	7.14034	-3.00347
C	18.54227	8.78520	-1.74004
H	18.96330	9.37969	-2.54116
C	18.52332	9.19187	-0.43457
C	17.96962	8.42470	0.62803
C	15.66713	6.79063	2.14317
C	14.70320	7.72712	1.77002
C	14.50120	8.35999	0.42406
H	14.88840	7.73982	-0.38193
H	14.99531	9.33392	0.34421
H	13.43885	8.52374	0.23212

C	13.87009	7.96630	2.90144
C	12.66492	8.86130	2.94914
H	12.81155	9.70330	2.26770
H	12.57351	9.29868	3.94767
C	11.34912	8.14836	2.59602
H	10.50373	8.84084	2.63497
H	11.15182	7.33165	3.29380
H	11.38878	7.72126	1.59121
C	14.31503	7.15716	3.93768
C	13.80162	7.04538	5.28840
H	13.39617	7.95096	5.72196
C	13.67192	5.90250	6.00846
C	13.09204	5.73089	7.33490
C	12.66539	6.87624	8.19247
H	13.49693	7.55704	8.39195
H	12.27436	6.53376	9.15001
H	11.88096	7.46231	7.70371
C	13.00075	4.39742	7.60081
C	12.42665	3.74329	8.82256
H	12.97271	2.81824	9.02648
H	12.59165	4.38557	9.69055
C	10.92488	3.43212	8.70228
H	10.55977	2.93180	9.60255
H	10.72288	2.78344	7.84774
H	10.34553	4.34790	8.56610
C	13.54166	3.65757	6.46743
C	13.60792	2.31214	6.28547
H	13.13519	1.68967	7.03324
C	14.24821	1.61617	5.20553
C	14.14817	0.27729	4.82994
C	13.20531	-0.73436	5.41127
H	13.03630	-0.51800	6.47022
H	13.67282	-1.72330	5.37944
C	11.84595	-0.80102	4.69529
H	11.20063	-1.55819	5.14872
H	11.96928	-1.05173	3.63950
H	11.33133	0.16082	4.74889
C	15.06186	0.05762	3.76165
C	15.27286	-1.23596	3.03754
H	16.14304	-1.19273	2.38137
H	14.41367	-1.50036	2.41232
H	15.42698	-2.06447	3.73467
C	15.70870	1.26432	3.49859
C	16.79585	1.54357	2.60577
H	17.35301	0.67784	2.27450
C	20.50340	7.80887	3.21376
H	20.83048	8.83404	3.39416
H	20.15810	7.76869	2.18026
H	21.37321	7.15800	3.29962
N	17.76453	7.55596	5.75695
H	16.75781	7.59015	5.86024
N	16.72963	10.23286	6.21893
N	15.37685	6.41608	3.44942

N	14.02372	4.61885	5.55919
H	13.95412	4.42873	4.56940
N	15.16339	2.21574	4.34936
N	16.61510	3.99593	2.32256
H	15.60765	4.04281	2.37415
N	16.93265	6.64534	8.66939
H	16.55557	7.37519	8.08958
N	15.96457	9.33650	9.13734
H	16.92748	9.21857	8.85545
C	15.43569	11.46459	7.99287
H	14.95105	12.42149	8.13476
C	15.44755	10.65661	9.08194
C	14.79575	10.90591	10.36092
C	14.07192	12.17525	10.67364
H	14.71903	13.04595	10.53472
H	13.71032	12.18900	11.70143
H	13.20717	12.31077	10.01609
C	14.90157	9.79052	11.13816
C	14.30084	9.55953	12.49350
H	14.98351	8.95096	13.09325
H	14.21310	10.51430	13.01723
C	12.92141	8.88015	12.45241
H	12.53926	8.71845	13.46330
H	12.97386	7.91190	11.95171
H	12.19949	9.49533	11.91153
C	15.64650	8.77925	10.40485
C	15.94244	7.50718	10.78074
H	15.66372	7.21711	11.78468
C	16.59050	6.49317	10.00147
C	17.02775	5.22498	10.39521
C	16.89384	4.63101	11.76800
H	16.94054	5.42460	12.51885
H	17.75401	3.98506	11.96757
C	15.60357	3.82026	11.97649
H	15.55910	3.40647	12.98774
H	15.54136	2.99109	11.26893
H	14.72067	4.44573	11.82734
C	17.62668	4.60764	9.26895
C	18.29067	3.26478	9.25882
H	18.44380	2.89440	8.24480
H	17.68748	2.51936	9.78223
H	19.26946	3.28819	9.75124
C	17.56493	5.51058	8.19937
C	18.23894	5.41134	6.94052
H	18.81399	4.50261	6.83043
H	17.37521	9.73319	6.80534
H	16.02961	5.91536	4.03214
H	15.66549	3.05201	4.60793

