Supplementary Materials

The Mechanistic Investigations of Photochemical Carbonyl Elimination and Oxidative Addition Reactions of (η^5-C_5H_5)M(CO)$_3$ (M = Mn and Re) Complexes

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(All were calculated at the CAS(14,13)/Def2-SVPD (geometry) and the MP2-CAS(14,13)/Def2-SVPD//CAS(14,13)/Def2-SVPD (energy) level of theory)

Mn-S0-Rea

Atomic Number	Coordinates (Angstroms) X	Y	Z
Mn	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.248000
C	1.368796	0.000000	1.819141
C	1.601953	-1.177293	1.085954
C	0.377549	-1.949087	1.081642
C	-0.583188	-1.233647	1.824915
H	-0.459439	0.727828	2.878790
H	2.084739	0.766546	2.018124
H	2.530086	-1.477933	0.653354
H	0.254360	-2.921036	0.658828
H	-1.583301	-1.550556	2.023671
C	-1.828041	0.198279	-0.478999
C	0.407005	1.796701	-0.375256
C	0.497943	-0.598443	-1.652263
O	-2.935738	0.295330	-0.747266
O	0.678889	2.891600	-0.578733
O	0.834856	-0.999856	-2.680500

Energy = -633.371131 hartree

Mn-T1-Min

Atomic Number	Coordinates (Angstroms) X	Y	Z
Mn	0.01237600	-0.01548500	-0.02081700
C	0.02864400	-0.03545100	2.28356600
C	1.39501700	-0.04364300	1.88176800
C	1.61750900	-1.20818100	1.12536100
C	0.39907200	-1.97492600	1.12145200
C	-0.55694200	-1.26785100	1.87426800
H	-0.45073500	0.72432500	2.90039800
H	2.12138600	0.74683800	2.07216700
H	2.55751600	-1.51100800	0.66537500
H	0.26971500	-2.95587700	0.66560000
H	-1.58419100	-1.57894600	2.06565700
C	-2.04627400	0.18387500	-0.54637600
C	0.48576800	1.99827500	-0.43623000
C	0.51302100	-0.61313000	-1.70656000
O	-3.13959700	0.27477500	-0.81160300
O	0.75588300	3.07502500	-0.64115100
O	0.86830200	-1.03018400	-2.71347300

Mn-T1-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
Mn	0.03997700	-0.25793700	-0.03759500
C	1.44614800	1.21644200	-1.07807900
C	1.99420700	-0.10333400	-1.18484500
C	2.28980600	-0.56647600	0.11396000
C	1.91257000	0.46733600	1.03621100
C	1.45043800	1.58072700	0.29106900
H	1.14923000	1.85505000	-1.91070000

H	2.14821800	-0.65280800	-2.11640200
H	2.72285400	-1.53351400	0.37586700
H	2.03407600	0.42455200	2.11909300
H	1.10821300	2.53095400	0.70954300
C	-1.84405700	1.58758800	0.33502900
C	-1.23534400	-0.95494700	-1.41886800
C	-0.57206200	-1.29361400	1.36457800
O	-2.58519300	2.39840200	0.58479100
O	-1.90379800	-1.41314300	-2.21536200
O	-0.86253900	-1.95752500	2.25659100

Mn-T1-IM

Atomic Number	Coordinates (Angstroms) X	Y	Z
Mn	0.00090200	0.00488200	0.74993200
H	2.20279400	-0.60695900	-1.13797100
C	1.16248800	-0.32510300	-1.11462500
C	0.66022900	1.00772100	-1.09909600
H	0.11820500	-2.29089400	-1.13913800
H	1.25781800	1.90509800	-1.09651500
C	-0.75232100	0.93964200	-1.06859000
H	-1.43398800	1.77456800	-1.06537200
C	-1.12398000	-0.44447600	-1.08043600
H	-2.13187500	-0.82671100	-1.08649100
C	0.06037700	-1.21380800	-1.13747000
C	-1.43003900	0.16809900	1.89921600
O	-2.35938300	0.28052400	2.56036800
C	1.42521100	-0.13863800	1.92216100
O	2.34356100	-0.23394600	2.59984700

Mn-Tl-Cpx

Atomic Number	Coordinates (Angstroms) X	Y	Z
Mn	-0.77593200	0.05031500	-0.02051400
C	-0.47006500	1.60552700	-0.98857900
8	-0.35719600	2.56390300	-1.61149700
C	-0.78968700	1.10002900	1.67263100
8	-0.85401700	1.70654900	2.62790500
Si	2.62005900	-0.53447000	-0.02982200
C	2.76466000	-0.36417800	-1.89489100
H	2.38252000	0.61664300	-2.23001400
H	2.18676600	-1.14878300	-2.41275000
H	3.81828500	-0.44945200	-2.21780500
C	3.47485600	0.88437200	0.85560400
H	3.06781300	1.85061900	0.50945800
H	4.56157000	0.88374800	0.66094400
H	3.32516600	0.82104500	1.94714800
C	3.19305200	-2.22082100	0.57425600
H	4.26104900	-2.39408500	0.35650100
H	2.61121000	-3.02110000	0.08533300
H	3.04724100	-2.31427800	1.66426200
H	1.15991800	-0.44184600	0.30613400
H	-0.26306800	-2.55599800	-1.48772200
C	-1.08398400	-2.01029700	-1.02046400
C	-1.49013500	-2.10612100	0.32948800
H	-1.84811500	-0.73988300	-2.70051500
H	-1.06519500	-2.76721300	1.08456400
C	-2.61803100	-1.24583200	0.50925000
H	-3.16896400	-1.11541600	1.44083500
C	-2.89013600	-0.60392300	-0.71465700
H	-3.68997400	0.10813600	-0.91065400
C	-1.90667900	-1.04103300	-1.65502000

