Supplementary Materials

The Mechanistic Investigations of Photochemical Decarbonylations and Oxidative Addition Reactions for $M(CO)_5$ (M = Fe, Ru, Os) Complexes

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(All geometries were calculated CASSCF(14,10)/Def2-SVP)

(1) Fe-S_0-Rea

Atomic Number	Coordinates (Angstroms) X	Y	Z
26	0.000000	0.000000	0.998568
6	0.000000	0.000000	-0.837166
8	0.000000	0.000000	-1.969707
6	1.587615	0.000000	1.919479
8	2.565798	0.000000	2.490197
6	-1.587615	0.000000	1.919479
8	-2.565798	0.000000	2.490197
6	0.000000	1.877121	0.997618
8	0.000000	3.003316	0.996854
6	0.000000	-1.877121	0.997618
8	0.000000	-3.003316	0.996854

CASSCF(14,10)/LANL2DZ = -1830.3284692

(2) Fe-T_1-Min

Atomic Number	Coordinates (Angstroms) X	Y	Z
26	-0.001248	-0.000419	1.120477
6	-0.004334	0.000095	-0.825387
8	-0.005120	0.000761	-1.975659
6	1.918884	-0.000074	1.836484
8	2.959513	-0.000169	2.301305
6	-1.916665	-0.001337	1.833084
8	-2.958535	-0.002401	2.295399
6	0.001310	2.135920	1.133639
8	0.003856	3.274173	1.071823
6	0.000562	-2.134074	1.134775
8	0.001778	-3.272474	1.074039

CASSCF(14,10)/LANL2DZ = -1830.3171546

(3) Fe-T_1-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
26	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.986013
6	2.027226	0.000000	-0.144124
6	0.487399	2.478478	-0.860592
6	-0.168939	-1.342002	-1.465627
6	-1.862571	0.776898	-0.239927
8	-0.007189	0.012239	3.129646
8	3.165108	-0.110112	-0.198749
8	0.765229	3.509524	-1.247107
8	-0.269855	-2.117174	-2.300618
8	-2.886008	1.261969	-0.391301

Vibrational Mode

-1	-0.05	-0.22	0.08
-2	-0.04	-0.19	0.06
-3	-0.10	0.04	-0.02
-4	0.09	0.51	-0.15
-5	-0.04	-0.20	0.09
-6	0.12	0.01	-0.01
-7	-0.03	-0.15	0.06
-8	-0.09	0.28	-0.10
-9	0.10	0.49	-0.17
-10	-0.04	-0.17	0.06
-11	0.22	0.19	-0.09

CASSCF(14,10)/LANL2DZ = -1830.3126925

(4) Fe-S_0-Int

Atomic Number	Coordinates (Angstroms) X	Y	Z
26	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.882068
6	1.817618	0.000000	-0.114896
6	-0.244670	0.509196	-1.798285
6	-1.083410	-1.460950	-0.119147

8	-0.026317	0.059852	3.008885
8	2.928185	-0.212425	-0.213895
8	-1.573105	-2.480125	-0.215214
8	-0.418614	0.864343	-2.855421

CASSCF(14,10)/LANL2DZ = -1716.9575843

(5) Fe-T_1/S_0-2

Atomic Number	Coordinates (Angstroms) X	Y	Z
26	-0.0919085	-0.0217508	1.1944324
6	-0.0788116	-1.8984185	1.4641525
8	-0.0491734	-3.0046254	1.6997147
6	-0.0670407	-0.0192786	-1.1466150
8	0.5682569	0.1411474	-2.0610209
6	-1.9572471	0.0173448	1.5576789
8	-3.0490790	0.0451820	1.8492041
6	-0.0261910	1.8615705	1.3736740
8	0.0348542	2.9777074	1.5519843
6	1.7937199	-0.0440417	1.2582961
8	2.9224926	-0.0547127	1.3514414
Derivative Coupling			
-1	-0.00197935	-0.00004608	0.14516168
-2	-0.00172868	-0.01085399	-0.03804965
-3	0.00068425	-0.00928431	0.01327994
-4	-0.02311027	-0.00601584	-0.03693525
-5	0.01995180	0.00511559	-0.00846081
-6	-0.01008904	-0.00051676	-0.03703049
-7	-0.00687924	0.00037024	0.01355906
-8	-0.00097093	0.00951704	-0.03809077
-9	0.00088275	0.01222593	0.01250713
-10	0.00640159	-0.00045986	-0.03631244
-11	0.01683712	-0.00005197	0.01037158

