Electronic Supplementary Material (ESI) for Dalton Transactions

Supporting Information for:

A Combined Experimental and Computational Study of Fluxional Process in Amine–Borane Sigma–Complexes of Rhodium and Iridium.

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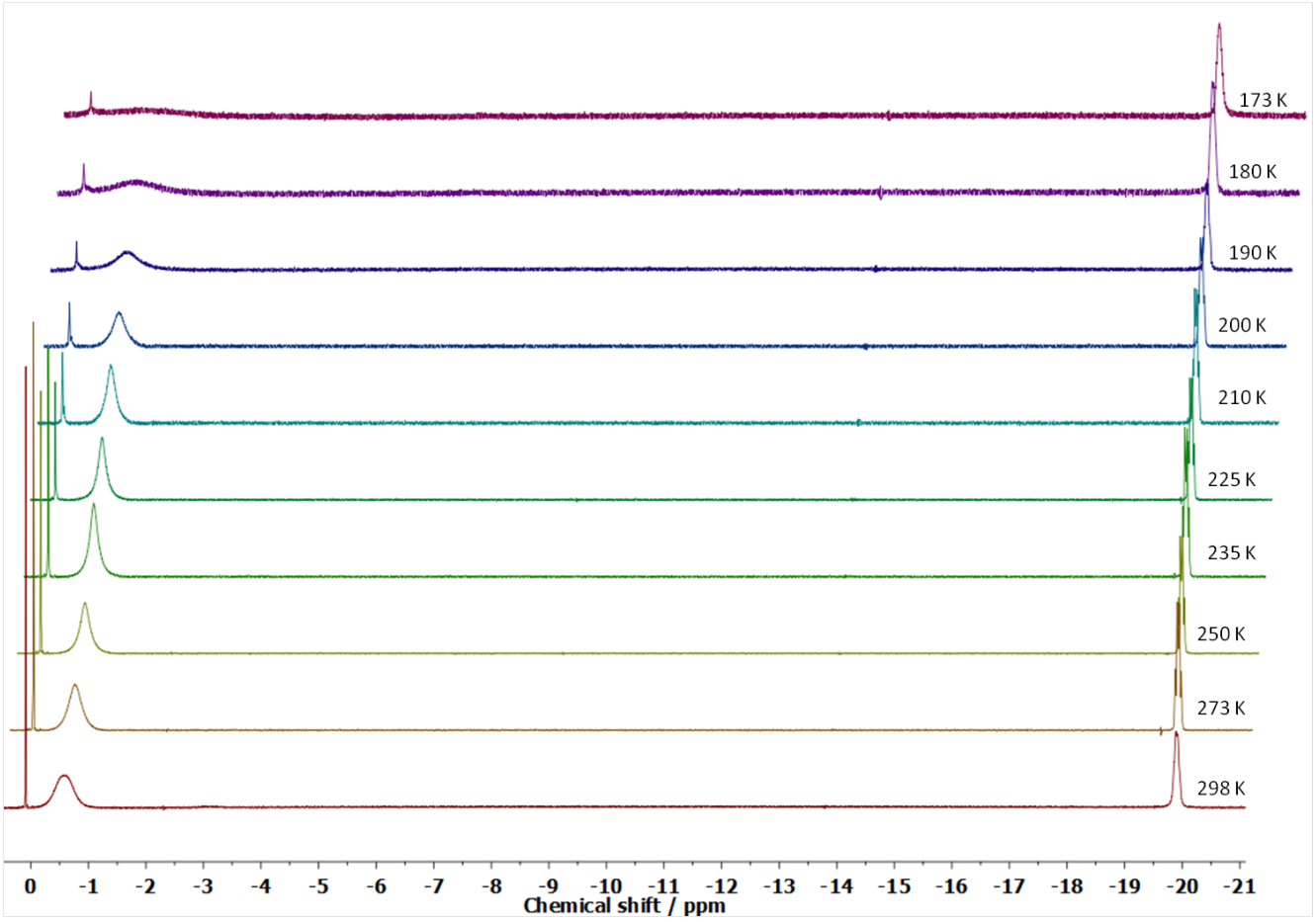

Figure S-1. Variable temperature ^{1}H NMR spectra of complex **1**, high field region.

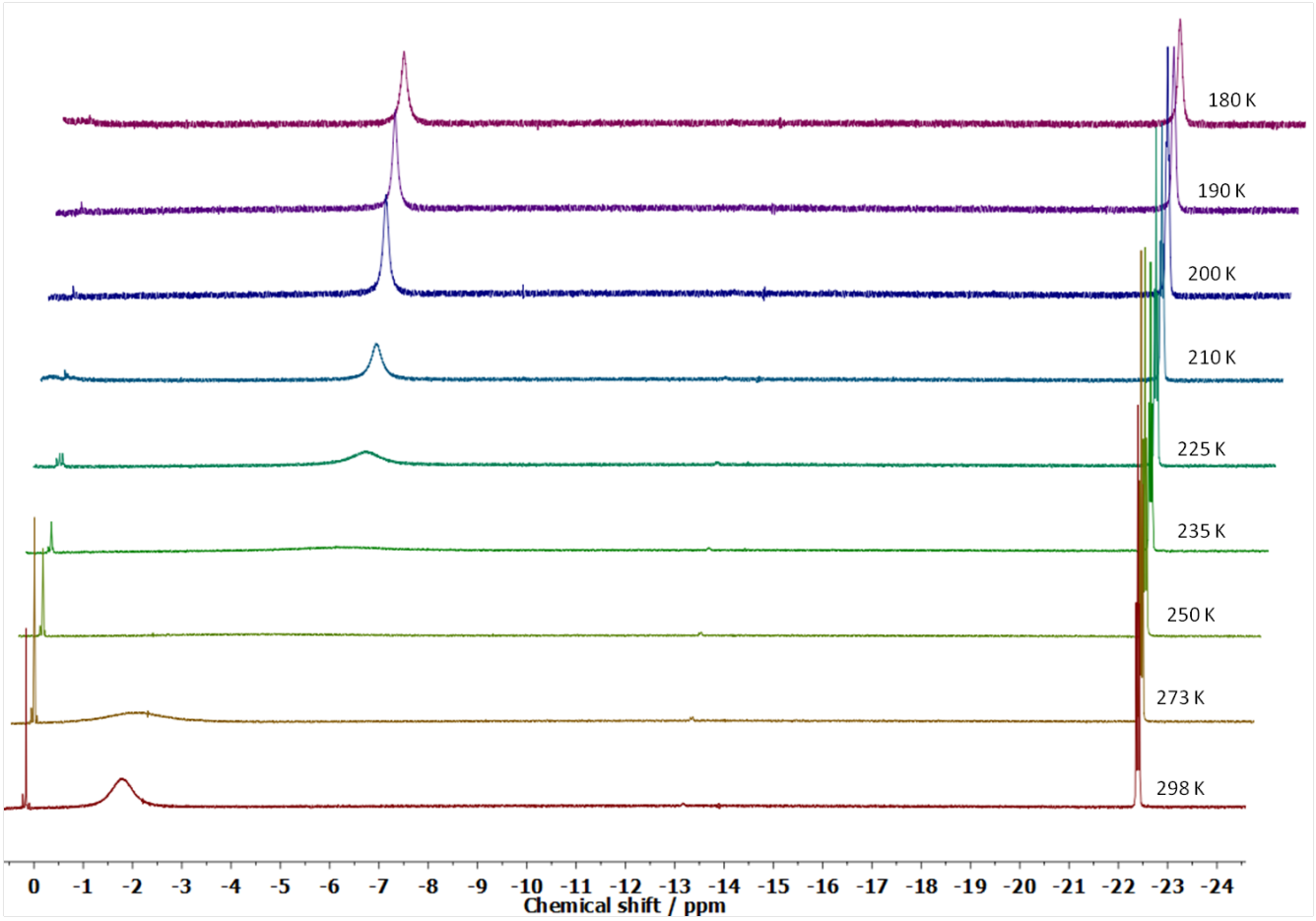

Figure S-2. Variable temperature ^{1}H NMR spectra of complex **2**, high field region.

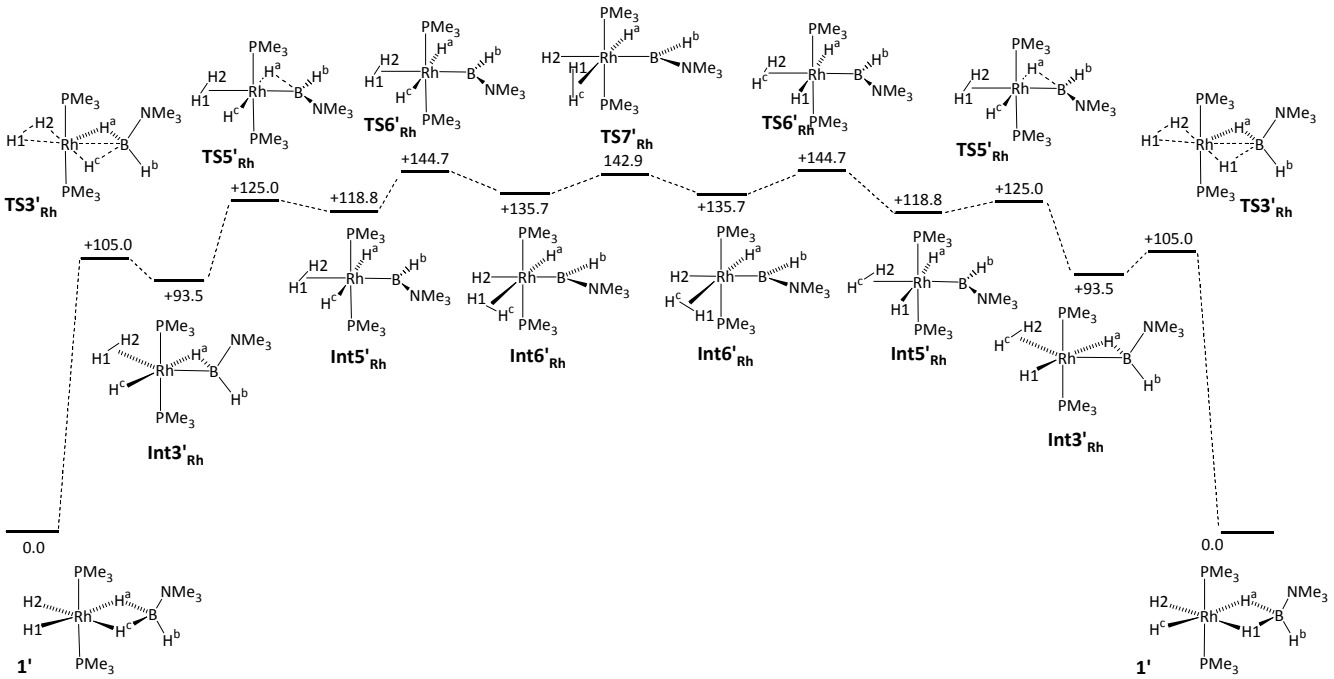

Figure S-3. Alternative free energy reaction profile (kJ/mol) for M—H/B–H bridging exchange in **1'** *via* **Int3'$_{Rh}$**. With $[Rh(PCy_3)_2(H)_2(\eta^2–H_3B{\cdot}NMe_3)]^+$ **TS3$_{Rh}$** and **TS7$_{Rh}$** have computed relative free energies of +134.2 and +143.7 kJ/mol, respectively.