TPSS/TZVP

C	18.56260	6.52028	5.84248
C	19.61708	6.51230	4.85476
C	20.73189	5.50242	4.83998

H	21.15396	5.44631	3.83142
H	20.32258	4.50673	5.05247
C	21.85855	5.81569	5.84885
H	22.63211	5.03992	5.81477
H	21.46737	5.86784	6.86965
H	22.32890	6.77781	5.61980
C	19.51379	7.63758	4.07020
C	18.32991	8.38179	4.47462
C	17.81328	9.56509	3.97346
C	18.32514	10.09449	2.68648
C	18.93311	11.39347	2.67657
H	18.97919	11.92779	3.62228
C	19.47157	11.97992	1.54364
H	19.93675	12.95939	1.62522
C	19.44049	11.32299	0.28392
H	19.86153	11.78605	-0.60413
C	18.84929	10.08562	0.28109
C	18.29554	9.46258	1.44491
C	16.86929	10.42360	4.68670
C	16.08970	11.51243	4.24510
C	15.86932	12.00377	2.84222
H	16.05295	11.22423	2.10273
H	16.52447	12.84798	2.58996
H	14.83509	12.34931	2.72299
C	15.46875	12.09107	5.38480
C	14.55812	13.28819	5.38209
H	13.84121	13.21579	6.20922
H	13.95841	13.28741	4.46276
C	15.30942	14.63331	5.48193
H	14.60755	15.47594	5.46618
H	16.00592	14.75415	4.64551
H	15.88980	14.68627	6.40947
C	15.83508	11.33906	6.51418
C	17.02955	2.57858	2.12785
C	18.30146	2.83478	1.60747
C	19.36876	1.80453	1.35826
H	20.34668	2.21305	1.64643
H	19.19821	0.93713	2.00736
C	19.44369	1.33213	-0.10961
H	20.23728	0.58645	-0.23971
H	19.65203	2.17099	-0.78194
H	18.49523	0.88192	-0.42269
C	18.41489	4.23956	1.39030
C	19.66370	4.91060	0.89619
H	19.69468	5.96392	1.17513
H	19.75144	4.86201	-0.19741
H	20.55049	4.41942	1.31560
C	17.19595	4.83404	1.75700
C	16.71306	6.20531	1.59365
C	17.34190	6.98712	0.50540
C	17.40240	6.40691	-0.80575
H	16.97742	5.41405	-0.92948
C	17.94859	7.04700	-1.90528

H	17.93240	6.54614	-2.87032
C	18.51745	8.34492	-1.80046
H	18.95295	8.84184	-2.66282
C	18.47824	8.90250	-0.54826
C	17.90990	8.25784	0.59627
C	15.67006	6.74796	2.32687
C	14.85714	7.93132	2.07815
C	14.82664	8.73787	0.81238
H	14.89837	8.08922	-0.06638
H	15.65611	9.44981	0.74849
H	13.89211	9.30296	0.74816
C	13.99926	8.10457	3.14019
C	12.93325	9.15388	3.28851
H	13.21606	10.04112	2.71337
H	12.88533	9.47460	4.33684
C	11.53602	8.67448	2.83839
H	10.79251	9.46656	2.98374
H	11.21987	7.79697	3.41108
H	11.54139	8.40104	1.77778
C	14.17760	7.01478	4.07378
C	13.50377	6.82147	5.25657
H	12.92013	7.66850	5.60515
C	13.39620	5.63582	6.04962
C	12.87784	5.46499	7.34240
C	12.50143	6.56339	8.29214
H	12.59121	7.54728	7.82254
H	13.15548	6.56704	9.17360
H	11.47015	6.45400	8.65053
C	12.82511	4.06994	7.61170
C	12.32965	3.42550	8.87749
H	12.84592	2.46997	9.03172
H	12.59672	4.05798	9.73372
C	10.80423	3.18442	8.89144
H	10.49071	2.72490	9.83650
H	10.50607	2.52146	8.07202
H	10.25669	4.12541	8.77222
C	13.30949	3.39576	6.48029
C	13.37244	1.99157	6.21020
H	12.83580	1.35041	6.90237
C	14.01962	1.37450	5.17122
C	14.00543	-0.03072	4.80472
C	13.13154	-1.05519	5.47206
H	13.10726	-0.86408	6.55265
H	13.57407	-2.04995	5.34610
C	11.68585	-1.06947	4.92937
H	11.08248	-1.81469	5.46017
H	11.67453	-1.31553	3.86240
H	11.21212	-0.09072	5.05438
C	14.86137	-0.21560	3.74576
C	15.16405	-1.48752	3.01462
H	16.24026	-1.70368	3.02569
H	14.85907	-1.42194	1.96240
H	14.64564	-2.33883	3.46371