CASSCF(14,10)/LANL2DZ = -1830.2653626

(6) Fe-T_1-Int

Atomic Number	Coordinates (Angstroms) X	Y	Z
26	-0.229655	0.145125	-0.102686
6	0.034534	-0.050515	1.861590
8	0.251136	-0.206529	2.962863
6	0.057001	-1.758811	-0.614688
8	0.288333	-2.839571	-0.864223
6	-1.859613	1.108615	-0.777482
8	-2.770839	1.648446	-1.150156
6	1.582888	0.832137	-0.562881
8	2.646218	1.158814	-0.778997

CASSCF(14,10)/LANL2DZ = -1716.9985852

(7) Fe-T_1/S_0-3

Atomic Number	Coordinates (Angstroms) X	Y	Z
26	-0.1659531	0.1001102	0.1345389
6	0.4333089	-0.2905916	1.8771350
8	0.6800134	-0.4585561	2.9656049
6	-0.4274170	-1.6412772	-0.3768902
8	-0.4022501	-2.6941804	-0.7961228
6	-1.3869011	0.8564950	-1.0850530
8	-2.1890441	1.3506790	-1.7064289
6	1.2555644	1.1643331	-0.3252218
8	2.2026815	1.6506990	-0.7142220
Derivative Coupling			
-1	-0.07202192	0.03453103	0.05755073
-2	-0.02528364	0.01334300	0.03739139
-3	0.01617424	-0.00973032	0.00250222
-4	0.05752293	-0.06074912	-0.05899310
-5	-0.02271198	-0.00391627	0.01253043
-6	-0.03826461	0.02145212	0.01588866
-7	0.00276399	-0.00123541	-0.01904621
-8	0.09284617	-0.01410169	-0.06261634
-9	-0.01102519	0.02040664	0.01479223

CASSCF(14,10)/LANL2DZ = -1716.95802126

(8) Fe-T_1-Cpx

Atomic Number	Coordinates (Angstroms) X	Y	Z
26	0.037535	0.369300	0.007795
6	-0.014448	0.179164	1.896546
6	1.914439	0.113433	-0.002552
6	-0.039315	0.106130	-1.871996
6	-1.541078	1.414667	-0.006327
8	-0.010330	0.158327	3.028221
8	3.043708	0.015434	-0.007937
8	-0.050807	0.058768	-3.003379
8	-2.452818	2.089584	-0.013876
14	-1.611849	-3.162752	0.143181
1	-0.429316	-2.259233	0.123572
6	-0.949955	-4.909916	0.301432
6	-2.558418	-2.925390	-1.454502
6	-2.684938	-2.702714	1.608062
1	-1.749783	-5.654161	0.319887
1	-0.370686	-5.010761	1.221161
1	-0.287233	-5.142665	-0.534337
1	-3.402377	-3.616964	-1.516931
1	-1.917087	-3.099083	-2.320451
1	-2.952929	-1.908436	-1.525402
1	-2.119869	-2.747129	2.540471
1	-3.535095	-3.383800	1.697458
1	-3.078411	-1.688747	1.499440

CASSCF(14,10)/LANL2DZ = -2126.808958

(9) Fe-T_1/S_0-4

Atomic Number	Coordinates (Angstroms) X	Y	Z
26	-0.1258166	-0.2945346	0.0386396
6	-0.2017658	-0.3178365	1.9674406

6	1.6473908	0.2465306	0.0120373
6	-0.2228337	-0.4318536	-1.8835136
6	-1.3249597	1.1090516	0.0034077
8	-0.2556510	-0.2986137	3.0946461
8	2.7045521	0.6588704	-0.0060328
8	-0.2884792	-0.4745947	-3.0095419
8	-1.9924215	2.0307520	-0.0177927
14	-1.5600390	-2.9704759	0.1268609
1	-0.2880462	-2.1305388	0.1024230
6	-0.8915166	-4.7091775	0.2790090
6	-2.4988469	-2.7654071	-1.4720420
6	-2.6059624	-2.5446732	1.6107124
1	-1.7144660	-5.4258725	0.2988618
1	-0.3182955	-4.8308718	1.1989496
1	-0.2434907	-4.9634696	-0.5596767
1	-3.3198639	-3.4842795	-1.5102692
1	-1.8565787	-2.9489042	-2.3344145
1	-2.9200465	-1.7643251	-1.5676970
1	-2.0334471	-2.6233635	2.5360842
1	-3.4445638	-3.2404206	1.6793993
1	-3.0059150	-1.5329357	1.5420447