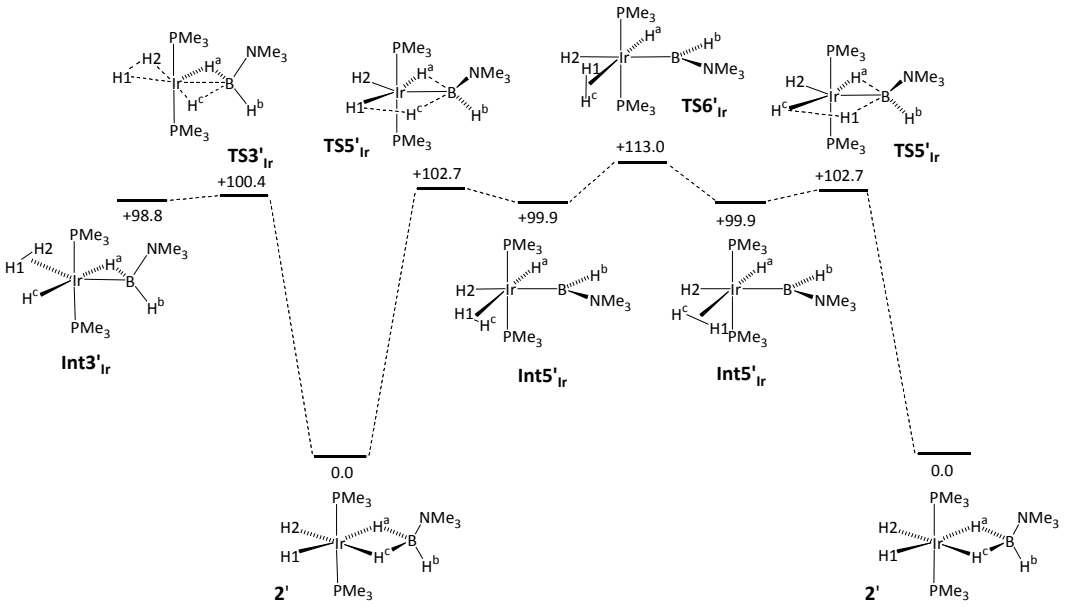

Figure S-4. Alternative free energy reaction profile (kJ/mol) for M—H/B–H bridging exchange in **2'** *via* **Int3'$_{Ir}$**. With $[Ir(PCy_3)_2(H)_2(\eta^2\text{–}H_3B{\cdot}NMe_3)]^+$ **TS3$_{Ir}$** and **TS7$_{Ir}$** have a computed relative free energies of 130.0 kJ/mol and 120.3 kJ/mol, respectively.

Computed Cartesian coordinates and associated energies (a.u.) for all species.

(a) B–H bridging/terminal exchange at $[ML_2(H)_2(\eta^2\text{–}H_3B\cdot NMe_3)]^+$

(i) M = Rh, L = PMe_3

1′

BP86 Energy = -565.553847067
Enthalpy 0K= -565.160317
Enthalpy 298K= -565.135029
Free Energy 298K= -565.214498
Nimag=0 (20.8467cm-1)
SCF PCM(DCM) = -565.605547910
D3 Correction = -0.05977992

C	-2.88463	-1.55706	1.46570
P	-1.74308	-1.73541	-0.00010
Rh	0.28555	-0.53708	-0.00005
P	2.60044	-0.14271	0.00005
C	3.61321	-1.70047	0.00004
C	-2.88502	-1.55666	-1.46556
C	-1.43634	-3.57175	-0.00040
B	-0.02848	1.72690	0.00003
N	-1.27727	2.77421	0.00007
C	-1.16966	3.64381	-1.22497
C	-1.17001	3.64332	1.22548
C	3.26813	0.78873	-1.46519
C	3.26801	0.78862	1.46542
H	0.68057	-1.68926	0.95661
H	-3.71364	-2.28083	1.39998
H	-2.31112	-1.74247	2.38713
H	-3.30232	-0.54008	1.51191
H	-2.38820	-4.12715	-0.00032
H	-0.85212	-3.84089	-0.89359
H	-0.85182	-3.84113	0.89251
H	-3.71388	-2.28061	-1.39990
H	-3.30293	-0.53975	-1.51124
H	-2.31173	-1.74161	-2.38721
H	0.68071	-1.68938	-0.95652
H	-0.19321	4.14617	1.21962
H	-1.97927	4.39130	1.22320
H	-1.24837	3.00957	2.12050
C	-2.61392	2.09984	-0.00026
H	-1.24767	3.01039	-2.12026
H	-1.97899	4.39171	-1.22268
H	-0.19291	4.14674	-1.21858
H	-0.13977	1.01299	-1.06108
H	-0.13986	1.01281	1.06103
H	0.96183	2.42334	0.00014
H	4.36218	0.89817	1.38997
H	2.79989	1.78341	1.50850
H	3.01725	0.23775	2.38514
H	4.36230	0.89827	-1.38965
H	3.01744	0.23793	-2.38497
H	2.80001	1.78353	-1.50823
H	4.68967	-1.46490	0.00011
H	3.36598	-2.29367	0.89367
H	3.36608	-2.29359	-0.89368
H	-3.41740	2.85419	-0.00015
H	-2.69194	1.47173	-0.89803
H	-2.69215	1.47124	0.89714

$TS1'_{Rh}$

BP86 Energy = -565.539872945
Enthalpy 0K= -565.147667
Enthalpy 298K= -565.122303
Free Energy 298K= -565.203553
Nimag=1 (-66.2188cm-1)
SCF PCM(DCM) = -565.593420365
D3 Correction = -0.05778237

C	3.39878	0.16265	-0.88143
P	2.32570	-1.08388	-0.00833
Rh	-0.00024	-0.79005	-0.00759
P	-2.32633	-1.08256	-0.00834
C	-2.89736	-2.69212	-0.74142
C	3.03559	-1.11868	1.71442
C	2.89580	-2.69406	-0.74079
B	0.00048	1.73903	0.59865
N	0.00095	3.25436	0.00017
C	-1.21994	3.50525	-0.83697
C	1.22202	3.50452	-0.83691
C	-3.03608	-1.11769	1.71446
C	-3.39881	0.16492	-0.88082
C	0.00121	4.21476	1.15937
H	4.46264	-0.11425	-0.80021
H	3.11492	0.20750	-1.94434
H	3.24486	1.15228	-0.42631
H	-0.00037	-1.24668	-1.45551
H	-0.00070	-2.33053	0.21809
H	0.00035	1.01689	-0.46768
H	-3.99272	-2.78959	-0.67068
H	-2.59281	-2.73808	-1.79849
H	-2.41619	-3.52317	-0.20374
H	4.12361	-1.29429	1.68307
H	2.83349	-0.15764	2.21276
H	2.55368	-1.92429	2.28993
H	3.99111	-2.79208	-0.67010
H	2.41422	-3.52462	-0.20271
H	2.59113	-2.74030	-1.79782
H	-1.02224	1.61540	1.24635
H	1.02307	1.61481	1.24645
H	-2.11190	3.35175	-0.21388
H	-1.20875	4.53814	-1.22206
H	-1.22950	2.79464	-1.67563
H	1.23119	2.79393	-1.67559
H	1.21148	4.53742	-1.22199
H	2.11387	3.35047	-0.21378
H	-4.12420	-1.29267	1.68314
H	-2.55457	-1.92380	2.28959

H -2.83340 -0.15697 2.21318
H -4.46281 -0.11145 -0.79962
H -3.24433 1.15427 -0.42527
H -3.11502 0.21008 -1.94372
H 0.00151 5.25181 0.78576
H -0.89461 4.03363 1.76928
H 0.89690 4.03312 1.76931

(ii) M = Ir, L = PMe_3

2′
BP86 Energy = -559.407832802
Enthalpy 0K= -559.013260
Enthalpy 298K= -558.988199
Free Energy 298K= -559.067611
Nimag=0 (26.0875cm-1)
SCF PCM(DCM) = -559.460106295
D3 correction = -0.062919160

C -2.94131 -1.47617 1.46664
P -1.79942 -1.63639 0.00002
Ir 0.24587 -0.44151 -0.00009
P 2.56835 -0.03234 0.00003
C 3.56243 -1.60065 -0.00027
C -2.94166 -1.47650 -1.46635
C -1.46885 -3.46789 0.00012
B -0.06582 1.77968 0.00001
N -1.33652 2.80604 -0.00000
C -1.23692 3.67695 -1.22553
C -1.23725 3.67656 1.22583
C 3.24095 0.89239 -1.46497
C 3.24066 0.89176 1.46557
H 0.64209 -1.60690 0.99619
H -3.74830 -2.22501 1.41059
H -2.35760 -1.63659 2.38633
H -3.39194 -0.47315 1.50714
H -2.41381 -4.03505 0.00019
H -0.88163 -3.72922 -0.89310
H -0.88154 -3.72914 0.89329
H -3.74900 -2.22491 -1.40965
H -3.39181 -0.47329 -1.50739
H -2.35828 -1.63780 -2.38609
H 0.64206 -1.60688 -0.99639
H -0.26415 4.18651 1.22227
H -2.05214 4.41810 1.21992
H -1.31468 3.04297 2.12120
C -2.66594 2.11872 -0.00032
H -1.31390 3.04364 -2.12113
H -2.05192 4.41836 -1.21969
H -0.26390 4.18707 -1.22144
H -0.17566 1.05662 -1.08659
H -0.17560 1.05659 1.08653
H 0.90364 2.50419 0.00008
H 4.33491 0.99892 1.39125
H 2.77640 1.88818 1.51250
H 2.98749 0.33848 2.38317
H 4.33516 0.99964 -1.39030
H 2.98811 0.33943 -2.38286
H 2.77660 1.88878 -1.51168
H 4.64150 -1.37732 -0.00018
H 3.30748 -2.19041 0.89331
H 3.30754 -2.19000 -0.89414
H -3.47562 2.86625 -0.00042
H -2.73748 1.48906 -0.89709
H -2.73786 1.48893 0.89633

