Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

A Model Study on the Photodecarbonyl Reaction of (η^5-C_5H_5)M(CO)$_2$ (M = Co, Rh, Ir)

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B3PW91/Def2-TZVPPD
(singlet)

Atomic Number	Coordinates (Angstroms) X	Y	Z
Co	0.000000	0.000000	0.000000
C	1.211873	0.000000	1.722987
C	-0.787946	0.955901	-1.215367
O	-1.307504	1.586207	-2.016760
H	2.289480	-0.038990	1.724139
C	0.332222	-1.136079	1.711676
H	0.635011	-2.171507	1.702546
C	-0.951273	0.743293	1.685389
H	-1.801098	1.407319	1.652957
C	-1.002834	-0.674252	1.736734
H	-1.897129	-1.275528	1.750147
C	0.420173	1.158495	1.716567
H	0.787756	2.171991	1.712084
C	0.806038	-0.971983	-1.191225
O	1.337324	-1.612648	-1.976401

SCF Done: E(B3PW91/Def2-TZVPPD) = -1803.0270035
Free energy: E(B3PW91/Def2-TZVPPD) = -1802.962336

(triplet)

Atomic Number	Coordinates (Angstroms) X	Y	Z
Co	0.000000	0.000000	0.000000
C	1.203093	0.000000	2.032646
C	-0.718104	1.437488	-1.183412
O	-1.122834	2.247671	-1.850396
H	2.280757	0.011398	2.086157
C	0.386472	-1.151135	1.979356
H	0.729781	-2.173702	1.985083
C	-0.980803	0.693437	2.003549
H	-1.861450	1.316061	2.031061

C	-0.966436	-0.721395	1.943504
H	-1.831130	-1.366844	1.917195
C	0.359973	1.139345	2.044500
H	0.684474	2.166418	2.109037
C	1.349660	-0.797978	-1.219269
O	2.114306	-1.250070	-1.910042

SCF Done: E(UB3PW91/Def2-TZVPPD) = -1802.999141

Free energy: E(UB3PW91/Def2-TZVPPD) = -1802.93875

B3LYP/TZP-DKH

(singlet)

Atomic Number	Coordinates (Angstroms) X	Y	Z
Co	0.000000	0.000000	0.000000
C	1.208437	0.000000	1.749450
C	-0.992001	0.769366	-1.219104
O	-1.640653	1.272441	-2.016255
H	2.286077	-0.039382	1.746177
C	0.330337	-1.141141	1.761901
H	0.630208	-2.177037	1.769872
C	-0.948240	0.747373	1.716310
H	-1.795154	1.414883	1.683434
C	-0.998709	-0.677578	1.776371
H	-1.890281	-1.282469	1.797128
C	0.418392	1.163516	1.753757
H	0.783034	2.177559	1.754312
C	0.998882	-0.802302	-1.193728
O	1.651458	-1.326451	-1.973597

SCF Done: E(B3LYP/TZP-DKH) = -1800.858765

Free energy: E(B3LYP/TZP-DKH) = -1800.925813

(triplet)

Atomic Number	Coordinates (Angstroms) X	Y	Z

Co	0.000000	0.000000	0.000000
C	1.204846	0.000000	2.001075
C	-1.322916	0.763708	-1.100995
O	-2.121744	1.224865	-1.765819
H	2.282678	0.003253	2.050832
C	0.381422	-1.145549	1.905516
H	0.722198	-2.169025	1.869833
C	-0.979655	0.701158	1.995990
H	-1.856377	1.328646	2.041216
C	-0.977618	-0.710431	1.907042
H	-1.850134	-1.344485	1.872759
C	0.367363	1.144470	2.023044
H	0.696433	2.169643	2.092545
C	1.531612	0.075980	-1.091624
O	2.456805	0.121877	-1.751035

SCF Done: E(UB3LYP/TZP-DKH) = -1800.9025418

Free energy: E(UB3LYP/TZP-DKH) = -1800.8450511

Co-S0-Rea

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	1.62624500	1.35935500	1.84665200
C	1.63202600	0.71208200	0.98477500
C	1.62288000	1.13464100	-0.37674700
H	1.62752900	-1.32580400	1.87149800
H	1.62488200	2.15895700	-0.71484600
C	1.66680000	-0.01132600	-1.20418800
H	1.68683800	-0.02150100	-2.28152100
C	1.62270500	-1.14179200	-0.35557300
H	1.62332700	-2.17216500	-0.67450100
C	1.63260200	-0.69438100	0.99790200
Co	-0.18795800	-0.00004800	-0.01555400
C	-1.43634500	1.33392200	-0.00737900
O	-2.18290800	2.18085000	0.01119700

C	-1.43661600	-1.33396400	-0.00575700
O	-2.18437500	-2.17992900	0.01061400

CAS, E = -1802.905266
MP2-CAS, E = -1802.839247

Co-T1-Min

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	1.43894500	1.33221200	1.95151700
C	1.53447000	0.70304000	1.08013000
C	1.71772300	1.14532100	-0.24986700
H	1.43544300	-1.34752800	1.94485100
H	1.78806000	2.17123100	-0.57625800
C	1.80939300	-0.00126100	-1.07973500
H	1.97552700	0.00085100	-2.14617700
C	1.71550700	-1.15107600	-0.25463100
H	1.78283900	-2.17568100	-0.58533900
C	1.53331700	-0.71415800	1.07680900
Co	-0.29971500	0.00055800	-0.22158600
C	-1.48116200	1.59253300	-0.00915300
O	-2.01566200	2.57257600	0.12894600
C	-1.48923500	-1.58639900	-0.00669000
O	-2.03041200	-2.56309400	0.12768400