Derivative Coupling

-1	-0.02061250	-0.07635574	0.00247952
-2	-0.00610789	-0.02557630	0.04966961
-3	0.06367071	0.07104969	-0.00260283
-4	-0.00689007	-0.02880203	-0.04718156
-5	-0.01849312	0.09234760	-0.00259438
-6	0.00136592	0.01214031	0.02124462
-7	0.01262261	-0.01338696	0.00038402
-8	0.00118046	0.01106944	-0.02255415
-9	-0.01756797	-0.00180875	0.00012720
-10	0.00929918	-0.02210879	0.00030317
-11	-0.01983531	-0.02862202	0.00105604
-12	-0.00293672	-0.00141813	0.00015983
-13	0.00239115	0.00309796	0.00065760
-14	0.00354096	0.00367045	-0.00066417
-15	0.00063482	-0.00086021	0.00008861
-16	-0.00012006	0.00018926	0.00010687
-17	-0.00015442	0.00023177	-0.00015032
-18	-0.00008666	0.00086568	0.00166728

-19	0.00022343	0.00082863	0.00059419
-20	-0.00098772	0.00068179	-0.00184901
-21	0.00026904	0.00077410	-0.00066054
-22	0.00012725	0.00085257	-0.00213501
-23	-0.00153308	0.00113967	0.00185342

CASSCF(14,10)/LANL2DZ = -2126.80559951

(10) Fe-S_0-Cpx

Atomic Number	Coordinates (Angstroms) X	Y	Z
26	-0.056630	-0.125463	0.018681
6	-0.046170	-0.087405	1.914136
6	1.773422	-0.020628	0.003550
6	-0.063981	-0.151355	-1.876301
6	-1.328123	1.185974	-0.001534
8	-0.044516	-0.077814	3.043629
8	2.901359	0.129318	-0.003826
8	-0.065238	-0.156949	-3.005842
8	-2.053960	2.064271	-0.012001
14	-1.659771	-2.967530	0.135668
1	-0.578688	-1.896174	0.101223
6	-0.787392	-4.617457	0.291422
6	-2.628090	-2.887111	-1.460562
6	-2.765021	-2.677652	1.614853
1	-1.526329	-5.422057	0.308177
1	-0.207763	-4.683321	1.212089
1	-0.115223	-4.803362	-0.545963
1	-3.372709	-3.685586	-1.487224
1	-1.979804	-3.011197	-2.328283
1	-3.151774	-1.936361	-1.559035
1	-2.200098	-2.682714	2.547298
1	-3.513719	-3.470356	1.679889
1	-3.290845	-1.726014	1.539492

CASSCF(14,10)/LANL2DZ = -2126.8040358

(11) Fe-T_1-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.483546	0.052910	1.675613
8	1.933406	0.098679	2.708441
26	0.704125	-0.006893	-0.134407
6	0.393072	1.816134	-0.209713
8	0.194976	2.930653	-0.235630
6	2.314668	-0.021721	-1.141307
8	3.252613	-0.032495	-1.767724
6	0.419437	-1.834666	-0.109510
8	0.241349	-2.952135	-0.064890
14	-1.747275	-0.006695	-0.155933
6	-2.627742	-1.542066	0.503597
1	-3.705788	-1.385594	0.417157
1	-2.402633	-1.744391	1.551604
1	-2.373667	-2.432836	-0.071248
6	-2.158315	0.077953	-1.999333
1	-3.242662	0.105093	-2.134529
1	-1.778970	-0.792828	-2.536803
1	-1.741842	0.970656	-2.468523
6	-2.577000	1.486570	0.654160
1	-2.200411	1.692235	1.656849
1	-3.651482	1.306424	0.729815
1	-2.432481	2.385903	0.054367
1	-1.022787	-0.170598	2.602508

Vibrational Mode

-1	0.04	0.00	-0.02
-2	0.06	0.01	-0.01
-3	-0.02	0.00	-0.01
-4	-0.01	0.01	-0.02
-5	0.00	0.01	0.00
-6	0.00	0.00	0.02
-7	0.02	0.00	0.00
-8	-0.01	-0.01	-0.01
-9	0.00	-0.01	-0.01
-10	-0.02	0.00	-0.01
-11	-0.03	0.00	0.03
-12	-0.03	-0.01	0.08

-13	-0.08	0.01	0.01
-14	0.00	-0.01	0.01
-15	0.03	0.00	0.00
-16	0.03	0.00	0.01
-17	0.03	0.00	0.00
-18	0.03	0.00	0.00
-19	-0.03	0.00	0.01
-20	-0.08	-0.04	-0.01
-21	-0.04	0.02	0.08
-22	0.02	0.01	-0.01
-23	0.48	0.03	0.85

