Supplementary Materials

A Mechanistic Study for The Photochemical Reactions of d^6 $M(CO)_5(CS)$ (M = Cr, Mo and W) Complexes

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(All were calculated at the CAS(12,10)/Def2-SVPD (geometry) and the MP2-CAS(12,10)/Def2-SVPD//CAS(12,10)/Def2-SVPD (energy) level of theory)

(1) Cr-S_0-Rea

Atomic Number	Coordinates (Angstroms) X	Y	Z
24	-0.001161	-0.002494	-0.000983
6	-0.003049	-0.003940	2.007295
6	2.008572	-0.001767	0.000851
6	0.002841	0.077570	-2.009528
6	-2.008199	0.076503	-0.001473
6	-0.032949	-2.087682	-0.041273
6	0.031303	1.817804	0.036731
8	-0.003295	0.041549	3.144745
8	3.145514	0.056287	0.003096
8	0.006008	0.173863	-3.143881
8	-3.143162	0.165992	-0.001216
8	-0.038479	-3.222315	-0.059410
16	0.049966	3.433950	0.070527

CAS-MP2/Def2-SVPD = -696.9050455

(2) Cr-S_1-FC

Atomic Number	Coordinates (Angstroms) X	Y	Z
24	-0.001161	-0.002494	-0.000983
6	-0.003049	-0.003940	2.007295
6	2.008572	-0.001767	0.000851
6	0.002841	0.077570	-2.009528
6	-2.008199	0.076503	-0.001473

6	-0.032949	-2.087682	-0.041273
6	0.031303	1.817804	0.036731
8	-0.003295	0.041549	3.144745
8	3.145514	0.056287	0.003096
8	0.006008	0.173863	-3.143881
8	-3.143162	0.165992	-0.001216
8	-0.038479	-3.222315	-0.059410
16	0.049966	3.433950	0.070527

CAS-MP2/Def2-SVPD = -696.7640118

(3) Cr-CI-1

Atomic Number	Coordinates (Angstroms) X	Y	Z
24	0.575231	-0.033525	0.002860
6	-0.406978	-0.082807	-1.833763
6	0.519844	1.974396	-0.004758
6	-0.423785	-0.077702	1.831560
6	0.702708	-2.037471	0.000414
6	-3.779831	-0.051266	-0.002867
6	2.507590	0.055580	0.017715
8	-0.891018	-0.107733	-2.863346
8	0.567144	3.117259	-0.013103
8	-0.922620	-0.101344	2.854265
8	0.848831	-3.172060	-0.001342
8	-4.914314	-0.072711	-0.027971
16	4.103643	0.125021	0.021513

Derivative Coupling

-1	0.0067605091	0.0002460607	-0.0002680091
-2	-0.0049613390	-0.0001448329	0.0068546820
-3	-0.0022769983	0.0003915542	0.0000251724
-4	-0.0051837081	-0.0003153848	-0.0066647799
-5	-0.0022315630	-0.0006188899	-0.0002276631
-6	-0.0010456307	-0.0000093894	-0.0000140962
-7	0.0069435766	0.0004035061	0.0002310116
-8	0.0013545457	0.0000409808	-0.0008648784
-9	0.0005278776	-0.0002574313	-0.0000082617
-10	0.0013932537	0.0000842249	0.0009124813

-11	0.0005046445	0.0002935418	0.0000415646
-12	0.0006617266	0.0000192777	0.0000200269
-13	-0.0024468948	-0.0001332179	-0.0000372504

Gradient Difference

-1	0.0010482392	-0.0005452310	0.0000873419
-2	-0.0139180323	-0.0010142967	-0.0090418355
-3	-0.0000576878	0.0002987179	0.0066437352
-4	0.0133119567	0.0002518460	-0.0096893700
-5	-0.0000576378	0.0001230837	0.0067182092
-6	-0.0000625715	0.0000034872	0.0002424147
-7	-0.0005441836	0.0009095235	0.0123867901
-8	0.0025250615	0.0001963531	-0.0003096523
-9	0.0000238697	-0.0000621618	-0.0014542702
-10	-0.0023469784	-0.0000339719	-0.0002306804
-11	0.0000135817	0.0000214833	-0.0014628015
-12	0.0000514198	0.0000063222	-0.0002290732
-13	0.0000129628	-0.0001551555	-0.0036608082