CAS, E = -1802.8919598
MP2-CAS, E = -1802.8350701

Co-T1-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	-1.29323500	-2.08459800	-1.36477400
C	-1.43952400	-1.21783800	-0.71563400
C	-1.76263200	0.10157900	-1.14656500
H	-1.28774800	-2.10144400	1.34136000
H	-1.89920100	0.42015300	-2.18181000

C	-1.96901200	0.89790600	0.00780500
H	-2.28767200	1.94177700	0.01475900
C	-1.75822300	0.08765500	1.15159800
H	-1.89090200	0.39352600	2.19119000
C	-1.43642700	-1.22679100	0.70344000
Co	0.24563100	0.07284500	0.00025100
C	1.19466200	1.67985700	-0.00387200
O	1.67205900	2.70726500	0.00162900
C	1.74951200	-1.34374000	0.00005400
O	2.64751600	-2.00826300	-0.00018700

-1	-0.24	0.06	0.00
-2	-0.19	0.07	0.00
-3	-0.08	0.10	0.00
-4	-0.24	0.06	-0.00
-5	-0.06	0.11	0.00
-6	-0.02	0.11	0.00
-7	0.05	0.14	0.00
-8	-0.08	0.10	0.00
-9	-0.06	0.10	0.00
-10	-0.19	0.07	-0.00
-11	-0.09	-0.10	-0.00
-12	0.10	-0.25	-0.00
-13	0.16	-0.27	0.00
-14	0.08	-0.05	0.00
-15	0.49	0.51	0.00

CAS, E = -1802.876195

MP2-CAS, E = -1802.8196451

Co-T1-Int

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	1.43894500	1.33221200	1.95151700
C	1.53447000	0.70304000	1.08013000
C	1.71772300	1.14532100	-0.24986700
H	1.43544300	-1.34752800	1.94485100
H	1.78806000	2.17123100	-0.57625800
C	1.80939300	-0.00126100	-1.07973500

H	1.97552700	0.00085100	-2.14617700
C	1.71550700	-1.15107600	-0.25463100
H	1.78283900	-2.17568100	-0.58533900
C	1.53331700	-0.71415800	1.07680900
Co	-0.29971500	0.00055800	-0.22158600
C	-1.48116200	1.59253300	-0.00915300
O	-2.01566200	2.57257600	0.12894600

CAS, E = -1689.5161959
MP2-CAS, E = -1689.4875957

Co-T1/S0-2

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	-2.0581862	1.9935503	-0.4438668
C	-1.8317962	0.9874327	-0.1269982
C	-1.5856902	0.5763042	1.2108906
H	-1.9560904	-0.1681627	-2.0305604
H	-1.5776421	1.2154792	2.0787190
C	-1.3353655	-0.8104309	1.1912813
H	-1.1080806	-1.4289972	2.0449090
C	-1.4513071	-1.2602135	-0.1559084
H	-1.3298407	-2.2781320	-0.4914058
C	-1.7885089	-0.1544800	-0.9658939
Co	0.2030714	0.1853874	-0.0385511
C	1.6803665	-0.9436041	0.0099151
O	2.5400801	-1.6726019	0.0483674
-1	-0.00132824	-0.00016155	0.00026013
-2	-0.04095417	0.00856217	0.00778129
-3	-0.00288069	0.01213818	-0.01687695
-4	-0.00035563	0.00001475	-0.00062369
-5	0.00050431	0.00079373	0.00045389
-6	-0.01315121	-0.02457932	-0.01031450
-7	-0.00026288	-0.00048818	0.00020381
-8	-0.02173371	-0.01901704	0.02002129
-9	-0.00086780	-0.00029886	0.00024838
-10	0.00828191	0.00977824	0.00297021
-11	-0.00937107	0.00017531	0.02082188

-12	0.05855802	-0.07385384	0.00053230
-13	-0.00277094	0.00344291	0.00106284

CAS, E = -1689.5099780
MP2-CAS, E = -1689.437196

Co-T1-Cpx

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	1.55173300	0.39976600	2.06233600
C	0.60248000	0.04295800	1.69233200
C	0.33800300	-1.25648800	1.19684500
H	-0.73706900	1.80303400	1.97560400
H	1.04404400	-2.07108300	1.14207300
C	-1.03995300	-1.32084200	0.85044100
H	-1.55897400	-2.18696900	0.47045600
C	-1.61640400	-0.06362600	1.13497800
H	-2.64988600	0.20692600	0.98064700
C	-0.60541500	0.78448100	1.64598300
Co	0.04874300	0.20125500	-0.50727800
C	-0.97229400	0.90177000	-1.94457300
O	-1.70514100	1.27302300	-2.72527000
Si	2.58882500	0.31522100	-2.21231000
C	4.42316500	0.20378300	-1.87549500
H	4.93280900	-0.19912600	-2.75614500
H	4.63897700	-0.45466600	-1.03105500
H	4.84875100	1.18514400	-1.66144300
C	2.23735500	1.42164900	-3.67644800
H	2.59025600	0.95843600	-4.60339300
H	2.74437900	2.38269500	-3.56376300
H	1.16647100	1.61688000	-3.78557300
C	1.87434700	-1.39973900	-2.45395100
H	2.39976700	-1.89921200	-3.27189800
H	0.81228000	-1.38692300	-2.70958200
H	1.99832500	-2.00712400	-1.55510200
H	1.93454100	0.93376300	-1.00198900

CAS, E = -2099.4876195

MP2-CAS, E = -2099.4436565

Co-S0-Int

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	2.28005800	-1.78310700	0.03444500
C	1.82671800	-0.80469000	0.01883500
C	1.50989700	-0.00907500	1.15398300
H	1.67942700	-0.35097100	-2.16178700
H	1.64713300	-0.29554300	2.18502100
C	1.00863900	1.22936500	0.69627600
H	0.68564600	2.04927000	1.31809700
C	1.02005200	1.21223200	-0.72234600
H	0.70781000	2.01674500	-1.36912600
C	1.52749700	-0.03775600	-1.14068500
Co	-0.35484400	-0.50414400	-0.00128100
C	-2.16375800	-0.04417600	-0.00319500
O	-3.22419300	0.33751100	0.00134300