TS1′$_{Ir}$
BP86 Energy = -559.390200249
Enthalpy 0K= -558.997212
Enthalpy 298K= -558.971934
Free Energy 298K= -559.054211
Nimag=1 (-52.6551cm-1)
SCF PCM(DCM) = -559.446470412
D3 Correction = -0.06076471

C 3.43764 0.37604 -0.71597
P 2.33789 -0.94145 0.00513
Ir -0.00000 -0.67189 -0.02407
P -2.33790 -0.94142 0.00513
C -2.91820 -2.47799 -0.86318
C 3.00508 -1.14141 1.73270
C 2.91816 -2.47803 -0.86317
B 0.00001 1.85530 0.64336
N 0.00002 3.35735 0.00271
C -1.22066 3.58986 -0.84007
C 1.22071 3.58984 -0.84007
C -3.00510 -1.14138 1.73269
C -3.43764 0.37609 -0.71596
C 0.00003 4.34337 1.14048
H 4.49756 0.08397 -0.63866
H 3.17960 0.52801 -1.77550
H 3.27991 1.31636 -0.16712
H -0.00001 -1.01616 -1.52889
H -0.00002 -2.25060 0.16465
H 0.00001 1.12825 -0.44090
H -4.01082 -2.59018 -0.77469
H -2.64080 -2.42098 -1.92715
H -2.41830 -3.35159 -0.41833
H 4.09213 -1.32356 1.71164
H 2.79937 -0.22822 2.31291
H 2.50293 -1.99183 2.21940
H 4.01079 -2.59024 -0.77468
H 2.41826 -3.35162 -0.41832
H 2.64077 -2.42102 -1.92714
H -1.02450 1.75123 1.28895
H 1.02452 1.75122 1.28895
H -2.11306 3.45385 -0.21387
H -1.20670 4.61288 -1.25040
H -1.23220 2.85884 -1.66098
H 1.23224 2.85882 -1.66098
H 1.20676 4.61287 -1.25040
H 2.11311 3.45382 -0.21387
H -4.09215 -1.32351 1.71164
H -2.50296 -1.99181 2.21940

H	-2.79937	-0.22819	2.31292
H	-4.49756	0.08403	-0.63866
H	-3.27989	1.31640	-0.16711
H	-3.17959	0.52806	-1.77549
H	0.00003	5.37152	0.74313
H	-0.89584	4.17596	1.75420
H	0.89589	4.17595	1.75420

(iii) M = Rh, L = PCy_3

1

BP86 Energy = -1737.68796088
Enthalpy 0K= -1736.575492
Enthalpy 298K= -1736.522981
Free Energy 298K= -1736.662415
Nimag=0 (10.7478cm-1)
SCF PCM(DCM) = -1737.73120181
D3 Correction = -0.217067240

B	0.21232	-2.49940	-0.69972
C	-2.16451	-3.43741	-1.28906
C	-0.56783	-4.84900	-0.09357
C	-0.20496	-4.30187	-2.45056
C	-2.49427	2.28081	0.34057
C	-1.89995	2.76932	1.68203
C	-2.15888	4.27693	1.89871
C	-1.62473	5.12223	0.73009
C	-2.20620	4.63546	-0.60797
C	-1.94584	3.12904	-0.82830
C	-3.28735	-0.24116	1.61175
C	-2.32104	-0.62811	2.75840
C	-3.08748	-0.97687	4.05161
C	-4.11996	-2.09354	3.81601
C	-5.06658	-1.73469	2.65755
C	-4.28933	-1.39211	1.36652
C	-3.47974	0.04209	-1.40606
C	-4.79180	0.86216	-1.43638
C	-5.72290	0.36091	-2.56280
C	-5.02186	0.39699	-3.93322
C	-3.69555	-0.38635	-3.90528
C	-2.76579	0.11062	-2.77724
C	2.74339	1.84604	0.17985
C	4.09575	2.24307	0.82047
C	4.18735	3.77725	0.98848
C	3.97779	4.51623	-0.34510
C	2.65127	4.10031	-1.00558
C	2.56442	2.56913	-1.17569
C	3.04392	-0.70304	1.70599
C	2.31358	-0.10428	2.93219
C	2.94631	-0.58705	4.25467
C	2.97990	-2.12356	4.33663
C	3.68886	-2.72658	3.11069
C	3.05256	-2.24631	1.78761
C	3.39535	-0.84058	-1.26705
C	4.91897	-0.58790	-1.17867
C	5.67734	-1.47728	-2.18928
C	5.16651	-1.26529	-3.62614
C	3.64372	-1.47896	-3.71426
C	2.88476	-0.58901	-2.70634
H	-3.59283	2.42622	0.38831
H	0.02439	0.67114	1.10639
H	0.06951	1.10367	-0.76740
H	-3.87579	0.64123	1.93652
H	-3.75759	-1.01834	-1.23880
H	1.93607	2.20502	0.85059
H	4.09652	-0.35654	1.72403
H	3.21985	-1.91445	-1.05301
H	-1.59622	0.18100	2.95253
H	-1.71914	-1.50015	2.43385
H	-2.37180	-1.27002	4.84054
H	-3.60587	-0.07047	4.42208
H	2.32049	1.00009	2.89574
H	-3.58964	-3.03714	3.57570
H	-4.69728	-2.28695	4.73719
H	3.66666	-3.83056	3.15324
H	-5.68593	-0.86223	2.94415
H	-5.76954	-2.56304	2.45684
H	-3.74115	-2.29846	1.03934
H	-5.00476	-1.14357	0.56445
H	-5.31531	0.81537	-0.46409
H	-4.55733	1.92816	-1.61674
H	-6.04091	-0.67679	-2.33784
H	-6.64321	0.97126	-2.58300
H	-4.81495	1.44965	-4.20937
H	-5.68880	-0.00556	-4.71582
H	-3.91488	-1.46335	-3.75197
H	-3.17900	-0.30758	-4.87876
H	-2.46467	1.15261	-2.99323
H	-1.82700	-0.47283	-2.75181
H	-0.13592	-2.15452	0.47720
H	-0.02464	-1.57147	-1.54605
H	1.34090	-2.92606	-0.75743
H	-2.27221	-2.68487	-2.08205
H	-2.53205	-3.02108	-0.34171
H	-2.73844	-4.34228	-1.54907
H	4.22874	1.76385	1.80548
H	4.93182	1.89902	0.18455
H	3.41837	4.10668	1.71542
H	5.16558	4.04075	1.42868
H	4.81544	4.27914	-1.03051
H	4.00377	5.60889	-0.18666
H	2.53561	4.59110	-1.98860
H	1.80377	4.44476	-0.37947
H	3.36279	2.24546	-1.87031
H	1.60226	2.28859	-1.64341
H	1.25022	-0.41223	2.89544
H	-1.11484	-5.75350	-0.40654
H	-0.97183	-4.47778	0.85897
H	0.49997	-5.07836	0.02896
H	3.97905	-0.19285	4.32985
H	2.38842	-0.16392	5.10924
H	3.47832	-2.44857	5.26699
H	1.94175	-2.50927	4.38525
H	4.75772	-2.43566	3.12588

H	3.60194	-2.68354	0.93497
H	2.01279	-2.61890	1.72218
H	5.12974	0.47333	-1.40975
H	5.29815	-0.77382	-0.15806
H	6.76019	-1.26765	-2.12795
H	5.54750	-2.54045	-1.90459
H	5.69123	-1.94226	-4.32338
H	5.40792	-0.23372	-3.95042
H	3.41238	-2.54297	-3.50474
H	3.28363	-1.27398	-4.73867
H	1.79873	-0.77626	-2.76645
H	3.03760	0.47092	-2.97991
H	0.84874	-4.58912	-2.33400
H	-0.28296	-3.50689	-3.20597
H	-0.80390	-5.17383	-2.76065
H	-2.32191	2.20470	2.53136
H	-0.80789	2.58112	1.68444
H	-3.24873	4.44569	2.00470
H	-1.70022	4.59481	2.85214
H	-0.51928	5.04566	0.69806
H	-1.86002	6.18966	0.88741
H	-1.78100	5.20965	-1.45041
H	-3.29840	4.82150	-0.62228
H	-2.39229	2.81530	-1.78738
H	-0.85523	2.95579	-0.91842
Rh	-0.04084	-0.28366	-0.10783
N	-0.71574	-3.77580	-1.13653
P	-2.31842	0.39583	0.07128
P	2.32789	-0.01993	0.07922

(iv) M = Ir, L = PCy_3

2

BP86 Energy = -1731.53993685
Enthalpy 0K= -1730.426559
Enthalpy 298K= -1730.374218
Free Energy 298K= -1730.513260
Nimag=0 (11.3596cm-1)
SCF PCM(DCM) = -1731.58375939
D3 Correction = -0.222115230