CAS-MP2/Def2-SVPD = -696.8083687

(4) Cr-CI-2

Atomic Number	Coordinates (Angstroms) X	Y	Z
24	0.488731	-0.373083	-0.473507
6	0.465755	1.120862	-1.817630
6	-0.023234	-1.745959	-1.984208
6	0.475366	-1.847984	0.891181
6	-1.154284	3.632347	4.465948
6	2.551863	-0.082093	-0.163017
6	-0.788140	0.517652	0.507917
8	0.406799	1.997314	-2.545174
8	-0.387258	-2.465134	-2.788799
8	0.416204	-2.654823	1.695259
8	-1.299200	4.339863	5.344779
8	3.647676	0.123602	0.067697
16	-1.949101	1.314910	1.380432

Derivative Coupling

-1	0.0190501058	0.0021470384	0.0013503150

-2	0.0016276178	-0.0011643590	-0.0036505292
-3	-0.0002276969	0.0066704993	0.0066242576
-4	0.0013546602	-0.0039036865	-0.0012127776
-5	0.0000271136	-0.0001823336	-0.0002339850
-6	0.0006956653	-0.0058312748	-0.0066913542
-7	-0.0278293587	0.0025856817	0.0042237921
-8	-0.0001741090	0.0009077187	0.0002767145
-9	0.0004341357	-0.0008629020	-0.0007937258
-11	-0.0001477995	0.0002428442	0.0009198266
-12	-0.0000301827	0.0001572852	0.0001900351
-13	-0.0005131900	0.0013619264	0.0015645692
-14	0.0057330385	-0.0021284378	-0.0025671383

Gradient Difference

-1	-0.0048442133	-0.0262277724	-0.0271741284
-2	0.0070672366	0.0009423476	-0.0054212628
-3	0.0176251543	-0.0009838344	-0.0006799064
-4	0.0069293116	-0.0052030559	-0.0005152743
-5	0.0000898118	-0.0002806693	-0.0003633439
-6	-0.0185206856	-0.0005255352	0.0008784680
-7	-0.0103037802	0.0395116396	0.0409245073
-8	-0.0016969527	0.0009447877	-0.0002586485
-9	-0.0040144200	0.0008284075	0.0008234365
-10	-0.0016389704	-0.0003858852	0.0010065307
-11	-0.0001610085	0.0001984223	0.0002333550
-12	0.0022140191	-0.0003204212	-0.0006633827
-13	0.0072544973	-0.0084984311	-0.0087903504

CAS-MP2/Def2-SVPD = -696.8028876

(5) Cr-CI-3

Atomic Number	Coordinates (Angstroms) X	Y	Z
24	-0.773289	-0.042378	0.007222
6	-0.758858	-0.045117	-1.989472
6	0.254308	1.747313	0.027606
6	-0.837552	-0.041484	2.002160
6	0.402508	-1.734407	0.034764
6	-2.835056	-0.116315	-0.035233

6	3.509595	0.053234	-0.046928
8	-0.764051	-0.049041	-3.136258
8	0.818221	2.738282	0.039465
8	-0.879237	-0.039876	3.148335
8	1.051679	-2.672137	0.050284
8	-3.974379	-0.176289	-0.060149
16	5.082781	-0.092235	-0.052256

Derivative Coupling

-1	-0.0002142930	-0.0024388313	0.0000106082
-2	0.0004655672	-0.0001814457	-0.0000660158
-3	-0.0007642024	-0.0012625576	-0.0000141092
-4	0.0004614856	-0.0001696449	0.0000813920
-5	0.0017956499	0.0013382409	0.0000307598
-6	-0.0014681087	0.0027692562	-0.0000386953
-7	0.0003152779	-0.0000159519	-0.0000047300
-8	-0.0001066464	-0.0000640064	0.0000365483
-9	0.0000876492	0.0003409779	0.0000017154
-10	-0.0001049128	-0.0000636314	-0.0000345334
-11	-0.0004820944	-0.0000004867	-0.0000092973
-12	0.0002007840	-0.0002712343	0.0000056514
-13	-0.0001861559	0.0000193154	0.0000007060

Gradient Difference

-1	0.0011786480	0.0003183659	0.0000423859
-2	0.0016415938	-0.0002468497	0.0001453156
-3	-0.0012469181	0.0016592670	-0.0000238974
-4	0.0016154662	-0.0002505132	-0.0001055361
-5	-0.0023519698	-0.0011446694	-0.0000416335
-6	0.0006847642	-0.0006032648	0.0000033788
-7	-0.0000867272	-0.0000108581	0.0000026041
-8	-0.0001556289	0.0000644661	-0.0000071437
-9	-0.0002585199	-0.0002523257	-0.0000055788
-10	-0.0001539732	0.0000646672	0.0000097416
-11	-0.0000674242	0.0002586473	-0.0000037199
-12	-0.0007510627	0.0001353577	-0.0000163242
-13	-0.0000482484	0.0000077097	0.0000004078