Mn-T1-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-1.18074800	1.68843800	-0.96106100
C	-0.79384200	1.91019000	0.38074400
C	-1.74202000	1.28241100	1.23850300
C	-2.67862400	0.61069600	0.42047500
C	-2.31515300	0.83475700	-0.94073400
Mn	-0.61732400	-0.42199300	0.03541300
C	-0.33756200	-1.22560200	-1.79868500
O	-0.36809400	-1.51570400	-2.90184700
C	-1.34743400	-1.93835500	1.26070600
O	-1.74564639	-2.76540042	1.92899824
H	-3.54023000	0.03624600	0.76211000
H	-1.73846900	1.31306900	2.32762400
H	0.05406100	2.51420400	0.70941300
H	-0.66112200	2.04556800	-1.85032700
H	-2.86599100	0.47917200	-1.81155000
Si	2.33908600	0.12983600	0.29066400
H	3.07367300	-1.95674600	-0.87282500
C	3.42461100	-1.37053700	-0.00651400
H	4.45680800	-1.03841600	-0.21882500
H	3.45807500	-2.03450900	0.87311100
H	1.85474700	0.67854700	-2.10745500
C	2.29933300	1.20636000	-1.24736700
H	1.73543100	2.13920600	-1.08496700
H	3.33853300	1.47674700	-1.51175100
C	2.91584700	1.12355700	1.77965300
H	3.26162400	0.45970700	2.59257000
H	2.09464800	1.74833400	2.17686300
H	3.75161700	1.79457400	1.50492000
H	0.99455200	-0.38929400	0.76982300

Mn-T1/S0-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-1.3725755	1.6874933	-0.9512499
C	-1.0574414	1.9737822	0.3982671
C	-1.9171666	1.2135011	1.2308790
C	-2.8109306	0.4916086	0.3824602
C	-2.4781356	0.7745750	-0.9561687
Mn	-0.6918980	-0.2163386	0.0006808
C	-0.1238799	-1.0383770	-1.5339311
O	0.1545289	-1.5114556	-2.5405051
C	-0.8490705	-1.8552886	0.9746659
O	-0.9866833	-2.8297106	1.5412130
H	-3.6028160	-0.1781823	0.7173930
H	-1.9363517	1.2266539	2.3193889
H	-0.2588824	2.6326078	0.7419878
H	-0.8990195	2.1213749	-1.8311815
H	-2.9737813	0.3780565	-1.8413116
Si	2.3378050	0.2202454	0.3348618
H	2.5264662	-1.9893827	-0.8208271
C	3.0325168	-1.4959940	0.0260953
H	4.1087808	-1.4320924	-0.2133723
H	2.9237297	-2.1375997	0.9167341
H	1.9203449	0.7397186	-2.0792764
C	2.3575439	1.2738691	-1.2199293
H	1.7929447	2.2103334	-1.0732571
H	3.3986629	1.5416404	-1.4751348
C	3.2541350	1.0929213	1.7276118
H	3.2269918	0.4988531	2.6566873
H	2.7964483	2.0747484	1.9390493
H	4.3112647	1.2609206	1.4585032
H	0.9368561	0.0865805	0.9073475
-1	0.00271252	-0.00245509	0.00498967
-2	-0.00427054	0.02467005	0.00990108
-3	0.00343301	0.00287065	-0.00544188
-4	-0.01889062	0.01889311	-0.00757508

-5	-0.02091962	0.00596999	0.00466603
-6	-0.01581939	0.00840570	-0.05187705
-7	0.00305851	0.00501219	0.02099203
-8	0.00553834	-0.01381301	-0.02653927
-9	0.00540773	-0.06563637	0.03492637
-10	0.00016179	0.00685479	-0.00453034
-11	0.00018205	-0.00087901	0.00023053
-12	0.00057804	-0.00047351	0.00059109
-13	-0.00126464	0.00083510	0.00040427
-14	0.00036701	-0.00094017	-0.00052874
-15	0.00056426	0.00009953	0.00002119
-16	0.00231221	-0.00188603	0.01401018
-17	-0.00017859	0.00030086	-0.00021751
-18	0.00191100	-0.00040468	-0.00136791
-19	0.00030616	-0.00067186	0.00009122
-20	0.00020739	0.00010979	0.00031486
-21	0.00017761	-0.00022925	-0.00030268
-22	-0.00284330	-0.00013116	-0.00112741
-23	0.00024519	0.00081560	-0.00021148
-24	-0.00009993	-0.00011508	0.00059975
-25	0.00599167	0.00100204	-0.00217584
-26	-0.00022120	-0.00032339	-0.00016546
-27	-0.00022275	0.00007116	-0.00008990
-28	0.00084222	0.00101815	0.00168591
-29	0.03073385	0.01102992	0.00872639