C	15.46066	1.06197	3.40237
C	16.44736	1.31137	2.48972
H	16.88439	0.44264	2.00637
C	20.56509	8.08962	3.09747
H	20.79226	9.15188	3.23186
H	20.25530	7.96375	2.05484
H	21.48672	7.51963	3.24661
N	17.81821	7.71859	5.63906
H	16.80369	7.64432	5.68414
N	16.67358	10.33252	6.06149
N	15.12343	6.14052	3.48839
N	13.71321	4.36778	5.56387
H	13.75641	4.17491	4.56899
N	14.84197	2.03459	4.22472
N	16.38839	3.80792	2.25689
H	15.38418	3.90410	2.34891
N	17.06062	6.78110	8.59484
H	16.68762	7.53226	8.02845
N	15.96767	9.41104	9.02406
H	16.97172	9.41723	8.85418
C	15.33347	11.51401	7.84793
H	14.77668	12.43750	7.98011
C	15.33879	10.69135	8.93908
C	14.58908	10.88263	10.16798
C	13.73434	12.08461	10.43209
H	14.31246	13.01190	10.33243
H	13.31007	12.05765	11.43937
H	12.90166	12.14405	9.71856
C	14.74438	9.77404	10.96478
C	14.07733	9.49505	12.28328
H	14.76504	8.93130	12.92631
H	13.88469	10.44354	12.79816
C	12.75185	8.71388	12.15221
H	12.31682	8.52543	13.14034
H	12.91183	7.75039	11.65842
H	12.02473	9.27862	11.55938
C	15.60956	8.83066	10.28419
C	15.97228	7.57092	10.67896
H	15.66584	7.26277	11.67390
C	16.69697	6.59703	9.92050
C	17.18330	5.33430	10.30949
C	17.03097	4.71395	11.67105
H	16.91792	5.50270	12.42495
H	17.95318	4.17755	11.93157
C	15.84067	3.73712	11.77867
H	15.78109	3.30374	12.78434
H	15.94004	2.91783	11.05886
H	14.89635	4.25091	11.56911
C	17.83348	4.76021	9.18834
C	18.52296	3.42766	9.14719
H	19.39983	3.44356	8.49001
H	17.85737	2.63352	8.78221
H	18.86569	3.13226	10.14479

C	17.75090	5.67796	8.11985
C	18.43306	5.61363	6.86718
H	19.05592	4.72993	6.75908
H	17.18395	9.67032	6.63069
H	15.74851	5.61353	4.09143
H	15.43139	2.79040	4.56568

B3LYP-D/TZVP

C	18.21807	5.93412	5.41634
C	19.28562	5.96655	4.43006
C	20.28609	4.86230	4.27037
H	20.71660	4.90581	3.26951
H	19.77332	3.89922	4.32716
C	21.40586	4.91615	5.32231
H	22.10429	4.08591	5.19079
H	20.99445	4.86131	6.33162
H	21.96746	5.84983	5.24256
C	19.30525	7.19067	3.83102
C	18.18718	7.98095	4.34415
C	17.73879	9.22868	4.00344
C	18.29310	9.97666	2.84986
C	18.85031	11.27425	3.07685
H	18.84907	11.64758	4.09362
C	19.38196	12.05708	2.07298
H	19.80038	13.02438	2.32543
C	19.39705	11.62475	0.72140
H	19.81377	12.24481	-0.06215
C	18.84830	10.39566	0.49516
C	18.29640	9.58202	1.52919
C	16.71994	9.94478	4.76919
C	15.77038	10.86179	4.34354
C	15.49183	11.29658	2.93743
H	15.64264	10.48348	2.23131
H	16.14511	12.12134	2.63613
H	14.46151	11.63860	2.83539
C	15.06223	11.32004	5.49498
C	13.91584	12.28632	5.49005
H	13.35138	12.19255	6.42125
H	13.21667	12.01821	4.69008
C	14.35259	13.74695	5.29913
H	13.49151	14.42031	5.28791
H	14.89196	13.87091	4.35779
H	15.02054	14.05840	6.10574
C	15.59170	10.68254	6.60833
C	17.50091	3.17941	2.65106
C	18.63566	3.35401	1.76320
C	19.71109	2.32536	1.59524
H	20.64593	2.80837	1.30386
H	19.90773	1.84430	2.55738
C	19.34863	1.25631	0.55117
H	20.14309	0.51168	0.46212
H	19.19531	1.71185	-0.42959
H	18.42566	0.74121	0.82433