CAS, E = -1689.4898887
MP2-CAS, E = -1689.4456070

Co-S0-Cpx

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	1.54894900	-2.32152300	-1.41392700
C	1.88573300	-1.55677300	-0.73118500
C	1.68115200	-1.55950100	0.68080700
H	2.96125200	-0.13133800	-2.06283200
H	1.17141300	-2.32785000	1.24254200
C	2.28184300	-0.40100900	1.20792000
H	2.30735500	-0.10740400	2.24512600
C	2.83030100	0.33313600	0.11737800
H	3.35831600	1.27135900	0.19432200
C	2.63500500	-0.41210500	-1.07426000
Co	0.68865100	0.21275000	-0.20859800

C	0.22167900	1.95991100	-0.05517000
O	-0.03358700	3.05757500	0.07454100
Si	-2.01863300	-0.36425900	-0.04209000
C	-2.72810500	-2.02734500	-0.51454500
H	-3.74485800	-2.12184600	-0.12292700
H	-2.13126900	-2.84333600	-0.10092100
H	-2.77053300	-2.14945500	-1.59765300
C	-3.05374600	1.02522500	-0.74194400
H	-4.00686700	1.09367000	-0.20829400
H	-3.26808500	0.84665300	-1.79830700
H	-2.55304000	1.99321600	-0.65747300
C	-1.86432900	-0.24428000	1.81354100
H	-2.84727800	-0.42407900	2.26030500
H	-1.51709400	0.73960000	2.12887600
H	-1.16867200	-0.98986900	2.20087300
H	-0.74080700	-0.33655900	-0.89987300

CAS, E = -2099.4539778
MP2-CAS, E = -2099.408399

Co-S0-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
Si	0.00000000	0.00000000	0.00000000
Co	0.00000000	0.00000000	3.07061600
H	1.28706500	0.00000000	0.72564500
C	0.06191500	1.80609200	3.34343700
C	1.08003300	-1.95885100	2.89483300
C	-0.17940800	-2.14774400	3.54070300
C	-0.16857500	-1.43644800	4.75750500
C	1.06454300	-0.73452000	4.81785700
C	1.85870900	-1.10908800	3.69521900
H	1.37712400	-2.40172100	1.95640400
H	2.85929300	-0.76769600	3.48389600
H	-0.98237500	-2.77131700	3.17727500
H	-0.96321000	-1.39564200	5.48438800
H	1.38148300	-0.08975400	5.62280000
O	0.13258100	2.92332600	3.51163900

C	-0.32207100	-1.75541400	-0.56323100
H	-1.19124800	-1.80081500	-1.22302300
H	-0.51319100	-2.40260700	0.29544700
H	0.53296300	-2.16053000	-1.10661400
C	0.05344700	1.18839800	-1.44192900
H	-0.88736900	1.16650800	-1.99564500
H	0.85540400	0.92084700	-2.13190200
H	0.22641600	2.21197100	-1.10610500
C	-1.45747500	0.51132900	1.08442500
H	-2.33608900	0.18267000	0.52003600
H	-1.53903400	1.59146300	1.19934600
H	-1.65583900	0.04006100	2.06994200

-1	-0.07	0.03	-0.00
-2	-0.06	0.02	-0.01
-3	-0.03	0.00	-0.01
-4	-0.12	0.11	0.03
-5	-0.01	-0.01	-0.01
-6	0.03	-0.05	-0.02
-7	0.05	-0.09	-0.02
-8	-0.01	-0.02	0.00
-9	-0.01	-0.02	-0.00
-10	-0.09	0.06	0.02
-11	0.03	0.03	0.11
-12	0.01	0.02	-0.12
-13	0.00	0.02	-0.01
-14	-0.04	-0.07	-0.12
-15	-0.08	-0.01	0.07
-16	-0.03	0.01	0.14
-17	-0.04	-0.01	0.02
-18	-0.16	-0.03	0.10
-19	-0.06	0.02	0.06
-20	-0.02	0.05	0.12
-21	-0.13	0.05	0.06
-22	-0.01	-0.01	0.03
-23	0.25	-0.05	-0.21
-24	0.30	-0.05	-0.12
-25	0.21	-0.03	-0.22
-26	0.27	-0.05	-0.22
-27	-0.35	-0.26	-0.38

CAS, E = -2099.320017
MP2-CAS, E = -2099.2417919

Co-T1-TS2

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	0.99471100	-2.36607900	-1.41109800
C	1.43020000	-1.63245500	-0.72770000
C	1.34263100	-1.66826500	0.66581000
H	2.63254800	-0.36875100	-2.10444600
H	0.82181800	-2.42229800	1.26032700
C	2.09529200	-0.60682800	1.16347300
H	2.27357400	-0.38705300	2.21887900
C	2.69232500	0.03982300	0.08003100
H	3.42176700	0.85094600	0.14774600
C	2.29095900	-0.59826600	-1.09304900
Co	0.52085800	0.21481500	-0.07479000
C	0.61320100	2.02015200	-0.01531600
O	0.64266300	3.14981100	0.01277400
Si	-1.73558400	-0.21457200	-0.05620400
C	-2.27983000	-1.98078000	-0.40074000
H	-3.35299200	-2.08886600	-0.21526900
H	-1.75273700	-2.68228500	0.25277400
H	-2.08821200	-2.27278800	-1.43774600
C	-2.81729200	1.01876000	-0.97446500
H	-3.87270400	0.83647800	-0.74904200
H	-2.69156700	0.94978900	-2.05934600
H	-2.57991100	2.04253600	-0.66973500
C	-2.17892600	0.06118800	1.74984300
H	-3.24811700	-0.10813000	1.91118700
H	-1.94937500	1.08530400	2.05987800
H	-1.62716900	-0.62634700	2.39837800
H	-1.01929700	-0.35691200	-1.58581800