CAS-MP2/Def2-SVPD = -696.7495101

(6) Cr-S_0-Prod1

Atomic Number	Coordinates (Angstroms) X	Y	Z
24	0.294367	0.001481	0.017554
6	0.351176	1.547179	-1.292943
6	0.369798	-1.309001	-1.527417
6	0.295553	-1.544460	1.328932
6	0.275159	1.313304	1.562906
6	9.868737	0.046723	0.027019
6	-1.474051	-0.007443	-0.029140
8	0.297653	2.412762	-2.028707
8	0.323692	-2.043452	-2.394647
8	0.207674	-2.410094	2.061228
8	0.177638	2.046529	2.426711
8	11.005861	0.046519	0.064062
16	-3.117556	-0.018050	-0.073333

M062X/Def2-SVPD = -696.8736770

(7) Cr-S_0-Prod2

Atomic Number	Coordinates (Angstroms) X	Y	Z
24	0.235300	-0.407699	0.349423
6	0.311068	1.090699	-0.921834
6	0.157314	-1.775262	-1.128612
6	0.305071	-5.066466	4.298703
6	0.119002	0.827590	1.937462
6	2.347890	-0.565013	0.507596
6	-1.575415	-0.360126	0.285145
8	0.305455	1.963280	-1.662711
8	0.031148	-2.542526	-1.960335
8	0.037407	-5.912047	5.010805
8	-0.027916	1.521029	2.828472
8	3.479053	-0.614256	0.559293
16	-3.199128	-0.341528	0.243717

CAS-MP2/DEF2-SVPD = -696.8644935

(8) Cr-S_0-Prod3

Atomic Number	Coordinates (Angstroms) X	Y	Z
24	0.092175	-0.000208	0.000472
6	0.030079	1.527771	-1.296511
6	0.045894	-1.296824	-1.528282
6	0.021525	-1.528939	1.296117
6	0.005988	1.295783	1.528149
6	2.038581	0.008391	0.016893
6	-8.708623	-0.046651	-0.091220
8	0.029443	2.399232	-2.035607
8	0.054008	-2.035997	-2.399650
8	0.015793	-2.400342	2.035268
8	-0.008425	2.035091	2.399307
8	3.190343	0.012402	0.025263
16	-10.287364	-0.048481	-0.101059

CAS-MP2/DEF2-SVPD = -696.8411261

(9) Mo-S_0-Rea

Atomic Number	Coordinates (Angstroms) X	Y	Z
42	-0.492218	0.005575	0.005548
6	-0.473772	1.403646	-1.625924
6	-0.387528	1.629007	1.385562
6	-0.463905	-1.368940	1.630693
6	-0.528445	-1.621482	-1.376143
6	-2.678277	0.070059	0.048850
6	1.488569	-0.051527	-0.024196
8	-0.450702	2.158725	-2.487374
8	-0.306794	2.495551	2.121935
8	-0.420846	-2.102085	2.502848
8	-0.516978	-2.490843	-2.113153
8	-3.816903	0.106497	0.075065
16	3.092826	-0.098724	-0.032821

CAS-MP2/DEF2-SVPD = -678.2159730

(10) Mo-S_1-FC

Atomic Number	Coordinates (Angstroms) X	Y	Z
42	-0.492218	0.005575	0.005548
6	-0.473772	1.403646	-1.625924
6	-0.387528	1.629007	1.385562
6	-0.463905	-1.368940	1.630693
6	-0.528445	-1.621482	-1.376143
6	-2.678277	0.070059	0.048850
6	1.488569	-0.051527	-0.024196
8	-0.450702	2.158725	-2.487374
8	-0.306794	2.495551	2.121935
8	-0.420846	-2.102085	2.502848
8	-0.516978	-2.490843	-2.113153
8	-3.816903	0.106497	0.075065
16	3.092826	-0.098724	-0.032821