CASSCF(14,10)/LANL2DZ = -2126.7296037

(12) Fe-S_0-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.063346	0.208622	-1.331774
8	1.476541	0.431727	-2.348566
26	0.644323	-0.026395	0.482220
6	0.374015	-1.885533	0.338526
8	0.213524	-2.998933	0.278644
6	2.440619	-0.054564	1.116528
8	3.501204	-0.055680	1.486749
6	0.322053	1.790016	0.764510
8	0.103741	2.878137	0.962993
14	-1.739126	0.004904	0.102846
6	-2.314737	1.417394	-0.970145
1	-3.403571	1.482866	-0.986610
1	-1.969969	1.071414	-1.948537
1	-1.908367	2.399488	-0.744138
6	-2.298716	0.142059	1.912469
1	-3.391889	0.123266	1.911676
1	-1.986933	1.065839	2.400907
1	-1.962301	-0.699415	2.520144
6	-2.425667	-1.530616	-0.687063
1	-1.976974	-1.473913	-1.692978
1	-3.510194	-1.438868	-0.772678

1	-2.191732	-2.476414	-0.205716
1	-1.366390	-0.440299	-3.385006

Vibrational Mode

-1	0.00	0.01	0.05
-2	0.17	-0.06	0.01
-3	-0.02	0.00	0.02
-4	-0.03	0.01	0.03
-5	-0.01	0.01	0.01
-6	-0.01	0.01	0.06
-7	-0.02	0.00	0.00
-8	-0.02	0.01	0.02
-9	0.00	0.01	0.01
-10	-0.02	0.00	-0.03
-11	-0.02	0.00	-0.03
-12	-0.02	0.02	0.01
-13	0.05	-0.01	-0.04
-14	-0.04	-0.01	-0.06
-15	-0.01	-0.02	-0.03
-16	-0.01	-0.02	-0.05
-17	0.00	-0.02	-0.02
-18	-0.01	-0.02	-0.03
-19	-0.03	0.01	-0.08
-20	0.02	0.05	-0.09
-21	-0.03	0.00	-0.05
-22	-0.05	-0.01	-0.13
-23	0.77	0.14	-0.53

CASSCF(14,10)/LANL2DZ = -2126.6698437

(13) Fe-T_1/S_0-1

Atomic Number	Coordinates (Angstroms) X	Y	Z
26	-0.2162414	0.0181189	1.0337565
1	-0.7550597	-1.4692144	1.3442073
6	-2.5726004	0.2233998	1.0673726
8	-3.6205382	-0.1570082	1.1733666
6	0.0277704	2.0898371	0.5857536
8	0.5213960	3.0700914	0.3365800

6	0.0757609	0.1022104	2.8653178
8	0.3160964	0.0620248	3.9699337
6	-0.0395071	-0.5998099	-0.7112240
8	0.1168432	-1.0496985	-1.7363681
14	2.3127552	0.1292091	0.9944268
6	3.0547923	0.3943344	-0.7212053
1	4.1436237	0.4508194	-0.6517200
1	2.7044309	1.3262974	-1.1701217
1	2.8044875	-0.4194547	-1.4026170
6	2.8966020	-1.5437565	1.6411319
1	3.9868982	-1.6080362	1.6035047
1	2.4880354	-2.3623952	1.0472117
1	2.5859910	-1.6966441	2.6758857
6	3.0530443	1.4736388	2.0955470
1	4.1430381	1.3992265	2.0805597
1	2.7272761	1.3802720	3.1324231
1	2.7896992	2.4733540	1.7462768

Gradient Difference

-1	0.06813164	-0.07294849	0.01195823
-2	-0.03194774	-0.01151184	0.00328508
-3	-0.03293755	0.02864104	-0.00425816
-4	-0.00786034	-0.01482796	0.00304812
-5	-0.03926490	0.03302758	-0.00516981
-6	0.02418181	0.00837604	-0.00306963
-7	-0.00477459	0.00691813	0.01237012
-8	0.00051701	0.00043790	0.00099964
-9	-0.00586083	0.00160638	-0.01478779
-10	0.00037199	0.00039128	-0.00007501
-11	0.02841725	0.02631191	-0.00539985
-12	0.00323808	-0.00128482	0.00051060
-13	0.00051602	-0.00001941	-0.00103178
-14	-0.00036901	-0.00011335	0.00081763
-15	0.00012008	-0.00012709	-0.00042105
-16	-0.00697402	-0.00314073	0.00126646
-17	-0.00096597	0.00171520	-0.00112007
-18	0.00089185	-0.00161297	0.00022559
-19	0.00058107	-0.00060580	0.00029546
-20	0.00395849	-0.00162666	0.00023405
-21	0.00062634	0.00100743	0.00070852
-22	-0.00003028	-0.00007232	0.00017178