-1	-0.14	0.17	-0.04
-2	-0.10	0.08	-0.02
-3	-0.12	0.02	-0.02
-4	0.05	0.01	0.02
-5	-0.19	0.06	-0.04

-6	-0.03	-0.10	0.01
-7	-0.03	-0.17	0.01
-8	0.05	-0.11	0.03
-9	0.12	-0.19	0.06
-10	0.01	-0.01	0.01
-11	0.11	0.09	0.04
-12	0.12	0.08	-0.00
-13	0.04	0.08	0.01
-14	-0.10	-0.11	-0.08
-15	-0.13	-0.06	0.09
-16	-0.07	-0.01	0.18
-17	-0.08	-0.06	0.04
-18	-0.23	-0.10	0.13
-19	-0.16	-0.07	0.05
-20	-0.11	-0.08	0.13
-21	-0.25	-0.04	0.06
-22	-0.14	-0.08	0.03
-23	0.09	-0.06	-0.16
-24	0.12	0.02	-0.12
-25	0.13	-0.08	-0.23
-26	0.08	-0.07	-0.16
-27	-0.28	-0.20	-0.23

CAS, E = -2099.4746959
MP2-CAS, E = -2099.4345830

Co-T1/S0-1

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	-3.3734927	0.7678585	-1.0374329
C	-2.7738306	0.0292734	-0.5303817
C	-2.4781289	0.0130543	0.8652789
H	-2.1529191	-1.3383263	-2.1668715
H	-2.8339983	0.7267653	1.5909460
C	-1.6894042	-1.1258545	1.1394397
H	-1.3183747	-1.4259254	2.1057403
C	-1.4326738	-1.7676571	-0.0949368
H	-0.8468090	-2.6644022	-0.2324255

C	-2.1351609	-1.0746853	-1.1220717
Co	-0.6086969	0.2429917	-0.2249828
C	-0.2439033	2.0175769	-0.0832265
O	-0.0383961	3.1286099	-0.0079055
Si	1.8612865	-0.3014804	-0.0212242
C	1.6826522	-1.0406824	1.6900257
H	1.1792711	-0.3636999	2.3787573
H	2.6848223	-1.2519522	2.0756141
H	1.1272034	-1.9785223	1.6585551
C	2.8537534	1.2819796	0.0450287
H	2.8438963	1.7932499	-0.9192704
H	3.8924634	1.0533922	0.2935502
H	2.4721487	1.9723526	0.7978369
C	2.7547020	-1.5641181	-1.0787991
H	2.9480251	-1.1848984	-2.0830983
H	2.1627683	-2.4770461	-1.1701232
H	3.7113404	-1.8294057	-0.6232800
H	0.7116398	-0.0341938	-1.0836969

-1	-0.00117521	-0.00047187	0.00036839
-2	-0.01626575	0.00823656	0.01844443
-3	-0.03895935	-0.00406570	0.00225815
-4	0.00005467	-0.00029422	-0.00060278
-5	-0.00099712	-0.00069833	0.00018643
-6	0.00353370	0.00870154	-0.01052194
-7	0.00086785	0.00055447	0.00087960
-8	-0.02003536	-0.03041522	-0.00868336
-9	-0.00154227	-0.00143864	0.00006043
-10	0.01144018	-0.01353582	0.00589211
-11	-0.01947205	-0.00027088	0.01952530
-12	-0.00105159	0.06669007	0.00849942
-13	-0.00183669	0.00082601	0.00006866
-14	0.04287515	-0.01452891	-0.04786831
-15	-0.01982869	0.00413226	-0.00139174
-16	-0.00011628	-0.00116417	0.00331831
-17	0.00068130	0.00430656	-0.00553522
-18	-0.00016672	0.00069915	0.00008406
-19	-0.00217392	0.00109046	0.00287667
-20	-0.00072312	-0.00082094	0.00017372
-21	-0.00048442	-0.00040917	0.00079783
-22	0.00109962	0.00132460	-0.00002346

-23	0.00628643	-0.00178414	0.00615637
-24	-0.00054434	0.00093547	0.00082528
-25	-0.00043235	0.00029595	0.00025079
-26	0.00114354	-0.00199442	-0.00152111
-27	0.05782280	-0.02590069	0.00548195

CAS, E = -2099.4792675
MP2-CAS, E = -2099.4342528

Co-S0-Pro

Atomic Number	Coordinates (Angstroms) X	Y	Z
H	1.26958600	-2.48948400	-0.71423300
C	1.67053800	-1.57287500	-0.31180100
C	1.57426400	-1.14635100	1.03675400
H	2.66303800	-0.65134300	-2.08517000
H	1.08454400	-1.67778600	1.83700900
C	2.19973400	0.11603100	1.13083000
H	2.28669000	0.71784500	2.02120900
C	2.73150200	0.44259100	-0.15299500
H	3.27221400	1.34255700	-0.39935200
C	2.41847500	-0.60676800	-1.03659200
Co	0.55727600	0.27715300	-0.27109000
C	-0.07804200	1.95981900	-0.07994000
O	-0.50241700	3.00128200	0.03394500
Si	-1.61580800	-0.42779800	-0.03298500
C	-1.79209100	-2.25880000	-0.41025000
H	-2.81737700	-2.57494500	-0.20036400
H	-1.12484800	-2.85932600	0.21063600
H	-1.57500200	-2.47932300	-1.45656800
C	-2.98283700	0.50770600	-0.92342400
H	-3.95832300	0.18966200	-0.54825500
H	-2.95317800	0.32226700	-1.99852400
H	-2.90567000	1.58569700	-0.76747800
C	-1.93429000	-0.19394700	1.81276400
H	-2.93778800	-0.55240400	2.06113100
H	-1.87313000	0.85871300	2.09579000
H	-1.21375200	-0.74616700	2.41706700