CAS-MP2/DEF2-SVPD = -678.0862539

(11) Mo-CI-1

Atomic Number	Coordinates (Angstroms) X	Y	Z
42	0.792842	0.008882	-0.026340
6	0.978074	0.009758	-2.121917
6	-0.718315	1.626464	-0.092634
6	0.788202	0.009571	2.077270
6	-0.647610	-1.666900	-0.089593
6	-3.949371	-0.194015	0.130694
6	2.782997	0.035486	0.062834
8	1.099865	0.008786	-3.258248
8	-1.432962	2.515278	-0.125923
8	0.807543	0.005359	3.219937
8	-1.337097	-2.575461	-0.123147
8	-5.081774	-0.265102	0.191656

16	4.404050	0.017531	0.136587

Derivative Coupling

-1	0.0161537855	-0.0242816211	0.0007692707
-2	0.0033267896	-0.0018410015	0.0021901355
-3	0.0038959520	0.0118565528	0.0001766821
-4	0.0035307036	-0.0018675142	-0.0018543403
-5	-0.0127941027	-0.0023290158	-0.0005570067
-6	0.0006505807	0.0001541323	-0.0000302320
-7	-0.0176162227	0.0265266008	-0.0008332478
-8	-0.0007673320	-0.0005771791	-0.0000638254
-9	-0.0025194858	-0.0019669714	-0.0001249343
-10	-0.0007710769	-0.0005737640	-0.0000129857
-11	0.0023916748	-0.0001907037	0.0001018474
-12	-0.0004753053	-0.0001164317	0.0000162200
-13	0.0049940392	-0.0047930834	0.0002224165

Gradient Difference

-1	0.0493995502	0.0019897104	0.0022994839
-2	0.0102032522	0.0002627939	0.0067992732
-3	-0.0141188099	0.0207672373	-0.0006307736
-4	0.0108537141	0.0002725400	-0.0057207179
-5	-0.0120336349	-0.0222847913	-0.0004601988
-6	0.0020758086	0.0002257018	-0.0000880549
-7	-0.0554337011	-0.0019297051	-0.0025951550
-8	-0.0023974078	0.0000546253	-0.0001921168
-9	-0.0000442607	-0.0025880984	-0.0000147333
-10	-0.0024227892	0.0000537037	-0.0000957557
-11	-0.0005813075	0.0026880019	-0.0000777233
-12	-0.0014989784	-0.0000970725	0.0000344189
-13	0.0159985642	0.0005853529	0.0007420532

CAS-MP2/DEF2-SVPD = -678.1019478

(12) Mo-CI-2

Atomic Number	Coordinates (Angstroms) X	Y	Z
42	-0.331041	0.267895	0.186675
6	-0.293718	1.716206	-1.369179
6	-0.767236	1.842150	1.666508

6	-0.293725	-1.186223	1.734126
6	-0.851111	-3.278975	-2.626116
6	-2.297091	-0.455612	-0.492678
6	1.400164	-0.358885	-0.393640
8	-0.243617	2.486646	-2.209608
8	-0.887806	2.670320	2.442840
8	-0.241506	-1.970662	2.561770
8	-0.865937	-4.178074	-3.320991
8	-3.277260	-0.881082	-0.893987
16	2.897675	-0.905450	-0.883444

Derivative Coupling

-1	-0.0159032872	-0.0221184805	-0.0206773219
-2	-0.0004145451	-0.0004861927	-0.0005053998
-3	0.0159970609	-0.0019265665	-0.0018654835
-4	-0.0004022165	-0.0004459773	-0.0004721935
-5	0.0001800972	0.0011524525	0.0009020026
-6	-0.0120082558	0.0078428771	0.0074150777
-7	0.0178088197	0.0238442155	0.0223953794
-8	-0.0003425451	-0.0004999961	-0.0005422343
-9	-0.0041245050	0.0004488162	0.0004465717
-10	-0.0003399037	-0.0006105517	-0.0004327511
-11	-0.0000072013	-0.0007498123	-0.0005943633
-12	0.0028164347	-0.0020540593	-0.0019329923
-13	-0.0032599529	-0.0043967250	-0.0041362916

Gradient Difference

-1	-0.0526816502	0.0216358300	0.0197290882
-2	-0.0105164373	0.0074787681	-0.0002430885
-3	-0.0081519550	-0.0206421307	-0.0192664222
-4	-0.0106254368	0.0002117088	0.0074110238
-5	-0.0002847862	0.0003827097	0.0002953759
-6	0.0183781614	0.0162426166	0.0154037651
-7	0.0831082854	-0.0328614070	-0.0299500104
-8	0.0020843577	-0.0003984255	-0.0010608021
-9	0.0031590024	0.0020390588	0.0018811797
-10	0.0020931336	-0.0010901441	-0.0003292027
-11	0.0004586902	-0.0000246031	-0.0000290560
-12	-0.0004293076	-0.0030819434	-0.0029546779
-13	-0.0265920577	0.0101079619	0.0091128271