-23	-0.00056640	-0.00054147	-0.00055813

CASSCF(14,10)/LANL2DZ = -2126.77740286

(14) Fe-S_0-Pro

Atomic Number	Coordinates (Angstroms) X	Y	Z
26	-0.220662	0.208026	0.997616
1	-0.169211	-1.295815	1.247540
6	-2.059057	0.040107	1.091116
8	-3.171817	-0.118854	1.161425
6	0.024594	2.016117	0.663572
8	0.241484	3.103003	0.449668
6	0.098568	0.184616	2.788402
8	0.344335	0.067173	3.886997
6	-0.030326	-0.414501	-0.703172
8	0.112418	-0.897245	-1.716010
14	2.194966	0.089269	1.002820
6	2.954665	0.295111	-0.711359
1	4.040731	0.358631	-0.612007
1	2.612240	1.210498	-1.198795
1	2.727849	-0.542730	-1.370427
6	2.770617	-1.562758	1.688880
1	3.862046	-1.603131	1.712339
1	2.412156	-2.383971	1.066610
1	2.404139	-1.728514	2.702922
6	2.965201	1.454561	2.053738
1	4.050641	1.329167	2.058861
1	2.626577	1.432356	3.090192
1	2.752440	2.445700	1.649071

CASSCF(14,10)/LANL2DZ = -2126.8237304

(15) Ru-S_0-Rea

Atomic Number	Coordinates (Angstroms) X	Y	Z

44	-0.000000	-0.000000	-0.000000
6	0.000000	-0.000000	2.052915
6	1.806265	-0.000000	-0.940433
6	-1.805815	-0.007915	-0.934910
6	-0.012893	2.007197	-0.028791
6	0.010910	-2.007408	-0.038736
8	-0.003177	0.001951	3.194837
8	2.825536	-0.003916	-1.458945
8	-2.826461	-0.014151	-1.450779
8	-0.025676	3.146219	-0.049407
8	0.021843	-3.146121	-0.069100

CASSCF(14,10)/LANL2DZ = -656.7186079

(16) Ru-S_1/S_0-CI

Atomic Number	Coordinates (Angstroms) X	Y	Z
44	0.230113	-0.055885	0.148828
6	0.934388	-0.042931	2.086567
6	2.062349	0.074265	-0.524709
6	-0.111779	1.945606	-0.130327
6	-0.296165	-2.024229	-0.119402
6	-3.316634	0.066624	-1.272812
8	1.282334	0.066152	3.171040
8	3.126334	0.224604	-0.923320
8	-0.227501	3.084087	-0.136746
8	-0.496435	-3.149916	-0.151203
8	-3.966776	-0.050931	-2.195593

Derivative Coupling

-1	-0.0025911105	0.0000343427	-0.0051503477
-2	-0.0127934058	0.0013310230	0.0006569003
-3	0.0028857260	-0.0000000044	-0.0129301813
-4	0.0064045390	0.0020423164	0.0120989033
-5	0.0081754633	-0.0034318139	0.0074448048
-6	0.0006202920	-0.0000875175	-0.0005921942
-7	0.0031722030	-0.0002572679	0.0001157044
-8	-0.0022539428	0.0000338757	0.0042572153
-9	-0.0019050609	0.0025676012	-0.0034985103

-10	-0.0021040118	-0.0022790724	-0.0026846887
-11	0.0003893085	0.0000465171	0.0002823942

Gradient Difference

-1	0.0142872012	-0.0069706083	-0.0302122305
-2	0.0050990170	0.0001422416	-0.0127926573
-3	0.0170413118	0.0003743140	0.0079790296
-4	-0.0228450232	0.0035239428	0.0164259276
-5	-0.0174637914	0.0035001748	0.0227463459
-6	-0.0053226934	-0.0002113218	-0.0037701048
-7	0.0004502048	-0.0000838068	0.0069021652
-8	-0.0061868307	-0.0000677780	-0.0027477399
-9	0.0066905340	-0.0022191065	-0.0030640089
-10	0.0058904364	0.0016632604	-0.0036971477
-11	0.0023596334	0.0003486878	0.0022304208

CASSCF(14,10)/LANL2DZ = -656.6462224866

(17) Ru-S_0-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
44	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.980973
6	1.603967	0.000000	-1.182893
6	-2.430504	0.016630	-1.480818
6	-0.028679	2.023790	-0.000861
6	-0.048065	-2.023591	-0.000086
8	0.179727	0.000002	3.120728
8	2.617753	-0.001142	-1.729426
8	-3.399262	0.023622	-2.070008
8	-0.046672	3.162307	-0.000180
8	-0.066746	-3.162098	0.006620