H	-0.46632600	0.02537800	-1.35531000

CAS, E = -2099.4815876
MP2-CAS, E = -2099.4341633

Co-T1-Pro ----------

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
	Co		-0.064052	0.016108	0.007512
	C		1.173973	0.020348	2.028847
	C		-1.546811	0.002939	-1.355179
	O		-1.990221	-0.031000	-2.414017
	H		2.248085	0.047088	1.952343
	C		0.368341	-1.135807	2.066111
	H		0.719792	-2.155202	2.034213
	C		-1.036847	0.665423	2.248916
	H		-1.915617	1.284442	2.337681
	C		-1.002293	-0.724618	2.244217
	H		-1.849615	-1.388465	2.317618
	C		0.308696	1.142563	2.069946
	H		0.610518	2.177878	2.078687
	Si		1.278994	1.523445	-1.298340
	H		1.122047	-0.524185	-0.916766
	C		0.306277	3.149614	-1.235508
	H		0.146432	3.503113	-0.215904
	H		0.868958	3.918638	-1.776337
	H		-0.669468	3.053650	-1.715210
	C		1.511080	1.096294	-3.122376
	H		0.555720	0.894390	-3.611367
	H		1.987418	1.927415	-3.651720
	H		2.139905	0.212105	-3.247045
	C		2.984135	1.816529	-0.543715
	H		2.924607	2.190295	0.480267
	H		3.524977	2.559837	-1.137010
	H		3.578075	0.900266	-0.534124

CAS, E = -2099.3663415
MP2-CAS, E = -2099.33636362

CO (singlet)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
	6		0.000000	0.000000	0.000000
	8		0.000000	0.000000	1.125018

CAS, E = -113.362853

MP2-CAS, E = -113.335285

CO (triplet)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
	6		0.000000	0.000000	0.000000
	8		0.000000	0.000000	1.201359

CAS, E = -113.1526371

MP2-CAS, E =-113.1154526

Rh-S0-Rea

Atomic Number	Coordinates (Angstroms) X	Y	Z
Rh	0.000000	0.000000	0.000000
C	1.220975	0.000000	1.830109
C	-1.673741	0.000236	-1.058690
O	-2.660731	0.000375	-1.682990
H	2.309331	0.001964	1.766393
C	0.372374	-1.200496	1.900582
H	0.694522	-2.239069	1.899711
C	-0.995100	0.737525	1.867747
H	-1.870018	1.385976	1.837993
C	-0.985664	-0.755731	1.863261
H	-1.849527	-1.418074	1.829670
C	0.366131	1.196342	1.903903
H	0.684525	2.236702	1.905915
C	1.668045	0.003598	-1.069601
O	2.651542	0.005719	-1.700248

CAS, E = -531.0083212
MP2-CAS, E = -530.946341

Rh-S1/S0-Cl

Atomic Number	Coordinates (Angstroms) X	Y	Z
Rh	0.392880	-0.097147	-0.682267
C	1.007597	-0.267965	1.583301
C	-1.610639	-0.904928	-1.529036
O	-2.595887	-1.522524	-1.594132
H	1.999107	-0.675671	1.586974
C	-0.203577	-1.043705	1.514910
H	-0.265030	-2.099593	1.352417
C	-0.702275	0.978946	2.459963
H	-1.258801	1.779004	2.903221

C	-1.232976	-0.271536	2.070660
H	-2.240054	-0.591282	2.193849
C	0.659257	0.968553	2.201778
H	1.336330	1.759732	2.420432
C	2.193148	0.766250	-1.573818
O	3.213741	1.221864	-1.748250

Gradient Difference :

-1	0.0035222130	0.0031087535	0.0072065670
-2	0.0062705868	-0.0025699154	0.0017780798
-3	0.0017823378	-0.0001359738	-0.0048236558
-4	-0.0014936424	-0.0000941507	-0.0000082290
-5	0.0007277131	-0.0006128631	-0.0003639649
-6	-0.0004597979	-0.0068470167	0.0034601379
-7	0.0011514829	-0.0010193843	-0.0006337642
-8	-0.0051308517	0.0031387776	0.0037393392
-9	0.0000132697	0.0002918182	-0.0006950678
-10	-0.0017239858	0.0000166444	-0.0036976758
-11	-0.0033902998	-0.0005629975	-0.0001585338
-12	0.0030433278	0.0038074849	-0.0037923176
-13	0.0019128013	0.0023125652	0.0002394291
-14	-0.0100875856	-0.0023503090	-0.0014803391
-15	0.0038624308	0.0015165667	-0.0007700048

Derivative Coupling

-1	0.0021168652	-0.0014573234	-0.0016007167
-2	-0.0028105609	0.0020729190	-0.0013050303
-3	-0.0009956377	-0.0012084326	0.0027404746
-4	0.0010094100	0.0008284210	-0.0006237840
-5	-0.0003479633	0.0003535050	0.0003436378
-6	0.0014233949	0.0006434711	0.0009133874
-7	-0.0001445315	0.0002100411	-0.0000912935
-8	-0.0017663364	-0.0025592969	-0.0007664862
-9	-0.0000350644	-0.0003068562	-0.0000107912
-10	0.0000969845	0.0022204035	0.0007269306
-11	0.0008708470	0.0004030839	0.0001472702
-12	0.0006339346	-0.0022300036	0.0009740233
-13	-0.0002584024	-0.0005773441	-0.0000422349
-14	-0.0009595681	0.0015623587	-0.0016058874
-15	0.0011666284	0.0000450536	0.0002005003