CAS-MP2/DEF2-SVPD = -678.1056651

(13) Mo-CI-3

Atomic Number	Coordinates (Angstroms) X	Y	Z
42	-0.807049	0.005575	-0.048882
6	0.149854	0.098915	-1.978472
6	-0.955134	2.104431	-0.136817
6	0.392408	0.117970	1.771860
6	-0.546442	-2.081665	-0.145975
6	-2.970290	-0.202818	0.164558
6	3.670321	-0.118124	0.344194
8	0.617916	0.146773	-3.021490
8	-1.000941	3.248792	-0.218646
8	0.991956	0.172222	2.740540
8	-0.362696	-3.211427	-0.236813
8	-4.097247	-0.312941	0.299790
16	5.214018	-0.438143	0.455693

Derivative Coupling

-1	-0.0007300398	-0.0000832986	-0.0022670079
-2	-0.0036955626	-0.0002704732	0.0089729472
-3	0.0010623697	-0.0002307472	0.0034949071
-4	0.0125929716	0.0011848621	-0.0046511668
-5	0.0010664623	0.0004341490	0.0033723850
-6	-0.0083256199	-0.0008255842	-0.0094532945
-7	0.0007984700	-0.0001150765	0.0000968517
-8	0.0001562938	0.0000112353	-0.0016897814
-9	-0.0004077607	0.0001774715	0.0001284154
-10	-0.0026272736	-0.0002525735	0.0004014755
-11	-0.0003835384	-0.0002471253	0.0001231149
-12	0.0010416461	0.0001012588	0.0015322195
-13	-0.0005484185	0.0001159018	-0.0000610658

Gradient Difference

-1	-0.0061270568	-0.0005564627	-0.0033025913
-2	0.0104923281	0.0009937997	-0.0017583414
-3	0.0109573076	0.0011655243	0.0026114961
-4	-0.0128489621	-0.0010108353	-0.0111707651
-5	0.0109677564	0.0008761001	0.0024982151
-6	-0.0056292278	-0.0005497061	0.0161206742

-7	0.0028816775	-0.0002742063	0.0004102465
-8	-0.0051987263	-0.0004995697	-0.0008350219
-9	-0.0014119454	-0.0002344496	-0.0007732243
-10	-0.0001977279	-0.0000490513	0.0009566979
-11	-0.0014595231	-0.0000134000	-0.0007445829
-12	-0.0011169607	-0.0001115509	-0.0038496476
-13	-0.0013089394	0.0002638078	-0.0001631554

CAS-MP2/DEF2-SVPD = -678.0628315

(14) Mo-S_0-Prod1

Atomic Number	Coordinates (Angstroms) X	Y	Z
42	3.563183	0.090555	-0.056577
6	3.491848	2.093915	-0.852936
6	3.589953	0.889671	1.927888
6	3.630929	-1.881585	0.746813
6	3.591330	-0.715378	-2.040021
6	-5.694721	-0.147586	0.072258
6	5.454466	0.122984	-0.070987
8	3.485647	3.168089	-1.251698
8	3.666909	1.315463	2.981960
8	3.733379	-2.930689	1.181475
8	3.671184	-1.143991	-3.092554
8	-6.831774	-0.175602	0.092145
16	7.087401	0.163488	-0.087794

CAS-MP2/DEF2-SVPD = -678.1816487

(15) Mo-S_0-Prod2

Atomic Number	Coordinates (Angstroms) X	Y	Z
42	-0.202666	-0.038513	-0.070052
6	-0.224276	1.952824	-0.883248
6	-0.294969	0.726507	1.814558
6	-0.087301	-2.007787	0.727622

6	-0.188847	-3.542213	-8.766606
6	-2.384451	-0.161709	-0.202524
6	1.766380	0.059082	0.019614
8	-0.188398	3.028491	-1.273199
8	-0.317078	1.158190	2.875639
8	0.019321	-3.055334	1.162836
8	-0.212816	-3.966610	-9.822245
8	-3.523564	-0.217850	-0.227334
16	3.373192	0.140454	0.091658