B	0.24546	-2.41588	-0.71536
C	-2.14307	-3.34138	-1.32372
C	-0.56012	-4.75840	-0.11494
C	-0.17832	-4.21317	-2.47008
C	-2.51783	2.26499	0.38625
C	-1.93002	2.73560	1.73717
C	-2.22258	4.23181	1.98758
C	-1.70938	5.11436	0.83713
C	-2.28125	4.64372	-0.51088
C	-1.98643	3.14887	-0.76414
C	-3.30411	-0.28244	1.60037
C	-2.34964	-0.69026	2.74937
C	-3.12951	-1.04843	4.03197
C	-4.16894	-2.15401	3.77569
C	-5.10251	-1.77546	2.61289
C	-4.31047	-1.42515	1.33290
C	-3.48434	0.06179	-1.41009
C	-4.80099	0.87552	-1.42238
C	-5.73024	0.39077	-2.55755
C	-5.03146	0.45882	-3.92794
C	-3.69879	-0.31418	-3.91721
C	-2.77244	0.16714	-2.77975
C	2.75185	1.86627	0.21758
C	4.09638	2.25802	0.87823
C	4.17755	3.78913	1.07703
C	3.97549	4.55382	-0.24314
C	2.65865	4.14195	-0.92489
C	2.58455	2.61386	-1.12671
C	3.07490	-0.71014	1.69300
C	2.34657	-0.14289	2.93545
C	2.99633	-0.64216	4.24334
C	3.04747	-2.17947	4.29725
C	3.75129	-2.75289	3.05427
C	3.09841	-2.25467	1.74592
C	3.41750	-0.78776	-1.28031
C	4.94007	-0.53166	-1.18381
C	5.70341	-1.39648	-2.21185
C	5.19387	-1.15703	-3.64486
C	3.67187	-1.37361	-3.73968
C	2.90937	-0.50640	-2.71489
H	-3.61838	2.39341	0.43874
H	0.02447	0.67221	1.17693
H	0.07007	1.17783	-0.75142
H	-3.89250	0.59592	1.93585
H	-3.76010	-1.00298	-1.26929
H	1.93565	2.20823	0.88603
H	4.12460	-0.35534	1.71254
H	3.24748	-1.86712	-1.09059
H	-1.61991	0.11025	2.95891
H	-1.75105	-1.56253	2.41967
H	-2.42249	-1.35632	4.82310
H	-3.64364	-0.14226	4.40889
H	2.33930	0.96192	2.91946
H	-3.64429	-3.09935	3.52980
H	-4.75572	-2.35258	4.68977
H	3.74048	-3.85764	3.07674
H	-5.71780	-0.90133	2.90311
H	-5.80982	-2.59626	2.39701
H	-3.76569	-2.33275	1.00386
H	-5.01621	-1.16529	0.52599
H	-5.32399	0.80714	-0.45111
H	-4.57272	1.94601	-1.58222
H	-6.04111	-0.65329	-2.35286
H	-6.65460	0.99524	-2.56460
H	-4.83319	1.51825	-4.18369
H	-5.69644	0.06645	-4.71736
H	-3.90899	-1.39599	-3.78642
H	-3.18381	-0.21073	-4.88922
H	-2.48224	1.21659	-2.97293
H	-1.82671	-0.40528	-2.76769
H	-0.09993	-2.08754	0.49044
H	-0.00197	-1.46884	-1.57100
H	1.36569	-2.85933	-0.78935

H	-2.24290	-2.59383	-2.12220
H	-2.51580	-2.91750	-0.38209
H	-2.71729	-4.24644	-1.58176
H	4.22381	1.76133	1.85514
H	4.94006	1.93088	0.24324
H	3.40016	4.09935	1.80343
H	5.15022	4.04926	1.53134
H	4.82139	4.33680	-0.92508
H	3.99216	5.64313	-0.06194
H	2.54927	4.65137	-1.89912
H	1.80229	4.46775	-0.30089
H	3.39498	2.31014	-1.81646
H	1.63093	2.33676	-1.61199
H	1.28719	-0.46319	2.90050
H	-1.10383	-5.66219	-0.43517
H	-0.97519	-4.38840	0.83339
H	0.50622	-4.98866	0.01892
H	4.02527	-0.23786	4.31729
H	2.44107	-0.24112	5.11018
H	3.55807	-2.51581	5.21692
H	2.01403	-2.57731	4.34850
H	4.81729	-2.45151	3.06492
H	3.64347	-2.67197	0.88057
H	2.06117	-2.63519	1.68526
H	5.14760	0.53511	-1.39127
H	5.31867	-0.73849	-0.16703
H	6.78531	-1.18393	-2.14466
H	5.57749	-2.46585	-1.94941
H	5.72191	-1.81797	-4.35485
H	5.43227	-0.11833	-3.94781
H	3.44353	-2.44253	-3.55278
H	3.31264	-1.14853	-4.76014
H	1.82338	-0.69143	-2.78108
H	3.06198	0.55912	-2.96530
H	0.87150	-4.51083	-2.34511
H	-0.24277	-3.41685	-3.22553
H	-0.78310	-5.07876	-2.78609
H	-2.33663	2.14265	2.57461
H	-0.83469	2.57209	1.73196
H	-3.31572	4.37408	2.09883
H	-1.76925	4.53889	2.94710
H	-0.60254	5.06378	0.80249
H	-1.96877	6.17247	1.01788
H	-1.87006	5.24580	-1.34075
H	-3.37743	4.80535	-0.52048
H	-2.42515	2.84634	-1.73027
H	-0.89274	3.00249	-0.85618
Ir	-0.02805	-0.25242	-0.10194
N	-0.69715	-3.68457	-1.15949
P	-2.32689	0.38624	0.07743
P	2.34879	0.00041	0.08330

TS1$_{Ir}$

BP86 Energy = -1731.52553951
Enthalpy 0K= -1730.413660
Enthalpy 298K= -1730.361239
Free Energy 298K= -1730.501425
Nimag=1 (-37.3027cm-1)
SCF PCM(DCM) = -1731.56921755
D3 Correction = -0.216905120

Ir	0.05889	-0.07998	0.04495
C	-0.25149	-4.89733	-1.86197
C	0.49845	-4.65883	0.45072
H	-0.56091	-5.93569	-1.65717
H	-0.88919	-4.46069	-2.64321
H	0.79521	-4.87351	-2.19474
H	0.19046	-5.69609	0.66361
H	1.53858	-4.64308	0.09806
H	0.41394	-4.04891	1.36142
H	1.23805	-2.66179	-1.36961
H	0.10488	1.49404	0.12844
H	0.15717	-0.01825	1.58504
P	2.42216	0.19325	-0.11347
P	-2.28589	0.35602	0.26669
B	0.09949	-2.54192	-0.97814
H	-0.67558	-2.10349	-1.80812
H	0.04486	-1.94790	0.17208
N	-0.38194	-4.06943	-0.61301
C	3.65245	-0.90826	0.82756
C	2.98602	1.97699	0.30339
C	-2.92141	0.14485	2.04896
C	-2.62007	2.20092	-0.08429
C	2.79123	-0.04440	-1.96175
C	-3.48415	-0.71310	-0.76801
H	4.62548	-0.38799	0.73621
C	3.27517	-0.97537	2.32752
H	2.27300	-1.43945	2.42061
H	3.18811	0.04002	2.75365
C	4.30469	-1.79411	3.13439
H	5.27696	-1.26336	3.12716
H	3.98878	-1.85107	4.19146
C	4.49183	-3.20444	2.54756
H	5.26592	-3.75589	3.10986
H	3.55008	-3.77736	2.66796
C	4.86036	-3.13721	1.05441
H	4.95294	-4.15337	0.62966
H	5.85597	-2.66412	0.94482
C	3.82490	-2.32695	0.24391
H	2.84933	-2.84576	0.26409
H	4.13687	-2.28163	-0.81451
H	2.65772	2.53196	-0.60104
C	4.51587	2.16955	0.45948
H	4.85094	1.66616	1.38727
H	5.07439	1.70828	-0.37144
C	4.87325	3.66935	0.56163
H	5.96650	3.78064	0.67437
H	4.60325	4.17278	-0.38781
C	4.13785	4.34596	1.73168
H	4.36266	5.42697	1.75401
H	4.51268	3.92787	2.68682
C	2.61878	4.11475	1.63925
H	2.21944	4.64794	0.75330
H	2.10781	4.54459	2.51959

C	2.27075	2.61530	1.51971
H	1.17917	2.48346	1.44028
H	2.58541	2.09665	2.44665
H	2.67998	-1.14116	-2.07777
C	4.17592	0.36386	-2.50697
H	4.31349	1.45571	-2.38994
H	4.98475	-0.12471	-1.93362
C	4.29967	0.00771	-4.00541
H	5.28845	0.32367	-4.38262
H	4.25550	-1.09315	-4.12312
C	3.17511	0.65742	-4.83296
H	3.26059	0.36512	-5.89442
H	3.28834	1.75908	-4.80131
C	1.78480	0.27370	-4.28881
H	1.62390	-0.81341	-4.42745
H	0.99040	0.78788	-4.85891
C	1.65803	0.61162	-2.78906
H	0.66347	0.27361	-2.41123
H	1.67815	1.71077	-2.65356
H	-2.00314	2.66784	0.71156
C	-2.04720	2.70539	-1.43094
H	-1.00555	2.35779	-1.55561
H	-2.62982	2.28422	-2.27080
C	-2.11070	4.24632	-1.50442
H	-1.44779	4.67389	-0.72595
H	-1.71502	4.58933	-2.47733
C	-3.54588	4.76408	-1.29405
H	-3.56156	5.86827	-1.30381
H	-4.17945	4.43457	-2.14131
C	-4.14370	4.23329	0.02168
H	-5.19192	4.56364	0.13246
H	-3.58769	4.66183	0.87899
C	-4.07503	2.69117	0.09702
H	-4.50127	2.34545	1.05564
H	-4.70830	2.26749	-0.70561
H	-3.08025	-1.72590	-0.57372
C	-4.97769	-0.72324	-0.36149
H	-5.09840	-0.94068	0.71397
H	-5.42141	0.27400	-0.53333
C	-5.75925	-1.77134	-1.18595
H	-5.39057	-2.78454	-0.92649
H	-6.82547	-1.74750	-0.89842
C	-5.60289	-1.54464	-2.70040
H	-6.08116	-0.58437	-2.97650
H	-6.13559	-2.33114	-3.26374
C	-4.11866	-1.50266	-3.10731
H	-4.01730	-1.28402	-4.18544
H	-3.66419	-2.50222	-2.94848
C	-3.33869	-0.45416	-2.28664
H	-3.74062	0.54809	-2.52548
H	-2.27334	-0.45128	-2.58126
H	-3.99949	0.39763	2.01398
C	-2.78268	-1.32073	2.52309
H	-1.71051	-1.60120	2.49103
H	-3.31647	-2.00128	1.83362
C	-3.32316	-1.51114	3.95663
H	-4.41595	-1.32944	3.95929
H	-3.18119	-2.56074	4.27206
C	-2.64430	-0.54999	4.94824
H	-1.56942	-0.80763	5.03131
H	-3.07488	-0.67349	5.95753
C	-2.78335	0.90949	4.48093
H	-2.25653	1.59086	5.17247
H	-3.85154	1.20222	4.50709
C	-2.23871	1.10683	3.04986
H	-2.38351	2.15799	2.74472
H	-1.14604	0.92388	3.04360
C	-1.80302	-4.13077	-0.14407
H	-1.91210	-3.49469	0.74555
H	-2.45609	-3.75745	-0.94503
H	-2.07571	-5.17069	0.10249