CASSCF(14,10)/LANL2DZ = -667.1235731

(18) Ru-S_0-Int

Atomic Number	Coordinates (Angstroms) X	Y	Z

44	0.000000	0.000000	-0.352360
6	0.000000	-1.862345	0.344533
8	0.000000	-2.868153	0.899609
6	-2.028193	-0.000000	-0.467662
8	-3.158628	-0.000000	-0.588796
6	2.028193	0.000000	-0.467662
8	3.158628	0.000000	-0.588796
6	-0.000000	1.862345	0.344533
8	-0.000000	2.868153	0.899609

CASSCF(14,10)/LANL2DZ = -543.9670656

(19) Ru-S_0-Cpx

Atomic Number	Coordinates (Angstroms) X	Y	Z
44	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.965577
6	1.715156	0.000000	-1.025547
6	-0.108537	-2.017006	0.018799
6	-0.100408	2.014060	0.021370
8	0.204007	0.002534	3.101423
8	2.800501	0.009140	-1.407882
8	-0.207249	-3.151456	0.048949
8	-0.207377	3.148410	0.040735
14	-2.396442	0.026001	-2.562183
1	-1.580288	0.010388	-1.279022
6	-1.230347	0.270530	-4.029708
6	-3.291480	-1.637309	-2.657213
6	-3.617873	1.461630	-2.405978
1	-0.686334	1.205875	-3.954102
1	-1.794213	0.287823	-4.957928
1	-0.503171	-0.531137	-4.097616
1	-3.928268	-1.792761	-1.792836
1	-2.592564	-2.465540	-2.711389
1	-3.919319	-1.678434	-3.542670
1	-4.260011	1.340785	-1.540083
1	-4.253484	1.514884	-3.285256

1	-3.105457	2.413456	-2.312169

CASSCF(14,10)/LANL2DZ = -667.1686034

(20) Ru-S_0-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.624753	-0.068103	1.887963
8	2.236939	-0.031638	2.850123
44	0.533221	-0.125843	0.161626
6	0.003123	1.807626	0.236660
8	-0.269624	2.915568	0.255206
6	2.148058	0.128013	-1.156989
8	3.007275	0.234853	-1.897822
6	0.469569	-2.130916	0.063460
8	0.405345	-3.269797	0.023302
14	-1.186533	-0.296528	-1.767211
6	-2.713696	-1.308151	-1.218017
1	-3.302127	-1.636382	-2.071918
1	-3.339761	-0.661250	-0.609053
1	-2.450985	-2.194752	-0.650852
6	-0.406398	-1.172238	-3.278250
1	-1.143032	-1.268367	-4.072513
1	-0.049730	-2.170188	-3.040619
1	0.430428	-0.605915	-3.677511
6	-1.864037	1.376819	-2.401564
1	-2.641080	1.720483	-1.722983
1	-2.320506	1.258375	-3.381557
1	-1.099896	2.140721	-2.497915
1	-4.347586	1.438999	-0.295224

Vibrational Mode

-1	-0.00	0.00	0.00
-2	-0.01	0.00	0.00
-3	-0.00	0.00	-0.00
-4	-0.00	0.00	-0.00
-5	-0.00	0.00	-0.00
-6	-0.00	0.00	0.00
-7	0.00	0.00	0.01

-8	-0.00	0.00	0.00
-9	0.00	0.00	0.00
-10	-0.00	-0.00	-0.01
-11	-0.00	-0.01	-0.02
-12	0.03	-0.03	-0.03
-13	-0.03	0.00	-0.06
-14	-0.01	0.01	0.01
-15	0.01	-0.00	0.00
-16	0.02	-0.01	-0.00
-17	0.01	-0.00	0.00
-18	0.01	-0.00	0.00
-19	-0.01	-0.01	-0.02
-20	-0.05	-0.04	-0.06
-21	0.05	-0.02	-0.05
-22	-0.03	0.01	0.02
-23	0.61	0.17	0.76

CASSCF(14,10)/LANL2DZ = -667.0677091

(21) Ru-S_0-Pro

Atomic Number	Coordinates (Angstroms) X	Y	Z
44	-0.261095	0.191729	0.994212
1	-0.101329	-1.451277	1.092430
6	-2.337074	-0.073608	1.072653
8	-3.454816	-0.277773	1.122989
6	-0.190762	2.219071	0.850030
8	-0.117522	3.355118	0.768187
6	-0.013066	0.136702	2.960839
8	0.166560	0.058989	4.085304
6	-0.147761	-0.130695	-0.964445
8	-0.062556	-0.365297	-2.077036
14	2.331632	0.034322	0.992343
6	3.081320	0.101335	-0.758062
1	4.165938	0.087317	-0.679352
1	2.804308	1.006377	-1.290078
1	2.787478	-0.748498	-1.365014
6	2.916522	-1.580013	1.808964