CAS, E = -530.9409089
MP2-CAS, E = -530.8885126

Rh-S0-IM

Atomic Number	Coordinates (Angstroms) X	Y	Z
Rh	-0.250259	0.000000	-0.117663
C	1.196226	-0.000000	1.812338
C	-1.758357	0.000000	-1.191099
O	-2.732392	0.000000	-1.848404
H	2.276738	-0.000000	1.751948
C	0.376120	-1.177018	1.947500
H	0.723747	-2.198067	1.976769
C	-0.970990	0.739491	1.955920
H	-1.850443	1.359098	2.056250
C	-0.970990	-0.739491	1.955920
H	-1.850443	-1.359098	2.056250
C	0.376120	1.177018	1.947500
H	0.723747	2.198067	1.976769

CAS, E = -417.5872673
MP2-CAS, E = -417.5700512

Rh-S0-Cpx

Atomic Number	Coordinates (Angstroms) X	Y	Z
Rh	0.000000	0.000000	0.000000
C	1.226665	0.000000	1.997810
C	-1.270457	0.006023	-1.341823
O	-2.074966	0.009836	-2.191525
H	2.306563	-0.000833	1.971639
C	0.384669	-1.170374	2.072705
H	0.721537	-2.195311	2.112261
C	-0.972559	0.717385	2.062794
H	-1.841838	1.358587	2.094308
C	-0.965723	-0.736450	2.086109

H	-1.823921	-1.390903	2.138158
C	0.381039	1.164833	2.057389
H	0.716837	2.191362	2.083697
Si	1.481967	1.213511	-1.478262
H	0.939919	-0.782078	-0.970015
C	0.725475	2.941636	-1.637987
H	1.377708	3.602988	-2.224790
H	-0.249566	2.900105	-2.137571
H	0.576616	3.394615	-0.651048
C	1.670665	0.487284	-3.213609
H	0.694934	0.306039	-3.680547
H	2.226204	1.179963	-3.858580
H	2.212845	-0.465190	-3.191956
C	3.176204	1.338044	-0.651583
H	3.093330	1.810047	0.334113
H	3.856095	1.946347	-1.262626
H	3.630543	0.349490	-0.518758

CAS, E = -827.5776195
MP2-CAS, E = -827.5310693

Rh-S0-TS1

Atomic Number	Coordinates (Angstroms) X	Y	Z
Rh	0.000000	0.000000	0.000000
C	1.204048	0.000000	2.142075
C	-1.166406	-0.605128	-1.290624
O	-1.910308	-0.991063	-2.113749
H	2.279791	0.058911	2.239834
C	0.442774	-1.185570	2.062838
H	0.820158	-2.196051	2.088497
C	-1.022110	0.663869	2.066022
H	-1.927152	1.251702	2.095498
C	-0.938066	-0.785776	1.884320
H	-1.760524	-1.474712	1.754198
C	0.295355	1.143392	2.182328
H	0.563524	2.181541	2.318154
Si	2.890010	0.644806	-1.332025

H	2.427016	-0.679336	-0.815325
C	1.401093	1.583448	-2.029661
H	1.730170	2.571726	-2.378002
H	0.958545	1.060709	-2.884265
H	0.594726	1.794814	-1.299719
C	4.150535	0.375319	-2.709267
H	3.765996	-0.307633	-3.474707
H	4.393825	1.326063	-3.199367
H	5.083068	-0.049359	-2.320559
C	3.653143	1.626334	0.090066
H	2.881846	1.981807	0.783162
H	4.192766	2.501742	-0.291451
H	4.363878	1.015811	0.659448

-1	0.06	-0.09	0.01
-2	-0.04	0.03	0.03
-3	0.00	0.05	-0.00
-4	-0.02	0.09	-0.00
-5	-0.04	0.02	0.05
-6	-0.06	0.02	0.11
-7	-0.06	0.02	0.18
-8	-0.02	0.05	-0.08
-9	-0.02	0.05	-0.14
-10	-0.03	0.02	0.04
-11	-0.04	0.03	0.04
-12	-0.02	0.04	-0.03
-13	-0.02	0.04	-0.06
-14	-0.11	0.10	-0.03
-15	-0.41	0.19	-0.02
-16	0.06	0.29	-0.12
-17	0.18	0.23	-0.17
-18	-0.00	0.30	-0.09
-19	0.10	0.35	-0.11
-20	-0.07	-0.13	0.05
-21	-0.10	-0.12	0.06
-22	0.05	-0.17	0.02
-23	-0.13	-0.21	0.11
-24	-0.03	-0.03	0.01
-25	-0.00	0.02	0.01
-26	0.06	-0.06	0.04
-27	-0.09	-0.11	-0.00

CAS, E = -827.4761954
MP2-CAS, E = -827.4364583

Rh-S0-Pro

Atomic Number	Coordinates (Angstroms) X	Y	Z
Rh	0.000000	0.000000	0.000000
C	1.220398	0.000000	1.978957
C	-1.193836	-0.064223	-1.404881
O	-1.950860	-0.104948	-2.295732
H	2.299245	-0.005838	1.930993
C	0.367977	-1.161534	2.073323
H	0.693905	-2.190341	2.108848
C	-0.976720	0.731119	2.107341
H	-1.840037	1.377350	2.172861
C	-0.980151	-0.713438	2.134443
H	-1.850521	-1.346967	2.224333
C	0.380282	1.168551	2.048363
H	0.714700	2.196170	2.061685
Si	1.226452	1.598870	-1.281875
H	0.938612	-0.848416	-0.893599
C	0.269916	3.230406	-1.220648
H	0.096881	3.556140	-0.188678
H	0.824908	4.023340	-1.740380
H	-0.707894	3.130328	-1.707100
C	1.450659	1.100957	-3.091037
H	0.489864	0.934529	-3.592413
H	1.978390	1.893780	-3.637601
H	2.038857	0.180296	-3.177335
C	2.931457	1.826170	-0.496946
H	2.856107	2.209720	0.527015
H	3.523187	2.542340	-1.083137
H	3.481330	0.878742	-0.465062