Mn-T1/SO-1

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	0.87493100	1.28597800	2.01093800
C	1.19032000	0.67712200	1.17909800
C	1.67737700	1.15726000	-0.07730700
H	0.89496600	-1.38770900	1.94382500

H	1.81166800	2.18943000	-0.35705500
C	1.98671600	0.02815200	-0.87180600
H	2.34861500	0.05685200	-1.88876200
C	1.69513500	-1.14481300	-0.13393000
H	1.84784000	-2.15950600	-0.46243600
C	1.20187200	-0.73376500	1.14394900
Mn	-0.14922100	-0.00146900	-0.38895000
C	-1.36863600	1.30470600	-0.10428500
O	-2.11985000	2.13817700	0.14248500
C	-1.37886400	-1.29887000	-0.10344400
O	-2.13902500	-2.12406100	0.14296500

Mn-SO-IM

Atomic Number	Coordinates (Angstroms) X	Y	Z
Mn	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.347899
C	1.349262	0.000000	1.865830
C	1.561353	-1.200492	1.138030
C	0.340729	-1.941789	1.147485
C	-0.609494	-1.201423	1.912268
H	-0.440723	0.743981	2.973975
H	2.079233	0.756598	2.052093
H	2.488351	-1.516739	0.711519
H	0.199955	-2.926908	0.758517
H	-1.608478	-1.512015	2.131338
C	-1.812223	0.124116	-0.747739
C	0.475651	1.646234	-0.544997
O	-2.872036	0.209889	-1.148053
O	0.809906	2.726175	-0.850613

Energy = -520.607049 hartree

Mn-SO-Cpx

Atomic Number	Coordinates (Angstroms) X	Y	Z
Mn	-0.688066	0.036969	0.005150
C	-0.423486	1.529697	-0.971437
O	-0.291306	2.491320	-1.614250
C	-0.743105	0.966888	1.608026
O	-0.821534	1.549844	2.599170
Si	2.539703	-0.487070	-0.070810
C	2.775750	-0.355085	-1.939938
H	2.457965	0.612203	-2.313079
H	2.212328	-1.117529	-2.467222
H	3.824407	-0.481572	-2.195652
C	3.408895	0.912328	0.850160
H	3.061369	1.881649	0.508805
H	4.481829	0.869280	0.686106
H	3.233575	0.852098	1.919237
C	3.037558	-2.189339	0.580786
H	4.091023	-2.378585	0.394983
H	2.469483	-2.977595	0.097672
H	2.869479	-2.263958	1.650191
H	1.081467	-0.361763	0.245184
H	-0.238966	-2.536712	-1.492619
C	-1.013858	-1.981391	-1.011491
C	-1.405164	-2.094677	0.355422
H	-1.832129	-0.743042	-2.663031
H	-1.005067	-2.776154	1.073457
C	-2.533463	-1.239100	0.553698
H	-3.070093	-1.118794	1.470083
C	-2.807665	-0.568264	-0.658528
H	-3.607335	0.116902	-0.835319
C	-1.860606	-1.032393	-1.635346

Energy = -643.694979 hartree

Mn-S0-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	1.323279	-1.328734	2.789700
C	2.087829	-0.537881	3.822365
C	1.299709	0.003240	4.925475
C	-0.248245	-0.340711	4.843929
C	-0.383871	-1.353158	3.267132
Mn	0.984685	-2.264483	4.859888
C	0.206247	-4.068372	3.931787
O	-0.275279	-5.184235	3.357641
C	0.762438	-1.983064	7.020672
O	0.626152	-1.810420	8.346056
Si	3.891859	-2.993963	4.961109
H	3.994031	-5.534320	5.225827
C	4.618363	-4.726005	5.612332
C	4.378494	-3.144049	3.047842
C	5.036275	-1.563434	5.700916
H	5.792895	-2.008579	6.350587
H	4.416221	-0.872937	6.276816
H	5.521885	-1.027989	4.882328
H	2.901691	-3.038182	6.460051

Mn-S0-Pro

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	-2.69461800	2.20301100	0.57626800
C	-2.67854400	1.15703600	0.28578100
C	-2.67556300	0.05189900	1.16950800
H	-2.66506900	1.25165400	-1.95352000
H	-2.68098300	0.10596400	2.25406800
C	-2.65795100	-1.13439300	0.39726600
H	-2.65916500	-2.14786400	0.78613100
C	-2.64849200	-0.76138000	-0.97844100
H	-2.64469100	-1.44092200	-1.82460900
C	-2.66133500	0.65558800	-1.04664400
Mn	-0.71992900	0.00049900	-0.07611100
C	0.06437600	-0.00294700	1.70284900
O	0.48349100	-0.00511500	2.76748200
C	-0.02820700	-1.73288000	-0.57367300
O	0.28565400	-2.76954000	-0.94148100
Si	0.25410715	1.54739902	-2.06166819
C	1.63207176	0.71354669	-3.05631398
H	2.01829270	1.45708445	-3.76901057
H	1.27443688	-0.14881227	-3.63049212
H	2.46811624	0.39172219	-2.42253341
C	1.00538963	3.17194678	-1.44501672
H	1.78970020	3.01200931	-0.69421640
H	0.25333469	3.85128038	-1.02769514
H	1.46668059	3.66880381	-2.31118089
C	-1.14230040	1.97442153	-3.25484748
H	-1.94335577	2.52370723	-2.74257119
H	-1.57521891	1.06818876	-3.69850054
H	-0.75335998	2.60588681	-4.06652823
H	-1.30612086	1.46943112	0.34554220