CAS-MP2/DEF2-SVPD = -678.17245681

(16) Mo-S_0-Prod3

Atomic Number	Coordinates (Angstroms) X	Y	Z
42	-0.083307	0.000009	0.001341
6	-0.120404	2.002047	-0.798589
6	-0.082525	0.782654	1.951618
6	0.010594	-1.938868	0.782645
6	-0.087336	-0.785891	-1.946851
6	-2.076880	-0.087268	0.038316
6	8.906099	0.210806	-0.087360
8	-0.155778	3.068900	-1.240484
8	-0.116224	1.206550	3.013669
8	0.014859	-3.003536	1.206483
8	-0.123237	-1.214798	-3.006898
8	-3.232291	-0.143130	0.061032
16	10.475447	0.239910	-0.088482

CAS-MP2/DEF2-SVPD = -678.14153320

(17) W-S_0-Rea

Atomic Number	Coordinates (Angstroms) X	Y	Z
74	0.000000	0.000000	0.000000
6	0.000000	0.000000	2.090914

6	2.090831	0.000000	0.001444
6	0.003725	0.089031	-2.088945
6	-2.088887	0.091937	0.000150
6	-0.046682	-2.152117	-0.044344
6	0.044544	2.001087	0.043455
8	0.001722	0.041686	3.226235
8	3.226169	0.042535	0.003047
8	0.007622	0.178933	-3.221487
8	-3.221203	0.184026	0.001230
8	-0.071042	-3.285264	-0.066951
16	0.079160	3.548521	0.077562

M062X/Def2-SVPD = -1069.2096980

(18) W-T_1-FC

Atomic Number	Coordinates (Angstroms) X	Y	Z
74	0.000000	0.000000	0.000000
6	0.000000	0.000000	2.090914
6	2.090831	0.000000	0.001444
6	0.003725	0.089031	-2.088945
6	-2.088887	0.091937	0.000150
6	-0.046682	-2.152117	-0.044344
6	0.044544	2.001087	0.043455
8	0.001722	0.041686	3.226235
8	3.226169	0.042535	0.003047
8	0.007622	0.178933	-3.221487
8	-3.221203	0.184026	0.001230
8	-0.071042	-3.285264	-0.066951
16	0.079160	3.548521	0.077562

M062X/Def2-SVPD = -1069.1171098

(19) W-T_1-Min

Atomic Number	Coordinates (Angstroms) X	Y	Z

74	-0.030601	-0.037229	-0.028369
6	-0.107501	-0.030168	2.065719
6	2.106519	-0.089279	-0.213229
6	-0.020078	0.128103	-2.123193
6	-2.131886	0.143286	0.084860
6	0.111940	-2.141859	0.100078
6	0.421456	2.029557	0.240071
8	-0.179645	-0.000526	3.196584
8	3.228913	-0.072061	-0.337152
8	-0.015367	0.242112	-3.251024
8	-3.259148	0.234765	0.144341
8	0.187069	-3.272607	0.190607
16	-0.308851	3.401652	-0.065019

M062X/Def2-SVPD = -1069.1277890

(20) W-T_1-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
74	0.036219	0.003110	-0.007251
6	-0.097642	1.336958	1.582094
6	0.913857	1.528886	-1.295216
6	0.101345	-1.394744	-1.542615
6	0.050329	-1.553690	1.350482
6	2.475977	-0.388215	0.485288
6	-1.735201	0.593436	-0.635699
8	-0.210606	2.059991	2.451936
8	1.300601	2.334344	-1.987046
8	0.097792	-2.164812	-2.378954
8	0.073520	-2.419945	2.102908
8	3.235576	-1.013438	1.050618
16	-3.248417	0.823245	-0.935332

Vibrational Mode

-1	0.11	0.00	0.01
-2	-0.01	-0.01	-0.02
-3	-0.09	0.00	0.12
-4	-0.02	0.01	-0.02
-5	-0.14	0.00	-0.11

-6	-0.60	-0.01	-0.53
-7	-0.04	-0.01	0.27
-8	-0.04	-0.01	-0.03
-9	-0.10	0.00	0.11
-10	-0.04	0.01	-0.03
-11	-0.05	0.00	-0.05
-12	-0.39	0.01	0.18
-13	0.05	0.00	-0.03

M062X/Def2-SVPD = -1069.1195355

(21) W-T_1-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
74	0.000000	0.000000	0.000000
6	0.000000	0.000000	2.391711
6	2.079775	0.000000	-0.022467
6	-0.000436	-0.208173	-2.033287
6	-2.074526	0.130102	-0.037578
6	-0.070553	-2.101734	0.327109
6	0.049305	1.907565	0.745030
8	0.012221	0.392447	3.453501
8	3.214611	0.019771	-0.057413
8	0.000774	-0.268714	-3.174091
8	-3.205574	0.222420	-0.079402
8	-0.107525	-3.219525	0.514643
16	0.090288	3.428332	1.103942