1	4.003577	-1.613812	1.831888
1	2.563644	-2.444554	1.257292
1	2.561356	-1.672397	2.830241
6	3.085288	1.491334	1.968129
1	4.168910	1.398646	1.983428
1	2.747378	1.514856	2.999607
1	2.846674	2.448945	1.515453

CASSCF(14,10)/LANL2DZ = -667.1787206

(22) Os-S_0-Rea

Atomic Number	Coordinates (Angstroms) X	Y	Z
76	0.000000	-0.000000	-0.000000
6	0.000000	0.000000	1.990589
6	1.757373	-0.000000	-0.931641
6	-1.766532	0.005496	-0.912684
6	-0.003319	2.000230	-0.025901
6	0.002077	-2.000072	-0.039158
8	-0.006249	0.004644	3.137499
8	2.777799	-0.001875	-1.457999
8	-2.793526	0.015759	-1.426238
8	-0.010205	3.138242	-0.046598
8	0.005925	-3.137808	-0.072567

CASSCF(14,10)/LANL2DZ = -653.8940456

(23) Os-S_1/S_0-CI

Atomic Number	Coordinates (Angstroms) X	Y	Z
76	-0.006984	-0.389473	0.039547
6	-1.964987	-0.088284	-0.280989
8	-3.105427	0.002606	-0.400306
6	1.911428	-0.095153	-0.323391
8	3.044941	-0.005146	-0.509998
6	0.035871	-2.275206	-0.403506

8	0.079248	-3.380972	-0.704924
6	0.024845	-0.907219	2.019383
8	0.075921	-1.181890	3.126387
6	-0.064306	3.245023	-0.634010
8	-0.013340	4.097101	-1.383600

Derivative Coupling

-1	0.0000290302	0.0056343189	0.0119521342
-2	-0.0041942542	-0.0140227313	0.0012083855
-3	-0.0016947608	0.0037354812	-0.0017443819
-4	0.0040195364	-0.0143401265	0.0020778595
-5	0.0015162378	0.0042894962	-0.0020213890
-6	0.0003101440	0.0039326099	-0.0144754429
-7	-0.0000809598	-0.0009767522	0.0051861018
-8	0.0000359451	0.0178498918	-0.0002499613
-9	-0.0000134671	-0.0037054447	-0.0009596391
-10	0.0000605612	-0.0025439821	-0.0007906077
-11	0.0000119871	0.0001472387	-0.0001830591

Gradient Difference

-1	0.0019753565	0.0123254685	0.0366806865
-2	0.0081025038	-0.0064353625	-0.0336150623
-3	-0.0005960890	0.0032841958	0.0072708417
-4	-0.0107594826	-0.0072438449	-0.0340221270
-5	0.0016791408	0.0034852384	0.0080866587
-6	0.0020337832	0.0032876515	0.0120754514
-7	-0.0005396415	-0.0062977503	-0.0025963028
-8	-0.0025353567	0.0024136438	0.0081733330
-9	0.0004462027	0.0014881957	-0.0037842990
-10	-0.0000633710	-0.0111754857	0.0047483687
-11	0.0002569537	0.0048680498	-0.0030175490

CASSCF(14,10)/LANL2DZ = -653.8029503123

(24) Os-S_0-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
76	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.953849
6	1.531820	0.000000	-1.226150

6	-2.649849	-0.078198	-1.430407
6	-0.058827	1.994929	-0.016508
6	-0.020889	-1.997977	0.007394
8	0.190870	0.004340	3.092968
8	2.531156	0.002880	-1.802256
8	-3.645359	-0.087512	-1.973235
8	-0.097854	3.135658	-0.024312
8	-0.031002	-3.139055	0.020657

Vibrational Mode

-1	-0.08	-0.03	-0.04
-2	0.03	0.02	-0.05
-3	-0.04	0.01	0.00
-4	0.62	0.15	0.26
-5	-0.09	0.02	-0.02
-6	0.00	0.01	0.04
-7	0.08	0.06	-0.05
-8	-0.04	0.05	0.00
-9	0.62	0.13	0.26
-10	-0.09	0.01	-0.01
-11	0.03	-0.00	0.05

CASSCF(14,10)/LANL2DZ = -664.2781346

(25) Os-S_0-Int

Atomic Number	Coordinates (Angstroms) X	Y	Z
76	-0.000000	0.000000	-0.337110
6	0.000000	-1.811399	0.372387
8	0.000000	-2.820906	0.932686
6	-1.992649	-0.000000	-0.488051
8	-3.121157	-0.000000	-0.636963
6	1.992649	0.000000	-0.488051
8	3.121157	0.000000	-0.636963
6	-0.000000	1.811399	0.372387
8	-0.000000	2.820906	0.932686