Mn-SO-Rea

Atomic Number	Coordinates (Angstroms) X	Y	Z
Mn	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.248000
C	1.368796	0.000000	1.819141
C	1.601953	-1.177293	1.085954
C	0.377549	-1.949087	1.081642
C	-0.583188	-1.233647	1.824915
H	-0.459439	0.727828	2.878790
H	2.084739	0.766546	2.018124
H	2.530086	-1.477933	0.653354
H	0.254360	-2.921036	0.658828
H	-1.583301	-1.550556	2.023671
C	-1.828041	0.198279	-0.478999
C	0.407005	1.796701	-0.375256
C	0.497943	-0.598443	-1.652263
O	-2.935738	0.295330	-0.747266
O	0.678889	2.891600	-0.578733
O	0.834856	-0.999856	-2.680500

Energy = -633.371131 hartree

Mn-T1-Min

Atomic Number	Coordinates (Angstroms) X	Y	Z
Mn	0.01237600	-0.01548500	-0.02081700
C	0.02864400	-0.03545100	2.28356600
C	1.39501700	-0.04364300	1.88176800
C	1.61750900	-1.20818100	1.12536100
C	0.39907200	-1.97492600	1.12145200

C	-0.55694200	-1.26785100	1.87426800
H	-0.45073500	0.72432500	2.90039800
H	2.12138600	0.74683800	2.07216700
H	2.55751600	-1.51100800	0.66537500
H	0.26971500	-2.95587700	0.66560000
H	-1.58419100	-1.57894600	2.06565700
C	-2.04627400	0.18387500	-0.54637600
C	0.48576800	1.99827500	-0.43623000
C	0.51302100	-0.61313000	-1.70656000
O	-3.13959700	0.27477500	-0.81160300
O	0.75588300	3.07502500	-0.64115100
O	0.86830200	-1.03018400	-2.71347300

Mn-T1-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
Mn	0.03997700	-0.25793700	-0.03759500
C	1.44614800	1.21644200	-1.07807900
C	1.99420700	-0.10333400	-1.18484500
C	2.28980600	-0.56647600	0.11396000
C	1.91257000	0.46733600	1.03621100
C	1.45043800	1.58072700	0.29106900
H	1.14923000	1.85505000	-1.91070000
H	2.14821800	-0.65280800	-2.11640200
H	2.72285400	-1.53351400	0.37586700
H	2.03407600	0.42455200	2.11909300
H	1.10821300	2.53095400	0.70954300
C	-1.84405700	1.58758800	0.33502900
C	-1.23534400	-0.95494700	-1.41886800
C	-0.57206200	-1.29361400	1.36457800
O	-2.58519300	2.39840200	0.58479100
O	-1.90379800	-1.41314300	-2.21536200
O	-0.86253900	-1.95752500	2.25659100

Mn-T1-IM

Atomic Number	Coordinates (Angstroms) X	Y	Z
Mn	0.00090200	0.00488200	0.74993200
H	2.20279400	-0.60695900	-1.13797100
C	1.16248800	-0.32510300	-1.11462500
C	0.66022900	1.00772100	-1.09909600
H	0.11820500	-2.29089400	-1.13913800
H	1.25781800	1.90509800	-1.09651500
C	-0.75232100	0.93964200	-1.06859000
H	-1.43398800	1.77456800	-1.06537200
C	-1.12398000	-0.44447600	-1.08043600
H	-2.13187500	-0.82671100	-1.08649100
C	0.06037700	-1.21380800	-1.13747000
C	-1.43003900	0.16809900	1.89921600
O	-2.35938300	0.28052400	2.56036800
C	1.42521100	-0.13863800	1.92216100
O	2.34356100	-0.23394600	2.59984700

Mn-T1-Cpx

Atomic Number	Coordinates (Angstroms) X	Y	Z
Mn	-0.77593200	0.05031500	-0.02051400
C	-0.47006500	1.60552700	-0.98857900
8	-0.35719600	2.56390300	-1.61149700
C	-0.78968700	1.10002900	1.67263100
8	-0.85401700	1.70654900	2.62790500

Si	2.62005900	-0.53447000	-0.02982200
C	2.76466000	-0.36417800	-1.89489100
H	2.38252000	0.61664300	-2.23001400
H	2.18676600	-1.14878300	-2.41275000
H	3.81828500	-0.44945200	-2.21780500
C	3.47485600	0.88437200	0.85560400
H	3.06781300	1.85061900	0.50945800
H	4.56157000	0.88374800	0.66094400
H	3.32516600	0.82104500	1.94714800
C	3.19305200	-2.22082100	0.57425600
H	4.26104900	-2.39408500	0.35650100
H	2.61121000	-3.02110000	0.08533300
H	3.04724100	-2.31427800	1.66426200
H	1.15991800	-0.44184600	0.30613400
H	-0.26306800	-2.55599800	-1.48772200
C	-1.08398400	-2.01029700	-1.02046400
C	-1.49013500	-2.10612100	0.32948800
H	-1.84811500	-0.73988300	-2.70051500
H	-1.06519500	-2.76721300	1.08456400
C	-2.61803100	-1.24583200	0.50925000
H	-3.16896400	-1.11541600	1.44083500
C	-2.89013600	-0.60392300	-0.71465700
H	-3.68997400	0.10813600	-0.91065400
C	-1.90667900	-1.04103300	-1.65502000