CAS, E = -827.5961953
MP2-CAS, E = -827.5520654

Ir-S0-Rea

Atomic Number	Coordinates (Angstroms) X	Y	Z
77	0.000000	0.000000	0.000000
6	1.200037	0.000000	1.969008
6	-1.261098	-0.000236	-1.326326
8	-2.047123	-0.000383	-2.153005
1	2.277983	0.000442	1.948032
6	0.368788	-1.157918	2.011978
1	0.695580	-2.183978	2.029362
6	-0.972085	0.715014	2.001880
1	-1.840322	1.353642	2.010383
6	-0.971512	-0.716647	2.001381
1	-1.838884	-1.356475	2.009436
6	0.367903	1.157276	2.012586
1	0.694141	2.183491	2.030522
6	1.254154	0.000989	-1.329263
8	2.037204	0.001607	-2.159209

CAS, E = -524.8394007
MP2-CAS, E = -524.774616

Ir-S1/S0-CI

Atomic Number	Coordinates (Angstroms) X	Y	Z
77	0.212505	0.236585	-0.354396
6	1.114533	0.165940	1.671806
6	-1.257002	0.076461	-1.530338
8	-2.184416	-0.083025	-2.202162
1	2.169795	0.196352	1.748523
6	0.321753	-1.029605	1.640996
1	0.686511	-2.014023	1.463577
6	-1.024044	0.654284	2.551370
1	-1.870081	1.189020	2.879884
6	-1.016801	-0.704323	2.198387
1	-1.827961	-1.394547	2.320129

6	0.218216	1.229956	2.133682
1	0.447233	2.275718	2.131757
6	1.967880	-0.291472	-1.535700
8	2.797859	-0.507420	-2.266316

Gradient Difference:

-1	0.0042856942	0.0211920049	-0.0030234418
-2	-0.0019729244	0.0339678773	0.0184292219
-3	-0.0064712109	0.0130270928	-0.0002167512
-4	0.0019025220	-0.0048096608	0.0001604120
-5	0.0026309015	0.0005911078	-0.0008409271
-6	-0.0225012831	-0.0121928381	0.0053740590
-7	-0.0001901319	-0.0015263945	-0.0001338555
-8	-0.0136271166	-0.0361029487	-0.0173238676
-9	-0.0059075665	0.0029826176	0.0033713831
-10	0.0095085038	0.0017042886	0.0111578979
-11	0.0044451208	0.0040712007	-0.0001734475
-12	0.0344110663	-0.0033974937	-0.0262161874
-13	0.0011529609	-0.0051348842	0.0024851026
-14	-0.0122938378	-0.0169161026	0.0110640549
-15	0.0046273018	0.0025441330	-0.0041136532

Derivative Coupling

-1	-0.0019056392	-0.0084821920	0.0175994965
-2	0.0004104664	-0.0094211611	-0.0087489736
-3	0.0072695402	-0.0037929292	-0.0186032916
-4	-0.0038186732	0.0010579246	0.0023930185
-5	0.0021868983	-0.0001367103	0.0000020441
-6	-0.0158746778	0.0038273293	0.0123384417
-7	0.0003258597	0.0004919108	0.0010511858
-8	0.0244771019	0.0369472462	-0.0066143899
-9	-0.0009588682	0.0022568686	0.0011027214
-10	0.0194503794	-0.0279708030	-0.0154713181
-11	0.0008202533	-0.0010050892	-0.0005847338
-12	-0.0223583228	0.0001451620	0.0161248750
-13	0.0000027122	-0.0008700469	0.0010666217
-14	-0.0121804718	0.0094780944	-0.0019982583
-15	0.0021534417	-0.0025256042	0.0003425605

CAS, E = -524.7369196

MP2-CAS, E =-524.6915971

Ir-S0-Int

Atomic Number	Coordinates (Angstroms) X	Y	Z
77	-0.422993	-0.221823	-0.052295
6	1.206862	0.024367	1.823783
6	-1.729892	0.287823	-1.198381
8	-2.592476	0.607599	-1.944989
1	2.282647	0.068979	1.732320
6	0.435374	-1.195855	2.083099
1	0.857642	-2.181695	2.213093
6	-1.040511	0.569109	1.816283
1	-1.941929	1.156896	1.902042
6	-0.928852	-0.865472	2.161277
1	-1.751904	-1.528813	2.379887
6	0.328057	1.120167	1.751346
1	0.586799	2.158717	1.612534

CAS, E = -411.4326762
MP2-CAS, E = -411.3882872

Ir-S0-Cpx

Atomic Number	Coordinates (Angstroms) X	Y	Z
77	-0.000000	0.000000	-0.000000
6	1.180886	0.000000	2.192165
6	-1.257018	0.061324	-1.302726
8	-2.078686	0.101409	-2.154272
1	2.245602	0.015890	2.377086
6	0.384776	-1.187578	2.104345
1	0.715478	-2.208263	2.205132
6	-0.985145	0.715131	1.860115
1	-1.853767	1.345675	1.748170
6	-0.960757	-0.767955	1.826490
1	-1.796532	-1.436009	1.686792
6	0.342640	1.166243	2.148018