C	18.55343	4.57561	1.16406
C	19.59552	5.14395	0.25243
H	19.74716	6.20682	0.42253
H	19.32369	5.03149	-0.79917
H	20.54993	4.63804	0.40129
C	17.31862	5.23150	1.61092
C	16.77817	6.44354	1.27166
C	17.40251	7.29332	0.22912
C	17.43328	6.91077	-1.14194
H	16.99677	5.95535	-1.40777
C	17.98129	7.70635	-2.13128
H	17.97007	7.35516	-3.15637
C	18.54604	8.97251	-1.84025
H	18.97343	9.58783	-2.62189
C	18.50340	9.34951	-0.52524
C	17.93992	8.53383	0.49362
C	15.60441	7.03391	1.90442
C	14.68920	7.95967	1.40393
C	14.55957	8.46863	-0.00033
H	14.85997	7.72332	-0.73425
H	15.18039	9.35418	-0.17217
H	13.52594	8.74632	-0.21459
C	13.84729	8.35885	2.47889
C	12.68413	9.30108	2.39879
H	12.87384	10.05048	1.62639
H	12.59611	9.85673	3.33689
C	11.35462	8.58870	2.10700
H	10.52727	9.30082	2.04568
H	11.12816	7.86575	2.89358
H	11.40597	8.04278	1.16196
C	14.23940	7.66036	3.61131
C	13.70773	7.76598	4.94135
H	13.20543	8.69515	5.17193
C	13.70741	6.81304	5.90345
C	13.09914	6.87148	7.22365
C	12.45605	8.10343	7.76776
H	13.05839	8.98719	7.55397
H	12.32847	8.04306	8.84805
H	11.46926	8.25876	7.31922
C	13.17892	5.63665	7.79359
C	12.61977	5.19931	9.10984
H	13.35453	4.57111	9.61804
H	12.47597	6.07248	9.74556
C	11.28865	4.44142	8.97522
H	10.92087	4.12689	9.95500
H	11.40047	3.55271	8.35187
H	10.52906	5.07538	8.51300
C	13.86947	4.74078	6.87850
C	14.12981	3.41950	7.03250
H	13.74642	2.94575	7.92483
C	14.85778	2.56755	6.14273
C	14.94612	1.17937	6.15561
C	14.18673	0.26356	7.06818

H	14.18718	0.66846	8.08547
H	14.70392	-0.69810	7.12843
C	12.73377	0.03474	6.62120
H	12.20814	-0.63572	7.30641
H	12.69988	-0.40355	5.62124
H	12.19135	0.98205	6.58439
C	15.82341	0.79101	5.10545
C	16.18658	-0.61691	4.75083
H	16.78649	-0.66182	3.84136
H	15.29565	-1.22931	4.58336
H	16.75830	-1.09823	5.55113
C	16.26579	1.94887	4.47295
C	17.25189	2.10121	3.44469
H	17.89758	1.24692	3.29699
C	20.38235	7.68967	2.92078
H	20.69802	8.69414	3.20567
H	20.05519	7.74833	1.88316
H	21.25181	7.03389	2.96124
N	17.61538	7.19302	5.36642
H	16.69132	7.39115	5.71354
N	16.57144	9.80951	6.15257
N	15.26616	6.80545	3.23441
N	14.26464	5.52423	5.77301
H	14.25472	5.09598	4.85751
N	15.62789	3.02753	5.07779
N	16.76469	4.36731	2.57465
H	15.77062	4.36506	2.74358
N	16.61258	5.96018	8.09224
H	15.97188	6.49629	7.52608
N	15.60927	8.57345	8.87524
H	16.32236	8.27324	8.23765
C	15.18537	10.82989	7.98596
H	14.73493	11.78179	8.23285
C	15.17959	9.89568	8.97213
C	14.58990	10.02503	10.30118
C	13.95447	11.28764	10.78177
H	14.65950	12.12297	10.74940
H	13.58873	11.19306	11.80361
H	13.10427	11.56157	10.14860
C	14.67851	8.82535	10.93980
C	14.16984	8.47408	12.30577
H	14.90582	7.84281	12.81237
H	14.09095	9.38317	12.90548
C	12.81066	7.75688	12.29320
H	12.46600	7.55754	13.31058
H	12.87630	6.80422	11.76691
H	12.05593	8.36551	11.79038
C	15.33539	7.87256	10.05342
C	15.58647	6.55452	10.27798
H	15.29970	6.16570	11.24462
C	16.22045	5.62652	9.39468
C	16.65920	4.32987	9.64495
C	16.48783	3.55282	10.91471