Int1$_{Ir}$

BP86 Energy = -1731.52622427
Enthalpy 0K= -1730.415002
Enthalpy 298K= -1730.361675
Free Energy 298K= -1730.504586
Nimag=0 (12.4203cm-1)
SCF PCM(DCM) = -1731.56863395
D3 Correction = -0.21868774

Ir	0.08690	-0.01960	0.10529
C	0.04647	-4.99983	-1.80272
C	0.79744	-4.45524	0.45858
H	-0.13609	-6.04469	-1.50105
H	-0.64774	-4.71183	-2.60451
H	1.07882	-4.88464	-2.16031
H	0.63480	-5.50108	0.76854
H	1.82222	-4.33241	0.08250
H	0.64367	-3.78193	1.31380
H	1.20655	-2.52988	-1.60911
H	0.11842	1.51373	0.48381
H	0.12062	-0.27837	1.63340
P	2.44085	0.27877	-0.10372
P	-2.26611	0.31226	0.32805
B	0.08629	-2.54834	-1.14964
H	-0.79420	-2.29693	-1.94364
H	-0.01236	-1.87219	-0.05356
N	-0.16557	-4.08397	-0.62930
C	3.76363	-0.89826	0.59315
C	2.99455	2.01205	0.47116
C	-2.90680	-0.01191	2.09176
C	-2.70040	2.14938	0.05930
C	2.56476	0.24746	-1.99960
C	-3.38411	-0.77813	-0.76998
H	4.67131	-0.27360	0.69809
C	3.35014	-1.38681	2.00290
H	2.40719	-1.96176	1.91674
H	3.12649	-0.52859	2.66168
C	4.44577	-2.26809	2.63760
H	5.34762	-1.65160	2.82061
H	4.10939	-2.62800	3.62649
C	4.81773	-3.45215	1.72697
H	5.63591	-4.04177	2.17685

H	3.94955	-4.13758	1.64619
C	5.21954	-2.96796	0.32177
H	5.44279	-3.82614	-0.33753
H	6.15605	-2.38093	0.39440
C	4.12604	-2.08790	-0.32335
H	3.22091	-2.69459	-0.51663
H	4.47760	-1.72938	-1.30692
H	2.45531	2.66984	-0.24320
C	4.50908	2.31547	0.36549
H	5.05664	1.70234	1.10753
H	4.91191	2.04925	-0.62513
C	4.78944	3.80475	0.66863
H	5.87406	3.99916	0.59166
H	4.30289	4.43119	-0.10506
C	4.26683	4.20377	2.06036
H	4.42729	5.28213	2.23637
H	4.85239	3.66960	2.83459
C	2.77662	3.85038	2.21932
H	2.17357	4.48440	1.53893
H	2.43290	4.07707	3.24457
C	2.49943	2.36642	1.89523
H	1.42327	2.14579	1.99572
H	3.02774	1.73126	2.63378
H	2.56311	-0.84004	-2.21251
C	3.76475	0.88759	-2.72677
H	3.79326	1.97302	-2.51227
H	4.71703	0.46423	-2.35938
C	3.64883	0.68402	-4.25413
H	4.50278	1.16776	-4.76036
H	3.71885	-0.39752	-4.48369
C	2.31908	1.23828	-4.79910
H	2.24054	1.05238	-5.88473
H	2.29927	2.33806	-4.66723
C	1.10812	0.61762	-4.07267
H	1.05819	-0.46571	-4.29448
H	0.16643	1.06427	-4.43830
C	1.22954	0.81337	-2.54721
H	0.34738	0.29630	-2.06226
H	1.13931	1.88748	-2.30034
H	-2.15867	2.61109	0.91072
C	-2.09160	2.76189	-1.22436
H	-1.02069	2.49976	-1.29362
H	-2.58665	2.33838	-2.11784
C	-2.26714	4.29604	-1.23257
H	-1.67918	4.73141	-0.39999
H	-1.84780	4.71411	-2.16549
C	-3.74529	4.69994	-1.07819
H	-3.84093	5.79946	-1.03982
H	-4.30954	4.36764	-1.97210
C	-4.36800	4.06535	0.17866
H	-5.44130	4.31681	0.24900
H	-3.88690	4.48825	1.08276
C	-4.19323	2.53012	0.18537
H	-4.64025	2.10671	1.10240
H	-4.75390	2.10505	-0.66885
H	-2.91119	-1.77125	-0.63193
C	-4.87585	-0.90622	-0.37693
H	-4.98803	-1.19061	0.68374
H	-5.38102	0.06920	-0.49630
C	-5.58573	-1.95303	-1.26510
H	-5.15362	-2.95383	-1.06117
H	-6.65242	-2.01358	-0.98458
C	-5.43768	-1.63017	-2.76282
H	-5.97565	-0.68808	-2.98715
H	-5.91660	-2.41536	-3.37431
C	-3.95722	-1.47165	-3.15417
H	-3.86509	-1.18676	-4.21762
H	-3.43899	-2.44598	-3.04577
C	-3.24831	-0.42441	-2.27012
H	-3.70782	0.56471	-2.45606
H	-2.18322	-0.34445	-2.55355
H	-3.99421	0.19884	2.05789
C	-2.71399	-1.49201	2.49800
H	-1.63085	-1.72735	2.46757
H	-3.21110	-2.16039	1.77057
C	-3.26085	-1.77207	3.91422
H	-4.35972	-1.63179	3.91268
H	-3.08217	-2.82969	4.18046
C	-2.62866	-0.83521	4.95839
H	-1.54557	-1.05602	5.04114
H	-3.06376	-1.02341	5.95571
C	-2.81899	0.63873	4.55962
H	-2.32412	1.30522	5.28830
H	-3.89773	0.88938	4.58919
C	-2.26999	0.92528	3.14528
H	-2.45315	1.98385	2.89090
H	-1.17149	0.78420	3.13969
C	-1.56249	-4.27234	-0.11968
H	-1.72786	-3.58693	0.72334
H	-2.26863	-4.03578	-0.92781
H	-1.70795	-5.31451	0.21112

(b) $M(H)_2/H_2$ exchange at $[ML_2(H)_2(\eta^2-H_3B{\cdot}NMe_3)]^+$

(i) M = Rh, L = PMe_3

$TS2'_{Rh}$

BP86 Energy = -566.720854421
Enthalpy 0K= -566.315557
Enthalpy 298K= -566.288060
Free Energy 298K= -566.371655
Nimag=1 (-276.4847cm-1)
SCF PCM(DCM) = -566.771757963
D3 Correction = -0.062932560

Rh	-0.37339	-0.61857	-0.06487
C	1.39256	4.00211	-0.83443
C	1.71260	3.18151	1.44746
H	2.28501	4.64189	-0.73705
H	1.25925	3.69875	-1.88240
H	0.49974	4.54702	-0.49884
H	2.58660	3.84450	1.55642

H	0.80133	3.70715	1.76490
H	1.84521	2.28248	2.06621
H	-0.71736	2.57352	0.14706
H	-1.01424	-1.98579	-0.44246
H	-0.64215	-1.18717	1.32500
P	-2.61481	0.09223	0.04746
P	1.58764	-1.91648	0.04408
B	0.20935	1.85610	-0.16592
H	0.17166	1.48670	-1.33020
H	0.34841	0.92216	0.69914
N	1.55409	2.76754	0.01140
H	-0.23863	-0.52460	-2.86183
H	-0.48986	-0.99117	-2.31261
C	2.69225	-1.64700	1.52284
H	2.10030	-1.79193	2.43985
H	3.53318	-2.35963	1.51493
H	3.09015	-0.62059	1.52639
C	2.77057	-1.84710	-1.39752
H	3.61319	-2.54035	-1.23996
H	2.23362	-2.13183	-2.31561
H	3.15946	-0.82539	-1.52230
C	1.23405	-3.73878	0.16695
H	0.68341	-4.06086	-0.73016
H	2.16879	-4.31614	0.25370
H	0.60208	-3.92479	1.04880
C	-3.06331	1.07104	1.56337
H	-2.44303	1.97851	1.60423
H	-4.12938	1.34983	1.54130
H	-2.86290	0.46081	2.45757
C	-3.21693	1.14773	-1.36201
H	-3.11403	0.58651	-2.30366
H	-4.27450	1.42096	-1.21349
H	-2.60192	2.05796	-1.41922
C	-3.83969	-1.30559	0.07986
H	-4.86914	-0.92063	0.16120
H	-3.74025	-1.89744	-0.84297
H	-3.62181	-1.95800	0.93929
C	2.78714	2.04259	-0.43241
H	2.90141	1.13474	0.17584
H	2.67240	1.76353	-1.48942
H	3.67353	2.68644	-0.30864

Int2'$_{Rh}$

BP86 Energy = -566.734212566
Enthalpy 0K= -566.325865
Enthalpy 298K= -566.298737
Free Energy 298K= -566.383280
Nimag=0 (14.3239cm-1)
SCF PCM(DCM) = -566.785589120
D3 Correction = -0.063295160