1	0.644011	2.192016	2.289574
14	2.718653	-0.518688	-1.579108
1	2.134062	-1.767209	-1.021401
6	1.505989	0.555611	-2.581824
1	2.171207	1.130426	-3.242378
1	0.838553	-0.041125	-3.210688
1	0.906730	1.289970	-2.033261
6	4.008951	-1.069846	-2.848973
1	3.558152	-1.705013	-3.619695
1	4.439833	-0.192862	-3.349391
1	4.828989	-1.629168	-2.385828
6	3.581006	0.518985	-0.252534
1	2.925853	1.291724	0.166732
1	4.441077	1.026945	-0.707393
1	3.958477	-0.099441	0.567983

CAS, E = -821.38976126
MP2-CAS, E = -821.3436158

Ir-S0-TS

Atomic Number	Coordinates (Angstroms) X	Y	Z
77	0.000000	-0.000000	0.000000
6	1.216444	-0.000000	2.038890
6	-1.331706	0.166987	-1.243055
8	-2.186866	0.274219	-2.041287
1	2.294574	-0.010701	2.071057
6	0.356649	-1.165811	2.129077
1	0.670631	-2.192154	2.240425
6	-0.981657	0.719135	1.927634
1	-1.850533	1.355650	1.861283
6	-0.987999	-0.732923	2.074597
1	-1.853685	-1.375111	2.137683
6	0.388600	1.167851	1.993099
1	0.728940	2.190668	1.984780
14	1.447129	0.934760	-1.447252
1	1.332227	-0.836513	-1.580619
6	1.020774	2.806826	-1.368955

	1			1.765996	3.384310	-1.933257
	1			0.034837	2.993926	-1.814550
	1			1.000103	3.175264	-0.336496
	6			1.423047	0.672862	-3.347501
	1			0.391694	0.590605	-3.716760
	1			1.884700	1.540718	-3.835369
	1			1.961779	-0.227692	-3.666893
	6			3.259831	0.854353	-0.863995
	1			3.361263	1.298423	0.135162
	1			3.891166	1.438792	-1.546533
	1			3.650925	-0.168457	-0.824962
-1	-0.01	0.00	0.01			
-2	-0.00	-0.01	0.01			
-3	0.01	-0.00	0.01			
-4	0.00	-0.00	0.00			
-5	0.00	-0.00	-0.00			
-6	-0.02	-0.01	0.01			
-7	-0.02	-0.01	0.01			
-8	0.03	0.01	-0.01			
-9	0.03	0.01	-0.01			
-10	-0.01	-0.01	0.00			
-11	-0.01	-0.01	0.01			
-12	0.02	-0.01	-0.00			
-13	0.02	-0.00	-0.00			
-14	0.01	0.00	-0.07			
-15	0.83	-0.21	-0.38			
-16	-0.02	0.01	-0.03			
-17	-0.03	0.00	-0.04			
-18	-0.02	0.01	-0.03			
-19	-0.03	0.01	-0.05			
-20	0.10	-0.00	0.06			
-21	0.02	-0.00	-0.00			
-22	0.06	0.06	0.15			
-23	0.21	-0.02	0.08			
-24	0.02	-0.03	0.03			
-25	0.01	-0.00	0.04			
-26	0.01	-0.02	0.05			
-27	0.03	-0.07	0.03			

CAS, E = -821.3428761

MP2-CAS, E = -821.3017868

Ir-S0-Pro

Atomic Number	Coordinates (Angstroms) X	Y	Z
77	0.000000	0.000000	0.000000
6	1.225812	0.000000	1.968535
6	-1.203392	-0.035671	-1.370456
8	-1.979491	-0.058677	-2.254300
1	2.303644	0.001417	1.922986
6	0.375019	-1.166208	2.051994
1	0.705269	-2.193199	2.079872
6	-0.984467	0.721453	2.085830
1	-1.853947	1.358639	2.143672
6	-0.980194	-0.723587	2.114280
1	-1.846182	-1.362866	2.197278
6	0.374956	1.166052	2.022302
1	0.705521	2.194057	2.024034
14	1.226400	1.630588	-1.257288
1	0.903054	-0.929198	-0.887967
6	0.288964	3.275844	-1.237201
1	0.117233	3.628033	-0.213065
1	0.850218	4.052383	-1.774094
1	-0.689338	3.170704	-1.721904
6	1.476339	1.111671	-3.057797
1	0.519792	0.935216	-3.564429
1	2.008894	1.895461	-3.612386
1	2.065904	0.189716	-3.122116
6	2.929285	1.879460	-0.466215
1	2.850396	2.261104	0.558886
1	3.513999	2.603914	-1.048927
1	3.490267	0.937989	-0.437385

CAS, E = -821.43387611
MP2-CAS, E = -821.3902814

SiMe3(H) in CAS(2,2)/Def2-SVPD

Atomic Number	Coordinates (Angstroms) X	Y	Z
Si	2.58883	0.31522	-2.21231
C	4.42317	0.20378	-1.8755
H	4.93281	-0.19913	-2.75615
H	4.63898	-0.45467	-1.03106
H	4.84875	1.18514	-1.66144
C	2.23735	1.42165	-3.67645
H	2.59026	0.95844	-4.60339
H	2.74438	2.3827	-3.56376
H	1.16647	1.61688	-3.78557
C	1.87435	-1.39974	-2.45395
H	2.39977	-1.89921	-3.2719
H	0.81228	-1.38692	-2.70958
H	1.99833	-2.00712	-1.5551
H	1.93454	0.93376	-1.00199

CAS, E = -409.947862

MP2-CAS, E = -409.932468

CO (singlet)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
	6		0.000000	0.000000	0.000000
	8		0.000000	0.000000	1.125018

CAS, E = -113.362853

MP2-CAS, E = -113.335285

CO (triplet)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
	6		0.000000	0.000000	0.000000
	8		0.000000	0.000000	1.201359

CAS, E = -113.1526371

MP2-CAS, E =-113.1154526