Mn-T1-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-1.18074800	1.68843800	-0.96106100
C	-0.79384200	1.91019000	0.38074400
C	-1.74202000	1.28241100	1.23850300
C	-2.67862400	0.61069600	0.42047500
C	-2.31515300	0.83475700	-0.94073400

Mn	-0.61732400	-0.42199300	0.03541300
C	-0.33756200	-1.22560200	-1.79868500
O	-0.36809400	-1.51570400	-2.90184700
C	-1.34743400	-1.93835500	1.26070600
O	-1.74564639	-2.76540042	1.92899824
H	-3.54023000	0.03624600	0.76211000
H	-1.73846900	1.31306900	2.32762400
H	0.05406100	2.51420400	0.70941300
H	-0.66112200	2.04556800	-1.85032700
H	-2.86599100	0.47917200	-1.81155000
Si	2.33908600	0.12983600	0.29066400
H	3.07367300	-1.95674600	-0.87282500
C	3.42461100	-1.37053700	-0.00651400
H	4.45680800	-1.03841600	-0.21882500
H	3.45807500	-2.03450900	0.87311100
H	1.85474700	0.67854700	-2.10745500
C	2.29933300	1.20636000	-1.24736700
H	1.73543100	2.13920600	-1.08496700
H	3.33853300	1.47674700	-1.51175100
C	2.91584700	1.12355700	1.77965300
H	3.26162400	0.45970700	2.59257000
H	2.09464800	1.74833400	2.17686300
H	3.75161700	1.79457400	1.50492000
H	0.99455200	-0.38929400	0.76982300

Mn-T1/S0-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
C	-1.3725755	1.6874933	-0.9512499
C	-1.0574414	1.9737822	0.3982671
C	-1.9171666	1.2135011	1.2308790
C	-2.8109306	0.4916086	0.3824602
C	-2.4781356	0.7745750	-0.9561687

Mn	-0.6918980	-0.2163386	0.0006808
C	-0.1238799	-1.0383770	-1.5339311
O	0.1545289	-1.5114556	-2.5405051
C	-0.8490705	-1.8552886	0.9746659
O	-0.9866833	-2.8297106	1.5412130
H	-3.6028160	-0.1781823	0.7173930
H	-1.9363517	1.2266539	2.3193889
H	-0.2588824	2.6326078	0.7419878
H	-0.8990195	2.1213749	-1.8311815
H	-2.9737813	0.3780565	-1.8413116
Si	2.3378050	0.2202454	0.3348618
H	2.5264662	-1.9893827	-0.8208271
C	3.0325168	-1.4959940	0.0260953
H	4.1087808	-1.4320924	-0.2133723
H	2.9237297	-2.1375997	0.9167341
H	1.9203449	0.7397186	-2.0792764
C	2.3575439	1.2738691	-1.2199293
H	1.7929447	2.2103334	-1.0732571
H	3.3986629	1.5416404	-1.4751348
C	3.2541350	1.0929213	1.7276118
H	3.2269918	0.4988531	2.6566873
H	2.7964483	2.0747484	1.9390493
H	4.3112647	1.2609206	1.4585032
H	0.9368561	0.0865805	0.9073475
-1	0.00271252	-0.00245509	0.00498967
-2	-0.00427054	0.02467005	0.00990108
-3	0.00343301	0.00287065	-0.00544188
-4	-0.01889062	0.01889311	-0.00757508
-5	-0.02091962	0.00596999	0.00466603
-6	-0.01581939	0.00840570	-0.05187705
-7	0.00305851	0.00501219	0.02099203
-8	0.00553834	-0.01381301	-0.02653927
-9	0.00540773	-0.06563637	0.03492637
-10	0.00016179	0.00685479	-0.00453034
-11	0.00018205	-0.00087901	0.00023053
-12	0.00057804	-0.00047351	0.00059109
-13	-0.00126464	0.00083510	0.00040427
-14	0.00036701	-0.00094017	-0.00052874
-15	0.00056426	0.00009953	0.00002119
-16	0.00231221	-0.00188603	0.01401018

-17	-0.00017859	0.00030086	-0.00021751
-18	0.00191100	-0.00040468	-0.00136791
-19	0.00030616	-0.00067186	0.00009122
-20	0.00020739	0.00010979	0.00031486
-21	0.00017761	-0.00022925	-0.00030268
-22	-0.00284330	-0.00013116	-0.00112741
-23	0.00024519	0.00081560	-0.00021148
-24	-0.00009993	-0.00011508	0.00059975
-25	0.00599167	0.00100204	-0.00217584
-26	-0.00022120	-0.00032339	-0.00016546
-27	-0.00022275	0.00007116	-0.00008990
-28	0.00084222	0.00101815	0.00168591
-29	0.03073385	0.01102992	0.00872639