H	16.22438	4.22520	11.73462
H	17.44264	3.09759	11.19874
C	15.42477	2.44742	10.79926
H	15.35506	1.86824	11.72357
H	15.66290	1.76093	9.98434
H	14.44205	2.87489	10.59066
C	17.31121	3.85611	8.47242
C	17.94304	2.51249	8.28763
H	18.89894	2.58228	7.76255
H	17.29574	1.85272	7.70025
H	18.13211	2.02579	9.24574
C	17.27352	4.87252	7.52276
C	17.97407	4.90624	6.28028
H	18.52058	3.99919	6.06317
H	17.34533	9.51302	6.72668
H	15.94999	6.45728	3.88795
H	16.10352	3.92013	5.13783

TPSS-D/TZVP

C	18.36592	6.21600	5.21554
C	19.49085	6.40221	4.33880
C	20.64042	5.43920	4.27908
H	21.22847	5.62721	3.37676
H	20.25177	4.41803	4.18390
C	21.55421	5.53596	5.51931
H	22.37124	4.80797	5.45683
H	20.98610	5.34148	6.43466
H	21.99051	6.53748	5.60032
C	19.42015	7.66102	3.77488
C	18.19907	8.29629	4.22804
C	17.63756	9.51729	3.86088
C	18.15171	10.18902	2.65654
C	18.59352	11.55284	2.70529
H	18.51206	12.07222	3.65709
C	19.13105	12.21389	1.61398
H	19.46467	13.24180	1.73414
C	19.27996	11.58060	0.34504
H	19.70632	12.11185	-0.50097
C	18.85138	10.27950	0.28579
C	18.28823	9.59258	1.40813
C	16.58388	10.18319	4.59823
C	15.67735	11.18676	4.19480
C	15.51578	11.79426	2.83282
H	15.75094	11.07831	2.04296
H	16.17491	12.65943	2.68768
H	14.48611	12.14020	2.69272
C	14.87818	11.52825	5.31762
C	13.78600	12.55966	5.35103
H	13.08994	12.33264	6.16760
H	13.19777	12.50395	4.42489
C	14.32288	13.99665	5.51588
H	13.50350	14.72518	5.53182
H	14.99511	14.25473	4.69077

H	14.88860	14.09131	6.44925
C	15.28436	10.73644	6.40215
C	17.48842	2.97429	2.91501
C	18.71295	3.15206	2.25389
C	19.82436	2.14290	2.19143
H	20.79004	2.64970	2.32210
H	19.73313	1.44265	3.03049
C	19.84780	1.35619	0.86464
H	20.67229	0.63346	0.84883
H	19.97101	2.03545	0.01451
H	18.90761	0.81195	0.72332
C	18.72390	4.44973	1.68084
C	19.90199	5.03249	0.95735
H	19.97915	6.10949	1.11642
H	19.84479	4.87236	-0.12655
H	20.82799	4.56368	1.30773
C	17.48589	5.06415	1.97557
C	16.96372	6.35717	1.58828
C	17.62620	7.06191	0.47871
C	17.80683	6.44871	-0.80406
H	17.45974	5.42559	-0.92636
C	18.37417	7.10889	-1.88106
H	18.45942	6.58793	-2.83166
C	18.82925	8.45752	-1.78709
H	19.26886	8.96137	-2.64308
C	18.66813	9.04808	-0.56008
C	18.08856	8.36917	0.55771
C	15.88508	6.99482	2.19731
C	15.09334	8.12077	1.73964
C	15.08449	8.71802	0.36134
H	15.32462	7.96936	-0.39793
H	15.81777	9.52623	0.25685
H	14.09583	9.13255	0.13988
C	14.21810	8.47260	2.74755
C	13.10914	9.48185	2.68819
H	13.31674	10.20931	1.89877
H	13.08663	10.04609	3.62924
C	11.73202	8.83086	2.43958
H	10.94229	9.59064	2.42113
H	11.49794	8.10689	3.22648
H	11.72320	8.30120	1.48079
C	14.38798	7.56913	3.85307
C	13.71962	7.63033	5.05724
H	13.16236	8.54555	5.22867
C	13.58888	6.63800	6.06187
C	12.90157	6.69886	7.29462
C	12.24247	7.91446	7.87763
H	12.54907	8.82861	7.36163
H	12.50206	8.03878	8.93533
H	11.14854	7.84111	7.81368
C	12.90966	5.40337	7.85789
C	12.27476	4.99745	9.15522
H	12.87809	4.21661	9.63320