Vibrational Mode

-1	0.04	0.02	-0.10
-2	-0.05	-0.10	0.74
-3	0.01	0.01	-0.02
-4	0.14	-0.01	0.08
-5	0.01	0.00	-0.02
-6	-0.07	-0.02	0.04
-7	0.14	0.01	-0.13
-8	-0.51	0.00	0.12
-9	0.00	0.00	0.02
-10	-0.01	0.01	-0.03

-11	-0.01	0.00	0.03
-12	-0.12	-0.03	0.10
-13	0.03	-0.04	0.22

M062X/Def2-SVPD = -1069.1257358

(22) W-T_1-TS3

Atomic Number	Coordinates (Angstroms) X	Y	Z
74	0.679331	-0.047824	0.079002
6	0.564257	1.242119	1.696078
6	0.436162	1.571346	-1.205136
6	0.702028	-1.323316	-1.558419
6	-0.696756	-1.276203	0.999283
6	2.656712	-0.417111	0.468212
6	-2.419626	0.625026	-0.792558
8	0.491268	1.950857	2.583620
8	0.288870	2.452536	-1.906765
8	0.700115	-2.018154	-2.459323
8	-1.467300	-1.952126	1.504343
8	3.748882	-0.644402	0.702972
16	-3.651909	-0.095154	-0.230496

Vibrational Mode

-1	-0.10	0.01	-0.01
-2	-0.10	0.01	-0.01
-3	0.12	0.01	-0.07
-4	-0.07	0.01	0.00
-5	0.02	0.00	0.10
-6	-0.09	-0.02	-0.07
-7	0.75	-0.18	0.41
-8	-0.06	0.01	-0.01
-9	0.12	0.01	-0.06
-10	-0.03	0.01	0.01
-11	0.07	0.00	0.14
-12	-0.10	-0.02	-0.05
-13	0.31	0.02	-0.07

M062X/Def2-SVPD = -1069.0941619

(23) W-T_1/S_0-1

Atomic Number	Coordinates (Angstroms) X	Y	Z
74	0.1932421	-0.0000812	0.0224240
6	0.2051811	-2.0816399	-0.0367781
6	0.0787230	0.0661956	-2.0619232
6	0.1857414	2.0804291	0.0969537
6	-1.1671270	-0.0568723	1.6052954
6	-3.3067755	0.0235615	-1.3142432
6	2.0562454	-0.0082868	0.5998053
8	0.2356579	-3.2179891	-0.0560999
8	0.0053049	0.1022320	-3.1961782
8	0.2065189	3.2158790	0.1502787
8	-1.9166860	-0.0873757	2.4621604
8	-4.0869878	0.0215593	-0.5034326
16	3.5410254	-0.0143453	1.0686142
Gradient Difference			
-1	0.06170729	-0.00061850	0.02943993
-2	-0.02037411	0.00047208	-0.00483019
-3	-0.07735502	-0.00107438	0.02249323
-4	-0.02033927	-0.00029094	-0.00483935
-5	-0.03556021	0.00231148	-0.07809279
-6	-0.00152134	0.00010289	-0.01534719
-7	0.07434882	-0.00045589	0.02418184
-8	0.00297097	0.00132910	0.00070079
-9	0.02493129	0.00037215	-0.00829140
-10	0.00297699	-0.00134863	0.00061095
-11	0.00955867	-0.00085493	0.02828771
-12	-0.00478483	-0.00006410	0.01117571
-13	-0.01655925	0.00011966	-0.00548925

M062X/Def2-SVPD = -1069.1308989

(24) W-T_1/S_0-2

Atomic Number	Coordinates (Angstroms) X	Y	Z

74	-0.4145723	-0.0309921	0.2191787
6	1.3131224	0.3729818	-2.7686892
6	-0.3794257	2.0299564	0.4968123
6	-1.4992587	-0.2559266	1.9243709
6	-0.3684718	-2.0943649	-0.0385676
6	-1.7219293	0.1785668	-1.4243365
6	1.5512182	-0.0693020	0.5558696
8	2.4253224	0.4009457	-2.9345596
8	-0.3388719	3.1528011	0.6709773
8	-2.0569218	-0.3861465	2.9106308
8	-0.3224081	-3.2244129	-0.1554928
8	-2.3418151	0.2991382	-2.3689968
16	3.0952204	-0.0869222	0.7266202