Mn-T1/S0-1

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	0.87493100	1.28597800	2.01093800
C	1.19032000	0.67712200	1.17909800
C	1.67737700	1.15726000	-0.07730700
H	0.89496600	-1.38770900	1.94382500
H	1.81166800	2.18943000	-0.35705500
C	1.98671600	0.02815200	-0.87180600
H	2.34861500	0.05685200	-1.88876200
C	1.69513500	-1.14481300	-0.13393000
H	1.84784000	-2.15950600	-0.46243600
C	1.20187200	-0.73376500	1.14394900
Mn	-0.14922100	-0.00146900	-0.38895000
C	-1.36863600	1.30470600	-0.10428500
O	-2.11985000	2.13817700	0.14248500
C	-1.37886400	-1.29887000	-0.10344400
O	-2.13902500	-2.12406100	0.14296500

Mn-SO-IM

Atomic Number	Coordinates (Angstroms) X	Y	Z
Mn	0.000000	0.000000	0.000000
C	0.000000	0.000000	2.347899
C	1.349262	0.000000	1.865830
C	1.561353	-1.200492	1.138030
C	0.340729	-1.941789	1.147485
C	-0.609494	-1.201423	1.912268
H	-0.440723	0.743981	2.973975
H	2.079233	0.756598	2.052093
H	2.488351	-1.516739	0.711519
H	0.199955	-2.926908	0.758517
H	-1.608478	-1.512015	2.131338
C	-1.812223	0.124116	-0.747739
C	0.475651	1.646234	-0.544997
O	-2.872036	0.209889	-1.148053
O	0.809906	2.726175	-0.850613

Energy = -520.607049 hartree

Mn-SO-Cpx

Atomic Number	Coordinates (Angstroms) X	Y	Z
Mn	-0.688066	0.036969	0.005150

C	-0.423486	1.529697	-0.971437
O	-0.291306	2.491320	-1.614250
C	-0.743105	0.966888	1.608026
O	-0.821534	1.549844	2.599170
Si	2.539703	-0.487070	-0.070810
C	2.775750	-0.355085	-1.939938
H	2.457965	0.612203	-2.313079
H	2.212328	-1.117529	-2.467222
H	3.824407	-0.481572	-2.195652
C	3.408895	0.912328	0.850160
H	3.061369	1.881649	0.508805
H	4.481829	0.869280	0.686106
H	3.233575	0.852098	1.919237
C	3.037558	-2.189339	0.580786
H	4.091023	-2.378585	0.394983
H	2.469483	-2.977595	0.097672
H	2.869479	-2.263958	1.650191
H	1.081467	-0.361763	0.245184
H	-0.238966	-2.536712	-1.492619
C	-1.013858	-1.981391	-1.011491
C	-1.405164	-2.094677	0.355422
H	-1.832129	-0.743042	-2.663031
H	-1.005067	-2.776154	1.073457
C	-2.533463	-1.239100	0.553698
H	-3.070093	-1.118794	1.470083
C	-2.807665	-0.568264	-0.658528
H	-3.607335	0.116902	-0.835319
C	-1.860606	-1.032393	-1.635346

Energy = -643.694979 hartree

Mn-S0-TS1

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

C	1.323279	-1.328734	2.789700
C	2.087829	-0.537881	3.822365
C	1.299709	0.003240	4.925475
C	-0.248245	-0.340711	4.843929
C	-0.383871	-1.353158	3.267132
Mn	0.984685	-2.264483	4.859888
C	0.206247	-4.068372	3.931787
O	-0.275279	-5.184235	3.357641
C	0.762438	-1.983064	7.020672
O	0.626152	-1.810420	8.346056
Si	3.891859	-2.993963	4.961109
H	3.994031	-5.534320	5.225827
C	4.618363	-4.726005	5.612332
C	4.378494	-3.144049	3.047842
C	5.036275	-1.563434	5.700916
H	5.792895	-2.008579	6.350587
H	4.416221	-0.872937	6.276816
H	5.521885	-1.027989	4.882328
H	2.901691	-3.038182	6.460051

Mn-SO-Pro

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	-2.69461800	2.20301100	0.57626800
C	-2.67854400	1.15703600	0.28578100
C	-2.67556300	0.05189900	1.16950800
H	-2.66506900	1.25165400	-1.95352000
H	-2.68098300	0.10596400	2.25406800
C	-2.65795100	-1.13439300	0.39726600
H	-2.65916500	-2.14786400	0.78613100
C	-2.64849200	-0.76138000	-0.97844100

H	-2.64469100	-1.44092200	-1.82460900
C	-2.66133500	0.65558800	-1.04664400
Mn	-0.71992900	0.00049900	-0.07611100
C	0.06437600	-0.00294700	1.70284900
O	0.48349100	-0.00511500	2.76748200
C	-0.02820700	-1.73288000	-0.57367300
O	0.28565400	-2.76954000	-0.94148100
Si	0.25410715	1.54739902	-2.06166819
C	1.63207176	0.71354669	-3.05631398
H	2.01829270	1.45708445	-3.76901057
H	1.27443688	-0.14881227	-3.63049212
H	2.46811624	0.39172219	-2.42253341
C	1.00538963	3.17194678	-1.44501672
H	1.78970020	3.01200931	-0.69421640
H	0.25333469	3.85128038	-1.02769514
H	1.46668059	3.66880381	-2.31118089
C	-1.14230040	1.97442153	-3.25484748
H	-1.94335577	2.52370723	-2.74257119
H	-1.57521891	1.06818876	-3.69850054
H	-0.75335998	2.60588681	-4.06652823
H	-1.30612086	1.46943112	0.34554220