CASSCF(14,10)/LANL2DZ = -541.1273525

(26) Os-S_0-Cpx

Atomic Number	Coordinates (Angstroms) X	Y	Z
76	0.000000	0.000000	0.000000
6	0.000000	0.000000	1.999558
6	1.957155	0.000000	-0.045801
6	-0.091265	-0.222653	-1.959659
6	-1.341881	1.406504	-0.051345
8	-0.014849	-0.035953	3.139749
8	3.098227	0.169432	-0.077962
8	-0.151925	-0.393443	-3.089323
8	-2.010204	2.349767	-0.091350
14	-1.907406	-3.350830	0.494876
1	-0.558507	-2.694289	0.468797
6	-1.663623	-5.211777	0.734619
6	-2.769317	-2.984942	-1.153294
6	-2.887309	-2.609952	1.938870
1	-2.622443	-5.721330	0.755309
1	-1.153875	-5.426230	1.668377
1	-1.076820	-5.641401	-0.070886
1	-3.732001	-3.485792	-1.200162
1	-2.179088	-3.329570	-1.996581
1	-2.948873	-1.922288	-1.280467
1	-2.369653	-2.749286	2.882805
1	-3.859041	-3.087809	2.023991
1	-3.058098	-1.546887	1.803153

CASSCF(14,10)/LANL2DZ = -664.3287665

(27) Os-S_0-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
6	1.585365	-0.039986	1.857504
8	2.209575	-0.013921	2.817296
76	0.507998	-0.093786	0.175950
6	-0.052524	1.806809	0.287394

8	-0.385957	2.896844	0.342868
6	1.988000	0.174813	-1.109614
8	2.841292	0.331321	-1.853917
6	0.453763	-2.072625	0.087888
8	0.386010	-3.210902	0.031501
14	-1.243874	-0.283573	-1.772881
6	-2.755486	-1.338758	-1.275378
1	-3.256792	-1.700619	-2.170217
1	-3.478895	-0.773947	-0.694058
1	-2.467138	-2.207058	-0.691923
6	-0.446951	-1.189891	-3.257664
1	-1.172742	-1.270472	-4.063884
1	-0.128678	-2.197768	-3.006790
1	0.413356	-0.654460	-3.648363
6	-1.839498	1.387230	-2.478650
1	-2.623179	1.843016	-1.879545
1	-2.240707	1.224605	-3.476089
1	-1.028961	2.103026	-2.573079
1	-3.540244	1.361496	0.089990

Vibrational Mode

-1	-0.01	0.00	0.00
-2	-0.01	0.00	0.00
-3	-0.00	0.00	-0.00
-4	0.01	0.00	-0.01
-5	0.02	0.01	-0.01
-6	-0.00	-0.00	0.00
-7	0.00	-0.00	0.01
-8	-0.00	0.00	0.00
-9	-0.00	0.00	0.00
-10	-0.00	-0.00	-0.01
-11	-0.00	-0.01	-0.02
-12	0.04	-0.06	-0.03
-13	-0.04	0.01	-0.09
-14	-0.02	0.02	0.03
-15	0.01	0.01	-0.00
-16	0.02	0.00	-0.01
-17	0.02	0.01	-0.00
-18	0.01	0.02	0.00
-19	-0.03	-0.01	-0.00
-20	-0.10	-0.07	-0.04

-21	0.04	-0.01	-0.03
-22	-0.07	0.04	0.07
-23	0.82	-0.10	0.52

CASSCF(14,10)/LANL2DZ = -664.2415873

(28) Os-S_0-Pro

Atomic Number	Coordinates (Angstroms) X	Y	Z
76	-0.274440	0.192678	0.992603
1	-0.126071	-1.484109	1.093641
6	-2.277592	-0.069500	1.069603
8	-3.399223	-0.266218	1.121878
6	-0.200710	2.173519	0.852848
8	-0.130142	3.312341	0.766250
6	-0.034424	0.146861	2.941837
8	0.147453	0.067425	4.067409
6	-0.163760	-0.111756	-0.949883
8	-0.083343	-0.342096	-2.064970
14	2.337430	0.043043	0.993200
6	3.083017	0.105390	-0.756603
1	4.166849	0.091903	-0.685499
1	2.804268	1.009513	-1.289378
1	2.787944	-0.745109	-1.362624
6	2.908974	-1.575643	1.810793
1	3.994561	-1.623681	1.829072
1	2.545596	-2.440539	1.265985
1	2.560396	-1.659657	2.835066
6	3.097469	1.493150	1.968393
1	4.179804	1.396746	1.991286
1	2.753883	1.521719	2.997788
1	2.866661	2.450836	1.511304

CASSCF(14,10)/LANL2DZ = -664.3736035