Rh	0.27969	-0.79330	-0.12412
C	-1.04733	4.31442	-0.86340
C	-2.48860	2.71141	0.28431
H	-1.56567	5.14165	-0.35114
H	-0.00344	4.59081	-1.06571
H	-1.55033	4.08325	-1.81257
H	-3.00502	3.53647	0.80215
H	-2.99057	2.49729	-0.66962
H	-2.50047	1.81259	0.91722
H	-0.93076	1.67624	-1.81098
H	0.75228	-2.26021	0.09009
H	0.30969	-0.82666	1.43585
P	-1.87587	-1.73105	0.04711
P	2.56980	-0.27920	0.04884
B	-0.28932	1.89748	-0.80713
H	0.84464	2.28151	-0.99906
H	-0.33207	0.92975	0.04664
N	-1.06361	3.08536	0.00546
C	-2.75754	-1.44471	1.66038
C	-1.90043	-3.58456	-0.09907
C	3.01239	1.10158	1.21178
C	-3.12262	-1.20397	-1.23266
H	-3.73975	-1.94474	1.66307
H	-1.47354	-3.87940	-1.07010
H	-3.24267	-0.11064	-1.20317
H	4.10492	1.24327	1.24517
H	0.16759	-0.52841	-1.94087
H	0.44722	-1.29703	-1.85497
H	-1.28009	-4.01651	0.70109
H	-2.92978	-3.97027	-0.01821
H	-2.89870	-0.36560	1.82566
H	-2.13853	-1.84339	2.47866
H	-4.09679	-1.68847	-1.05518
H	-2.75444	-1.48476	-2.23192
H	2.53316	2.02801	0.86257
H	2.64194	0.85977	2.21968
C	3.61286	-1.68892	0.66229
H	3.51676	-2.53933	-0.03008
H	4.67134	-1.39045	0.73408
H	3.24847	-2.00157	1.65284
C	3.40347	0.21505	-1.53943
H	2.89872	1.10305	-1.95002
H	4.46844	0.44181	-1.36770
H	3.32081	-0.60907	-2.26527
C	-0.37599	3.39569	1.30275
H	-0.36758	2.49091	1.92735
H	0.65748	3.70187	1.08931
H	-0.90353	4.20950	1.82709

TS3'$_{Rh}$

BP86 Energy = -566.714285815
Enthalpy 0K= -566.309515
Enthalpy 298K= -566.282815
Free Energy 298K= -566.366225
Nimag=1 (-560.5413cm-1)
SCF PCM(DCM) = -566.766064369
D3 Correction = -0.064024050

Rh	-0.05210	-0.83813	-0.02218
C	-0.18796	4.41109	0.82852
C	1.67196	3.26163	-0.26179

H	0.06555	5.33409	0.28178
H	-1.26819	4.37414	1.02567
H	0.35551	4.37559	1.78289
H	1.92744	4.18554	-0.80623
H	2.20653	3.23373	0.69802
H	1.95152	2.38731	-0.86687
H	0.47179	1.88691	1.87901
H	-0.10958	-1.94598	-1.13260
H	-0.05920	-0.49372	-1.61841
P	2.28455	-1.16826	0.00282
P	-2.41387	-0.89973	0.00513
B	-0.20057	1.88788	0.87589
H	-1.39878	1.90810	1.03780
H	0.18702	0.93901	0.07220
N	0.19695	3.20989	0.00549
C	3.20864	-0.65590	-1.52721
C	2.76769	-2.95085	0.19978
C	-3.30097	0.31794	-1.08180
C	3.19203	-0.32830	1.38887
H	4.28343	-0.88007	-1.42935
H	2.35402	-3.33519	1.14475
H	3.01111	0.75589	1.34575
H	-4.39070	0.16285	-1.02306
H	-0.03581	-0.92777	1.60199
H	-0.14835	-2.19493	0.76349
H	2.34775	-3.53604	-0.63265
H	3.86456	-3.05736	0.20797
H	3.07674	0.42306	-1.70077
H	2.79509	-1.19908	-2.39081
H	4.27402	-0.52893	1.32631
H	2.79958	-0.70420	2.34617
H	-3.05955	1.33744	-0.74709
H	-2.96489	0.18795	-2.12183
C	-3.09960	-2.53392	-0.55202
H	-2.70324	-3.33357	0.09228
H	-4.20035	-2.53097	-0.49811
H	-2.78274	-2.72727	-1.58849
C	-3.18111	-0.65134	1.67660
H	-2.86545	0.32428	2.07609
H	-4.28070	-0.69106	1.61152
H	-2.82174	-1.44172	2.35332
C	-0.53905	3.25525	-1.30175
H	-0.29153	2.35388	-1.88097
H	-1.61860	3.27320	-1.09818
H	-0.25343	4.15825	-1.86586

(ii) M = Ir, L = PMe_3

TS2′$_{Ir}$

BP86 Energy = -560.571944431
Enthalpy 0K= -560.165724
Enthalpy 298K= -560.138377
Free Energy 298K= -560.221908
Nimag=1 (-298.4245cm-1)
SCF PCM(DCM) = -560.623144363
D3 Correction = -0.066021050

Ir	-0.32468	-0.52879	-0.03141
C	1.47517	4.08025	-0.80774
C	1.80239	3.20619	1.45325
H	2.37833	4.70407	-0.70634
H	1.32625	3.80170	-1.86050
H	0.59451	4.63116	-0.45064
H	2.68369	3.85819	1.56876
H	0.89913	3.73382	1.78987
H	1.93175	2.29294	2.05160
H	-0.64559	2.66847	0.14103
H	-0.98277	-1.91912	-0.42894
H	-0.58090	-1.07014	1.39975
P	-2.56329	0.23050	0.04754
P	1.65254	-1.81753	0.04482
B	0.26626	1.93773	-0.18113
H	0.22785	1.58573	-1.35030
H	0.40225	1.00402	0.70897
N	1.62790	2.82524	0.00971
H	-0.18917	-0.44937	-2.88758
H	-0.42889	-0.88246	-2.30435
C	2.78821	-1.54556	1.49892
H	2.21219	-1.67904	2.42777
H	3.62268	-2.26539	1.48126
H	3.19602	-0.52310	1.48814
C	2.80309	-1.76301	-1.42202
H	3.64583	-2.45895	-1.27882
H	2.24348	-2.05256	-2.32493
H	3.19409	-0.74446	-1.56439
C	1.29147	-3.63610	0.18640
H	0.72353	-3.95988	-0.69907
H	2.22416	-4.21830	0.26114
H	0.67364	-3.81225	1.08015
C	-3.01591	1.22742	1.54963
H	-2.39158	2.13236	1.58519
H	-4.08019	1.51175	1.51949
H	-2.82371	0.62528	2.45110
C	-3.14367	1.27638	-1.37680
H	-3.03709	0.70377	-2.31119
H	-4.19990	1.56069	-1.24160
H	-2.52058	2.18084	-1.43870
C	-3.79570	-1.15896	0.08237
H	-4.82358	-0.76810	0.15367
H	-3.69204	-1.75799	-0.83522
H	-3.58678	-1.80570	0.94820
C	2.84805	2.09511	-0.46024
H	2.95018	1.16833	0.12062
H	2.72522	1.84833	-1.52432
H	3.74413	2.72216	-0.32162

Int2′$_{Ir}$

BP86 Energy = -560.591205878
Enthalpy 0K= -560.181982
Enthalpy 298K= -560.155098
Free Energy 298K= -560.239547
Nimag=0 (14.3970cm-1)

SCF PCM(DCM) = -560.642852872
D3 Correction = -0.066107680

C	-3.59842	-1.48242	0.69729
P	-2.53660	-0.10003	0.05770
C	-2.96517	1.31064	1.18795
Ir	-0.24647	-0.67976	-0.08084
P	1.92285	-1.61946	0.05700
C	3.15417	-1.09949	-1.23839
C	-3.35439	0.36962	-1.54460
C	2.82233	-1.33709	1.65953
C	1.93111	-3.47183	-0.08983
B	0.34706	2.01599	-0.83627
N	1.13348	3.17563	0.00381
C	0.45863	3.45758	1.31460
C	1.11502	4.42513	-0.83627
C	2.55955	2.78903	0.26056
H	1.64314	5.23670	-0.30934
H	1.60774	4.21410	-1.79551
H	0.07082	4.71225	-1.02121
H	0.99798	4.25269	1.85510
H	-0.57356	3.77861	1.11785
H	0.44656	2.53661	1.91508
H	-0.78567	2.40602	-1.00954
H	-0.74485	-2.15936	0.20523
H	-0.23613	-0.59760	1.51658
H	0.98595	1.80207	-1.84067
H	0.40295	1.02963	0.01904
H	-4.65368	-1.17066	0.75762
H	-2.83431	1.23980	-1.97382
H	-2.59425	1.08827	2.20012
H	3.80027	-1.84509	1.65510
H	-0.15984	-0.47294	-1.86703
H	-0.44481	-1.28233	-1.74232
H	-3.28009	-0.47297	-2.24991
H	-4.41669	0.61631	-1.38548
H	-3.24155	-1.77640	1.69624
H	-3.50843	-2.34878	0.02428
H	-4.05621	1.46244	1.22060
H	-2.48026	2.22532	0.81643
H	2.97385	-0.25887	1.82132
H	2.20654	-1.72856	2.48364
H	1.48997	-3.76228	-1.05576
H	2.95790	-3.86631	-0.02153
H	1.31690	-3.89860	0.71773
H	3.28171	-0.00701	-1.20983
H	4.12786	-1.58990	-1.07628
H	2.76945	-1.37673	-2.23242
H	3.08293	3.59880	0.79507
H	2.57310	1.87438	0.87023
H	3.05268	2.59773	-0.70276

TS3′$_{Ir}$

BP86 Energy = -560.583854932
Enthalpy 0K= -560.176639
Enthalpy 298K= -560.150403
Free Energy 298K= -560.232553
Nimag=1 (-273.7894cm-1)
SCF PCM(DCM) = -560.635717865
D3 Correction = -0.06692950