H	12.28623	5.85461	9.83805
C	10.82380	4.49892	8.99034
H	10.39132	4.22044	9.95877
H	10.78593	3.62444	8.33155
H	10.19540	5.27777	8.54520
C	13.58759	4.54723	6.96705
C	13.77263	3.14169	7.02811
H	13.23231	2.62653	7.81418
C	14.53129	2.36043	6.19003
C	14.61384	0.91724	6.16925
C	13.76671	0.02237	7.02740
H	13.67570	0.45542	8.03133
H	14.26632	-0.94482	7.15463
C	12.35660	-0.20085	6.44024
H	11.75749	-0.84001	7.09877
H	12.42060	-0.68027	5.45776
H	11.83488	0.75349	6.31586
C	15.52023	0.54509	5.20094
C	15.91534	-0.84118	4.79478
H	17.00073	-0.98297	4.87767
H	15.64191	-1.03925	3.75064
H	15.42849	-1.59427	5.42002
C	16.04387	1.73861	4.57448
C	17.01517	1.81776	3.61002
H	17.51295	0.88659	3.35593
C	20.52530	8.30014	2.98362
H	20.60498	9.36739	3.20758
H	20.36893	8.21219	1.90251
H	21.48062	7.82264	3.22317
N	17.66268	7.44147	5.22461
H	16.66209	7.47704	5.39808
N	16.28937	9.89575	5.93197
N	15.31002	6.58432	3.42630
N	14.03648	5.32876	5.90757
H	14.23753	4.92628	4.99887
N	15.36708	2.84474	5.14967
N	16.77451	4.15945	2.76487
H	15.77406	4.22165	2.91083
N	16.64608	5.98014	7.76376
H	16.86927	6.95366	7.59035
N	15.42778	8.50318	8.53020
H	15.09918	8.03960	7.67904
C	14.82861	10.78147	7.75729
H	14.31734	11.69554	8.04478
C	14.93359	9.81917	8.72850
C	14.55044	9.92805	10.11722
C	14.05659	11.19869	10.73715
H	14.77986	12.01223	10.60114
H	13.87535	11.07755	11.80850
H	13.11481	11.52146	10.27360
C	14.73617	8.70561	10.72399
C	14.46330	8.34636	12.15676
H	15.24664	7.66847	12.51877

H	14.52343	9.24740	12.77771
C	13.08299	7.68487	12.35616
H	12.91003	7.45444	13.41345
H	13.01177	6.75295	11.78654
H	12.28361	8.34990	12.01209
C	15.23874	7.77455	9.73832
C	15.53428	6.44417	9.91905
H	15.28530	6.02148	10.88691
C	16.16246	5.56153	8.99989
C	16.49222	4.19578	9.13676
C	16.23724	3.33548	10.34363
H	15.87500	3.95676	11.17098
H	17.19848	2.91903	10.67882
C	15.25526	2.17060	10.11962
H	15.20065	1.53322	11.01005
H	15.56615	1.55391	9.27113
H	14.25146	2.54740	9.90456
C	17.20795	3.80597	7.98063
C	17.78797	2.45102	7.70312
H	18.66784	2.51593	7.05404
H	17.06847	1.78585	7.20918
H	18.09671	1.96477	8.63560
C	17.32790	4.93796	7.14447
C	18.12097	5.09170	5.97937
H	18.71742	4.22446	5.71337
H	16.93611	9.41895	6.54899
H	15.93268	6.14211	4.09701
H	15.95098	3.65511	5.37489