Gradient Difference

-1	-0.02175476	-0.01290672	0.09842832
-2	-0.01366320	0.00234329	-0.01797281
-3	0.00677433	0.00270996	-0.01802676
-4	-0.06936048	-0.00493974	0.03668348
-5	0.00673957	0.00203348	-0.01807740
-6	0.06306490	0.00235355	-0.01689578
-7	0.00681466	0.01213286	-0.09322788
-8	0.01751152	-0.00063847	0.00540150
-9	-0.00129834	-0.00313913	0.00192233
-10	0.02139661	0.00160569	-0.01195665
-11	-0.00129963	0.00250146	0.00264354
-12	-0.01865537	-0.00093120	0.00685109
-13	0.00373021	-0.00312503	0.02422703

M062X/Def2-SVPD = -1069.1311433

(25) W-T_1/S_0-3

Atomic Number	Coordinates (Angstroms) X	Y	Z
74	-1.0323086	0.0664723	-0.3573233
6	-0.3194465	1.4071409	-1.7761357
6	-0.4461694	1.3608998	1.1697032
6	-1.7317035	-1.2735332	1.0611830

6	-0.2742658	-1.5231813	-1.4611438
6	-2.9335854	0.4205870	-0.9591305
6	3.3241953	-2.8139335	-1.4207554
8	0.0503043	2.1452370	-2.5593157
8	-0.0965072	2.0493025	2.0066827
8	-2.1341890	-2.0069905	1.8331236
8	0.1556919	-2.4001447	-2.0467526
8	-4.0063381	0.6156110	-1.2977823
16	3.6029830	-4.0869244	-2.2218233

Gradient Difference

-1	-0.07513985	0.01919991	-0.01893085
-2	0.02040283	-0.00242108	0.00758715
-3	0.06514615	-0.05524768	-0.01985483
-4	0.01994215	-0.00289599	0.00804707
-5	0.07130053	0.01422694	0.04889651
-6	-0.07701623	0.01846665	-0.02128596
-7	0.00002296	0.00216864	0.00120510
-8	-0.00355086	-0.00109826	0.00043826
-9	-0.01989350	0.01917966	0.00811496
-10	-0.00201223	0.00186908	-0.00267657
-11	-0.02158887	-0.00564090	-0.01620395
-12	0.02205571	-0.00537703	0.00607653
-13	0.00033122	-0.00242993	-0.00141342

M062X/Def2-SVPD = -1069.0852378

(26) W-S_0-Prod1

Atomic Number	Coordinates (Angstroms) X	Y	Z
74	0.000000	0.000000	0.000000
6	0.000000	0.000000	2.091120
6	2.091261	0.000000	0.003306
6	0.005531	0.162780	-2.085572
6	-2.085476	0.162820	0.004540
6	0.075376	1.878154	0.075596
8	0.003810	0.105531	3.222177
8	3.222299	0.105924	0.009846
8	0.012580	0.356773	-3.204748

8	-3.204652	0.357100	0.012161
16	0.139582	3.445288	0.139784

M062X/Def2-SVPD = -955.9682741

(27) W-S_0-Prod2

Atomic Number	Coordinates (Angstroms) X	Y	Z
74	0.000000	0.000000	0.000000
6	0.000000	0.000000	2.086627
6	2.158936	0.000000	-0.056030
6	-0.113290	0.094796	-2.082728
6	-1.985268	0.086973	0.064567
6	0.003978	1.940300	0.044958
8	-0.048207	0.077533	3.219774
8	3.288225	0.099274	-0.080521
8	-0.221247	0.224309	-3.206886
16	-3.528959	0.223339	0.125534
8	-0.023074	3.088691	0.072469

M062X/Def2-SVPD = -955.9588759

(28) W-S_0-Prod3

Atomic Number	Coordinates (Angstroms) X	Y	Z
74	0.000000	0.000000	0.000000
6	0.000000	0.000000	2.082446
6	2.082660	0.000000	-0.000121
6	-0.000901	0.106095	-2.079555
6	-2.079581	0.103112	0.002661
6	0.048447	1.936557	0.050227
8	0.000976	0.079447	3.217257
8	3.217504	0.078725	0.002079
8	-0.000414	0.244175	-3.208794
8	-3.209095	0.238999	0.006700
8	0.077138	3.085842	0.080075

M062X/Def2-SVPD = -633.0893095