C	-3.22118	-0.25081	1.57811
P	-2.39197	-0.82376	0.01714
C	-3.27483	0.09884	-1.33251
Ir	-0.02285	-0.70746	-0.01855
P	2.34003	-0.95675	0.01449
C	3.17831	-0.77743	-1.63173
C	-3.02700	-2.55755	-0.17804
C	3.30643	0.16652	1.13373
C	2.85947	-2.64750	0.58105
B	0.44760	2.00901	-0.91682
N	0.10302	3.31210	-0.00455
C	-1.37852	3.50757	0.13255
C	0.68315	4.50498	-0.72003
C	0.71439	3.21462	1.36362
H	0.47703	5.42029	-0.14169
H	1.76740	4.36249	-0.82610
H	0.22706	4.57741	-1.71716
H	-1.58786	4.43006	0.69832
H	-1.82095	3.57515	-0.87122
H	-1.80042	2.64402	0.66621
H	-0.12686	2.11917	-1.97189
H	-0.06161	-2.01842	0.88702
H	0.00911	-0.22907	1.56492
H	1.64753	1.89409	-0.96086
H	-0.16570	1.06754	-0.22247
H	-4.31315	-0.38689	1.51759
H	-2.67306	-2.96686	-1.13672
H	-3.02544	1.16891	-1.27590
H	4.37638	-0.09665	1.11181
H	-0.03520	-0.70733	-1.67255
H	-0.04915	-2.00914	-0.96615
H	-2.63382	-3.18196	0.63875
H	-4.12860	-2.57412	-0.15616
H	-2.99600	0.81251	1.75342
H	-2.82134	-0.83195	2.42315
H	-4.36602	-0.03029	-1.24766
H	-2.93220	-0.28436	-2.30599
H	3.18209	1.20594	0.79641
H	2.92244	0.06866	2.16051
H	2.40836	-3.40577	-0.07717
H	3.95668	-2.74657	0.55621
H	2.49820	-2.81200	1.60785
H	2.97187	0.22493	-2.03606
H	4.26640	-0.92365	-1.53570
H	2.76581	-1.52797	-2.32355
H	0.45768	4.10845	1.95521
H	0.33604	2.30836	1.85850
H	1.80551	3.14211	1.25803

(iii) M = Rh, L = PCy$_3$

TS2$_{Rh}$

BP86 Energy = -1738.84934137
Enthalpy 0K= -1737.727034
Enthalpy 298K= -1737.671022
Free Energy 298K= -1737.818821
Nimag=1 (-115.0044cm-1)
SCF PCM(DCM) = -1738.89469874
D3 Correction = -0.219818850

C	2.22533	-1.75655	2.56656
C	2.87720	-0.54695	1.85789
C	2.61593	0.75282	2.65550
C	3.09809	0.63054	4.11643
C	2.45799	-0.57871	4.82093
C	2.70750	-1.87450	4.02907
P	2.34193	-0.35161	0.04336
C	3.53027	0.98720	-0.62900
C	4.97928	0.99328	-0.08330
C	5.75233	2.22634	-0.60422
C	5.74284	2.30511	-2.14124
C	4.30504	2.27002	-2.68928
C	3.53414	1.03624	-2.17533
Rh	-0.00100	0.02684	-0.19090
P	-2.37936	-0.23643	-0.12073
C	-3.35907	1.18290	-0.94583
C	-4.87137	1.28523	-0.63785
C	-5.46508	2.57427	-1.24962
C	-5.21739	2.64715	-2.76735
C	-3.72092	2.49836	-3.09735
C	-3.12381	1.21845	-2.47463
C	-3.03322	-0.28027	1.66151
C	-2.42794	-1.43907	2.48813
C	-3.02249	-1.47826	3.91185
C	-2.82883	-0.13692	4.64196
C	-3.40241	1.03098	3.81931
C	-2.81541	1.06583	2.39139
C	-3.07241	-1.81733	-0.96162
C	-4.42932	-2.31288	-0.39956
C	-4.99355	-3.46918	-1.25437
C	-3.99645	-4.63657	-1.35247
C	-2.63549	-4.15398	-1.88481
C	-2.06750	-2.98997	-1.04430
C	2.78129	-2.03730	-0.72564
C	2.19094	-2.23413	-2.14264
C	2.36847	-3.69432	-2.61140
C	3.84535	-4.12948	-2.55949
C	4.44178	-3.91338	-1.15667
C	4.26934	-2.45188	-0.68578
B	0.12645	2.77233	-0.98603
N	0.15107	4.17095	-0.13682
C	-1.13199	4.36696	0.61392
C	0.32023	5.30135	-1.11305
C	1.29168	4.19399	0.83579
H	0.33931	6.26394	-0.57524
H	1.26103	5.15599	-1.66171
H	-0.51746	5.28198	-1.82383
H	-1.10887	5.32249	1.16444
H	-1.96331	4.37064	-0.10494
H	-1.26297	3.53224	1.31715
H	-0.83327	2.82964	-1.72361
H	-0.02213	-1.51065	-0.00383
H	-0.05520	-0.00664	1.32062
H	1.19259	2.68628	-1.55469
H	-0.02925	1.88901	-0.07881
H	-4.12352	-0.45299	1.57106
H	-1.33089	-1.29989	2.55124
H	-2.58699	-2.40902	1.98522
H	-4.10400	-1.71003	3.84957
H	-2.55992	-2.30167	4.48476
H	-3.29999	-0.16989	5.64008
H	-1.74650	0.03288	4.81171
H	-3.21002	1.99423	4.32564
H	-4.50337	0.92766	3.75387
H	-1.72572	1.26673	2.44549
H	-3.26777	1.89892	1.82313
H	-3.24677	-1.46906	-1.99965
H	-4.28955	-2.67556	0.63643
H	-5.16629	-1.49393	-0.35016
H	-5.95188	-3.81052	-0.82380
H	-5.22265	-3.09270	-2.27094
H	-4.40092	-5.43454	-1.99986
H	-3.85954	-5.08570	-0.34882
H	-2.75250	-3.81641	-2.93399
H	-1.90868	-4.98577	-1.90344
H	-1.11329	-2.64252	-1.47781
H	-1.83127	-3.35274	-0.02458
H	-2.85746	2.07621	-0.52227
H	-5.39762	0.41520	-1.07328
H	-5.06588	1.26393	0.44897
H	-6.54644	2.62527	-1.03001
H	-5.00496	3.45473	-0.75708
H	-5.60917	3.59561	-3.17569
H	-5.78259	1.83549	-3.26638
H	-3.16688	3.37671	-2.70933
H	-3.56397	2.48863	-4.19077
H	-2.04538	1.15486	-2.70228
H	-3.60532	0.33974	-2.94627
H	2.21871	-2.72098	-0.05668
H	1.11823	-1.96045	-2.14263
H	2.69241	-1.56015	-2.86097
H	1.76791	-4.35938	-1.95942
H	1.96700	-3.80945	-3.63418
H	3.94307	-5.18806	-2.85830
H	4.42549	-3.54096	-3.29762
H	5.51287	-4.18296	-1.14464
H	3.94032	-4.58819	-0.43496
H	4.68938	-2.33264	0.32910
H	4.85440	-1.79119	-1.35344
H	3.03046	1.91378	-0.28014
H	4.99283	0.99690	1.02028
H	5.50545	0.07534	-0.40262
H	5.29068	3.14444	-0.18733
H	6.78855	2.19984	-0.22242
H	6.31058	1.44799	-2.55392

H	6.26429	3.21712	-2.48202
H	4.30937	2.27301	-3.79395
H	3.76648	3.18709	-2.37556
H	4.02241	0.12492	-2.56948
H	2.50133	1.04463	-2.56573
H	3.97103	-0.72042	1.82426
H	1.52582	0.95814	2.64398
H	3.10688	1.61586	2.16924
H	4.20040	0.52063	4.12669
H	2.87307	1.56408	4.66327
H	1.36618	-0.41105	4.91481
H	2.84887	-0.67525	5.84914
H	2.20456	-2.72957	4.51492
H	3.79110	-2.10464	4.03648
H	2.45100	-2.69546	2.03134
H	1.12408	-1.63962	2.54795
H	0.21104	-0.08996	-3.76805
H	0.14419	0.61999	-3.52869
H	1.29742	5.14542	1.39384
H	1.18189	3.35023	1.53175
H	2.23224	4.08452	0.27786

Int2$_{Rh}$

BP86 Energy = -1738.87059730
Enthalpy 0K= -1737.743059
Enthalpy 298K= -1737.688973
Free Energy 298K= -1737.831720
Nimag=0 (11.1727cm-1)
SCF PCM(DCM) = -1738.91303421
D3 Correction = -0.222173790

C	2.24745	-1.53503	2.63825
C	2.86684	-0.36315	1.84262
C	2.56776	0.98235	2.54275
C	3.04951	0.98004	4.00953
C	2.44009	-0.19035	4.80098
C	2.72789	-1.53268	4.10613
P	2.34318	-0.33201	0.01402
C	3.46820	1.00515	-0.75779
C	4.91807	1.11278	-0.22412
C	5.63092	2.34381	-0.82856
C	5.61414	2.31817	-2.36712
C	4.17779	2.18269	-2.90308
C	3.46313	0.95306	-2.30395
Rh	-0.00610	0.00123	-0.30400
P	-2.38011	-0.28857	-0.13609
C	-3.38178	1.13240	-0.93552
C	-4.88187	1.23891	-0.56944
C	-5.49440	2.53222	-1.15265
C	-5.30929	2.60753	-2.67869
C	-3.82809	2.45470	-3.06824
C	-3.20861	1.17182	-2.47274
C	-3.00011	-0.35224	1.65503
C	-2.38526	-1.52264	2.45722
C	-2.95338	-1.57527	3.89178
C	-2.74324	-0.24286	4.63308
C	-3.33169	0.93393	3.83439
C	-2.76930	0.98446	2.39689
C	-3.06238	-1.87048	-0.97867
C	-4.42526	-2.36106	-0.42591
C	-4.98926	-3.51406	-1.28529
C	-3.99742	-4.68617	-1.37760
C	-2.62996	-4.20910	-1.89774
C	-2.06287	-3.04896	-1.05085
C	2.87778	-2.05912	-0.59851
C	2.36020	-2.43505	-2.00741
C	2.65032	-3.92010	-2.31864
C	4.14578	-4.25509	-2.17434
C	4.66929	-3.85986	-0.78222
C	4.38752	-2.37251	-0.47400
B	0.06451	2.80253	-1.05910
N	0.05441	4.17541	-0.16518
C	-1.20811	4.29325	0.63391
C	0.13886	5.33763	-1.11464
C	1.22614	4.22564	0.76761
H	0.13621	6.28539	-0.55068
H	1.06444	5.24855	-1.70002
H	-0.72226	5.30042	-1.79603
H	-1.20705	5.23274	1.21196
H	-2.06361	4.28192	-0.05602
H	-1.27845	3.43371	1.31552
H	-0.91228	2.84781	-1.77367
H	-0.00637	-1.53179	-0.09897
H	-0.04899	0.00444	1.25211
H	1.12010	2.78017	-1.65327
H	-0.02805	1.87378	-0.18260
H	-4.09171	-0.52253	1.57440
H	-1.28732	-1.38831	2.49894
H	-2.56246	-2.48617	1.94813
H	-4.03642	-1.80417	3.84818
H	-2.48143	-2.40596	4.44620
H	-3.19486	-0.28654	5.63983
H	-1.65762	-0.07585	4.78299
H	-3.12941	1.89164	4.34730
H	-4.43373	0.83142	3.78822
H	-1.67882	1.18144	2.43415
H	-3.23119	1.82430	1.84634
H	-3.22546	-1.52279	-2.01918
H	-4.29229	-2.72520	0.61050
H	-5.15953	-1.53980	-0.37946
H	-5.95200	-3.85076	-0.86106
H	-5.20999	-3.13559	-2.30297
H	-4.40058	-5.48071	-2.02997
H	-3.87093	-5.13801	-0.37384
H	-2.73611	-3.86951	-2.94744
H	-1.90663	-5.04395	-1.91120
H	-1.10296	-2.70873	-1.47595
H	-1.84042	-3.41403	-0.02909
H	-2.86278	2.02380	-0.53019
H	-5.42828	0.37333	-0.98811
H	-5.03529	1.21411	0.52354
H	-6.56542	2.58649	-0.88787
H	-5.01082	3.40963	-0.67736