Re-S_0-Rea

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	1.98416200	-1.10965800	-1.99559800
C	1.98254600	-0.58646100	-1.05256600
C	1.98376300	-1.19237400	0.23314900

H	2.00544000	1.55045700	-1.67662200
H	2.00718400	-2.24942700	0.43941200
C	1.98245700	-0.14644500	1.19716200
H	1.98416200	-0.27593800	2.26755900
C	1.98656100	1.09143700	0.51392500
H	2.00260500	2.06761100	0.97008300
C	1.98699600	0.81787100	-0.88658800
Re	-0.05309000	0.00013800	-0.00058900
C	-1.19163400	-0.98220800	-1.17390800
O	-1.84425800	-1.58448900	-1.89338900
C	-1.18261900	1.51363700	-0.26395400
O	-1.83076300	2.44181200	-0.42274600
C	-1.19075600	-0.52664900	1.43644100
O	-1.84319200	-0.84810700	2.31831100

Energy = -611.732864 hartree

Re-S_1S_0-CI

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	2.086572	-1.118823	-1.973987
C	2.062165	-0.605632	-1.056009
C	2.034709	-1.205012	0.239214
H	1.977432	1.520212	-1.701191
H	2.077253	-2.261629	0.428334
C	1.982304	-0.162660	1.193818
H	1.994598	-0.297244	2.261853
C	1.971936	1.084398	0.507733
H	1.992623	2.062578	0.959731
C	1.959852	0.809230	-0.894463
Re	-0.071560	0.009282	0.019284
C	-1.226867	-0.995148	-1.198598

O	-1.890479	-1.583320	-1.962968
C	-1.567831	2.051484	-0.333685
O	-2.230834	2.960518	-0.491168
C	-1.215133	-0.515396	1.485205
O	-1.878022	-0.819140	2.361236

Derivative Coupling

-1	0.0016738369	0.0002166014	-0.0037919873
-2	-0.0089687170	-0.0095896018	0.0073946545
-3	0.0292339935	0.0198667053	-0.0179275358
-4	-0.0030334261	-0.0002135546	0.0008404822
-5	-0.0037655761	0.0023379296	-0.0007916454
-6	-0.0301494156	-0.0360569091	0.0135073103
-7	0.0020832973	0.0008206616	-0.0027179389
-8	0.0130746159	0.0258058080	-0.0043980020
-9	0.0017727614	0.0027706892	0.0018995933
-10	0.0037319162	-0.0166920063	-0.0028837538
-11	-0.0052684528	0.0148316165	0.0159237686
-12	-0.0051762968	-0.0067444527	0.0004402402
-13	0.0000035894	0.0028127192	0.0005765301
-14	0.0098178354	-0.0081466693	0.0057821195
-15	-0.0023858618	0.0030213739	-0.0018034094
-16	-0.0036686130	0.0054140116	-0.0127503076
-17	0.0010245131	-0.0004549224	0.0006998815

Unscaled Gradient Difference

-1	0.0102770236	-0.0035071101	0.0001307568
-2	-0.0427938155	0.0051238832	0.0132984335
-3	0.0086436284	0.0296534947	-0.0060224703
-4	-0.0086609876	-0.0016359273	0.0018203075
-5	-0.0086918380	-0.0033165123	-0.0015803500
-6	-0.0375849706	-0.0124812142	-0.0259715365
-7	-0.0029549073	0.0050629814	0.0037877229
-8	-0.0265102807	0.0070123412	0.0131575354
-9	0.0030379887	-0.0008889160	-0.0006506971
-10	0.0361359092	-0.0151908622	-0.0245243842
-11	0.1143855592	-0.0616028736	0.0618968979
-12	-0.0437773856	0.0349952399	-0.0208906602
-13	0.0129282771	0.0038507727	0.0145084101
-14	-0.0105593109	0.0007744255	-0.0127642428
-15	0.0045730777	-0.0045200163	0.0021919550
-16	-0.0173092794	0.0160048448	-0.0123633084

-17	0.0088613117	0.0006654485	-0.0060243698

Re-S_0-Int

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	-0.84285900	-1.36798700	2.08589900
C	-1.21211200	-0.72914100	1.30076900
C	-1.87770200	-1.15521500	0.10524300
H	-0.83339900	1.31961900	2.11639200
H	-2.07140000	-2.17199900	-0.19208600
C	-2.23848700	0.01177000	-0.60910200
H	-2.71474600	0.02433700	-1.57818500
C	-1.87063200	1.15834700	0.13156300
H	-2.05494500	2.18326400	-0.14298200
C	-1.20560400	0.70102900	1.31676500
Re	0.11072500	-0.00135200	-0.30525800
C	1.40559200	-1.33597600	0.06489900
O	2.12518500	-2.16596200	0.40017000
C	1.39461200	1.34535800	0.06115900
O	2.10468700	2.18309900	0.39702000

Energy = -498.317584 hartree

Re-S_0-Cpx

Atomic Number	Coordinates (Angstroms) X	Y	Z
Re	-0.461314	0.182468	-0.056067

C	0.340814	0.989217	-1.623543
C	-0.920427	2.006550	0.515103
Si	2.040557	-0.341168	0.271832
H	2.186111	-2.252440	-1.375566
C	2.715772	-1.315401	-1.223100
H	3.764668	-1.559460	-1.061944
H	2.653448	-0.750257	-2.148489
H	1.789816	-2.364140	1.765309
C	2.367617	-1.443543	1.787704
H	3.418111	-1.724182	1.828853
H	2.127215	-0.931128	2.715296
H	3.039429	1.865049	-0.407416
C	3.129334	1.202816	0.449689
H	2.864965	1.775768	1.334328
H	4.178214	0.925676	0.537384
H	0.484130	0.463915	1.305032
O	-1.212334	3.036401	0.863593
O	0.777034	1.433251	-2.568805
C	-1.443114	-1.580273	-1.224812
C	-1.513511	-1.622657	1.065848
C	-2.517946	-0.742965	0.617589
C	-2.478466	-0.704085	-0.804379
C	-0.842191	-2.142611	-0.074004
H	-1.179578	-1.801524	-2.239130
H	-0.063730	-2.876057	-0.065526
H	-1.297646	-1.864754	2.085861
H	-3.204393	-0.207163	1.241369
H	-3.152894	-0.170765	-1.441323

Energy = -904.4629 hartree

Re-S_0-TS1

Atomic	Coordinates (Angstroms)		
Number	X	Y	Z

Re	0.49492200	0.10383200	-0.10421100
C	1.33718600	1.73240200	-0.79711300
C	-0.24375000	1.33450300	1.11274600
Si	-2.05146800	-0.15944800	-0.21648200
H	-0.31500800	-1.06402000	-4.14433800
C	2.33712200	-1.30138500	-0.33046700
C	2.18726000	-0.84616100	1.01788100
C	0.96013500	-1.37702200	1.51607500
C	0.35341200	-2.13627400	0.47542800
C	1.21603600	-2.09600500	-0.65711300
H	3.15880200	-1.07426800	-0.99025300
H	2.89728700	-0.26060500	1.57744200
H	0.56867500	-1.24447700	2.51198700
H	-0.56714800	-2.69102100	0.54542600
H	1.01502500	-2.53756500	-1.62117600
C	-2.47615800	-1.54098200	-1.41794000
C	-2.76890100	-0.58736200	1.46711100
C	-2.81336100	1.43396400	-0.84556400
H	-2.19057100	-2.52743600	-1.05064800
H	-3.55922300	-1.54136600	-1.57556900
H	-1.96530400	-1.36738700	-2.36308700
H	-2.60045800	0.20003700	2.20240300
H	-3.84877000	-0.72571300	1.36746800
H	-2.35537400	-1.51845900	1.85999900
H	-3.89708400	1.30604700	-0.92406900
H	-2.61651500	2.27495200	-0.17981400
H	-2.43082500	1.67542600	-1.83841200
O	1.87410800	2.67650000	-1.13046400
O	-0.65235500	2.05433300	1.90833500

-1	0.00	0.00	-0.01
-2	0.00	0.00	0.00
-3	0.00	0.00	0.00
-4	0.00	0.00	0.00
-5	0.25	0.38	0.89
-6	0.00	0.00	0.00
-7	0.00	0.00	0.00
-8	0.00	0.01	0.00

-9	0.00	0.00	0.00
-10	0.00	0.00	0.00
-11	0.00	0.00	0.00
-12	0.00	0.00	0.00
-13	0.00	0.00	0.00
-14	0.00	0.00	0.00
-15	0.00	0.01	0.00
-16	-0.01	0.00	0.01
-17	0.00	0.00	0.00
-18	0.00	0.00	0.00
-19	0.00	0.00	0.00
-20	-0.02	-0.02	0.02
-21	-0.02	0.01	0.01
-22	0.00	0.00	0.00
-23	0.00	0.00	0.00
-24	0.00	0.00	0.00
-25	0.00	0.00	0.00
-26	0.00	0.00	0.00
-27	0.00	-0.01	0.00
-28	0.00	0.00	0.00
-29	0.00	0.00	0.00

Energy = -907.908487 hartree

Re-S_0-Pro

Atomic Number	Coordinates (Angstroms) X	Y	Z
Re	-0.395268	-0.205143	0.341581
C	0.108960	1.471352	-0.365068
O	0.388813	2.485391	-0.828387
C	-0.653028	0.789668	1.955178
O	-0.814222	1.375482	2.922534

Si	2.057520	-0.412748	-0.135730
C	2.299756	-0.264258	-2.002230
H	1.944454	0.695945	-2.380194
H	1.773915	-1.056702	-2.539479
H	3.362948	-0.349978	-2.242851
C	3.114231	0.895966	0.696092
H	2.825607	1.903396	0.392654
H	4.165809	0.753553	0.435666
H	3.023634	0.832413	1.782385
C	2.774829	-2.086845	0.354954
H	3.788921	-2.184358	-0.040719
H	2.187977	-2.924523	-0.026419
H	2.826390	-2.186625	1.440994
H	0.819789	-0.631572	1.387522
H	0.170378	-2.708298	-1.324177
C	-0.668754	-2.156020	-0.933827
C	-1.323817	-2.393666	0.307365
H	-1.103156	-0.697851	-2.562575
H	-1.048732	-3.138152	1.036545
C	-2.396519	-1.478282	0.412735
H	-3.077937	-1.399753	1.244814
C	-2.423373	-0.677637	-0.759040
H	-3.138529	0.096148	-0.983463
C	-1.349845	-1.099814	-1.592973

Energy = -908.094240 hartree