H	-5.71362	3.55829	-3.06903
H	-5.89744	1.79899	-3.15579
H	-3.25562	3.33014	-2.70166
H	-3.71428	2.44564	-4.16694
H	-2.14024	1.11403	-2.74667
H	-3.70978	0.29480	-2.92660
H	2.33355	-2.70930	0.11709
H	1.27527	-2.24463	-2.07587
H	2.84823	-1.80326	-2.77281
H	2.06473	-4.55448	-1.62369
H	2.29558	-4.16014	-3.33695
H	4.31751	-5.33034	-2.35803
H	4.71988	-3.70926	-2.94908
H	5.75390	-4.05394	-0.70454
H	4.18176	-4.48911	-0.01150
H	4.76827	-2.12121	0.53186
H	4.95052	-1.74879	-1.19406
H	2.92984	1.92997	-0.46786
H	4.93517	1.18715	0.87687
H	5.48635	0.20288	-0.48811
H	5.12796	3.26537	-0.47143
H	6.66803	2.39033	-0.45116
H	6.21948	1.46172	-2.72409
H	6.09244	3.22772	-2.77170
H	4.17878	2.11123	-4.00540
H	3.59912	3.09293	-2.64808
H	3.98470	0.03783	-2.64268
H	2.42843	0.89775	-2.68818
H	3.96541	-0.50593	1.82246
H	1.47285	1.15394	2.51434
H	3.03947	1.81943	1.99615
H	4.15432	0.90092	4.02926
H	2.79799	1.94508	4.48567
H	1.34379	-0.04644	4.88048
H	2.83029	-0.20021	5.83394
H	2.24661	-2.36379	4.65175
H	3.81736	-1.73167	4.13222
H	2.50124	-2.50455	2.17534
H	1.14406	-1.44764	2.60883
H	-0.37393	-0.08142	-2.07492
H	0.45740	-0.04606	-2.05472
H	1.21291	5.16460	1.34639
H	1.17474	3.36417	1.44792
H	2.15020	4.16674	0.17542

TS3$_{Rh}$

BP86 Energy = -1738.84776531
Enthalpy 0K= -1737.723593
Enthalpy 298K= -1737.669854
Free Energy 298K= -1737.812148
Nimag=1 (-564.6493cm-1)
SCF PCM(DCM) = -1738.89018391
D3 Correction = -0.220393260

Rh	0.00863	-0.00527	-0.04173
C	-0.20020	-5.29880	-0.97710
C	1.30074	-4.29362	0.66493
H	-0.16615	-6.24726	-0.41572
H	-1.16974	-5.19322	-1.48294
H	0.60236	-5.27469	-1.72724
H	1.32101	-5.23689	1.23612
H	2.10100	-4.29675	-0.08844
H	1.44245	-3.44165	1.34380
H	0.87845	-2.81762	-1.69012
H	0.02836	1.09969	1.06819
H	0.03971	-0.30945	1.55961
P	2.39720	0.28979	-0.08976
P	-2.38042	0.31336	0.02903
B	-0.06583	-2.77894	-0.93772
H	-1.14855	-2.75087	-1.46833
H	0.07968	-1.83745	-0.05615
N	-0.01636	-4.14151	-0.03389
C	3.25317	0.13662	1.59897
C	2.95697	1.98518	-0.78855
C	-3.10728	0.25512	1.78780
C	-2.81851	2.08914	-0.53105
C	3.26357	-1.00820	-1.19147
C	-3.41272	-0.97149	-0.92780
H	4.32529	0.31768	1.38565
C	2.77831	1.19856	2.61812
H	1.69637	1.05961	2.80586
H	2.90072	2.21728	2.21157
C	3.54753	1.07626	3.95168
H	4.61617	1.31204	3.77951
H	3.17217	1.83196	4.66447
C	3.42662	-0.33687	4.54903
H	4.02030	-0.41482	5.47681
H	2.37208	-0.52439	4.83409
C	3.87644	-1.40447	3.53580
H	3.73700	-2.41867	3.95196
H	4.96137	-1.29327	3.34168
C	3.11036	-1.27949	2.20067
H	2.03332	-1.47722	2.37503
H	3.47223	-2.04515	1.49054
H	2.90607	1.80718	-1.88206
C	4.41667	2.37049	-0.43174
H	4.48885	2.56862	0.65477
H	5.11506	1.54598	-0.64819
C	4.85956	3.63847	-1.19475
H	5.89708	3.89182	-0.91267
H	4.87328	3.42316	-2.28143
C	3.91762	4.82192	-0.91727
H	4.22318	5.70415	-1.50691
H	3.99934	5.11282	0.14870
C	2.45904	4.44657	-1.23296
H	2.35268	4.27499	-2.32261
H	1.77981	5.28005	-0.97930
C	2.01514	3.17385	-0.47976
H	0.97580	2.92578	-0.75722
H	2.00602	3.37598	0.60880
H	2.79127	-1.94501	-0.83415
C	4.79723	-1.16240	-1.05102
H	5.30017	-0.25425	-1.43122

H	5.09952	-1.27625	0.00487
C	5.29655	-2.37244	-1.87225
H	6.39213	-2.46440	-1.76533
H	4.86242	-3.30217	-1.45188
C	4.90467	-2.24697	-3.35544
H	5.23585	-3.13831	-3.91727
H	5.43729	-1.38261	-3.79889
C	3.38694	-2.04557	-3.51449
H	2.85641	-2.96224	-3.18868
H	3.12464	-1.89414	-4.57678
C	2.87364	-0.85157	-2.68078
H	1.77805	-0.75979	-2.78280
H	3.31761	0.07968	-3.08406
H	-2.18147	2.67713	0.16285
C	-2.37595	2.46352	-1.96596
H	-1.33586	2.14737	-2.15647
H	-3.00568	1.92867	-2.70036
C	-2.52120	3.98272	-2.20079
H	-1.83013	4.52286	-1.52316
H	-2.20721	4.22873	-3.23094
C	-3.96291	4.45948	-1.94754
H	-4.03413	5.55454	-2.07110
H	-4.63267	4.01405	-2.70945
C	-4.44474	4.04722	-0.54556
H	-5.50088	4.33493	-0.39729
H	-3.86070	4.59382	0.22141
C	-4.28734	2.52799	-0.30925
H	-4.63870	2.27665	0.70618
H	-4.94242	1.98565	-1.01673
H	-2.97694	-1.91847	-0.54819
C	-4.93421	-1.00256	-0.64353
H	-5.14204	-1.05239	0.43947
H	-5.40299	-0.07249	-1.01416
C	-5.59157	-2.21184	-1.34674
H	-5.19977	-3.14696	-0.89790
H	-6.67869	-2.20499	-1.15084
C	-5.31312	-2.21652	-2.86042
H	-5.81156	-1.34295	-3.32497
H	-5.75626	-3.11333	-3.32863
C	-3.80213	-2.14953	-3.14775
H	-3.61533	-2.09789	-4.23525
H	-3.31535	-3.07887	-2.78977
C	-3.14577	-0.93922	-2.45110
H	-3.57236	-0.01283	-2.87834
H	-2.06041	-0.91931	-2.65199
H	-4.19329	0.42129	1.64565
C	-2.91944	-1.12798	2.45036
H	-1.83314	-1.31869	2.55967
H	-3.32619	-1.92896	1.80620
C	-3.59160	-1.18353	3.83929
H	-4.68792	-1.08275	3.71602
H	-3.41967	-2.17451	4.29716
C	-3.07630	-0.06432	4.76150
H	-2.00345	-0.23591	4.98077
H	-3.60265	-0.09411	5.73176
C	-3.24612	1.31580	4.10211
H	-2.82688	2.10844	4.74708
H	-4.32554	1.53983	3.99292
C	-2.57309	1.37291	2.71281
H	-2.73827	2.36925	2.26666
H	-1.47918	1.25316	2.83284
H	-0.01274	1.33811	-0.82830
H	-0.02730	0.02766	-1.66719
C	-1.11557	-4.16548	0.98457
H	-0.98874	-3.31048	1.66286
H	-2.07937	-4.07561	0.46415
H	-1.08478	-5.10888	1.55500

(iv) M = Ir, L = PCy_3

$TS2_{Ir}$

BP86 Energy = -1732.69832392
Enthalpy 0K= -1731.575209
Enthalpy 298K= -1731.519249
Free Energy 298K= -1731.666966
Nimag=1 (-116.7137cm-1)
SCF PCM(DCM) = -1732.74601665
D3 Correction = -0.2247850

C	2.25976	-1.73540	2.58876
C	2.91110	-0.53328	1.86603
C	2.67031	0.77138	2.66232
C	3.17394	0.65068	4.11610
C	2.53544	-0.55103	4.83487
C	2.76277	-1.85168	4.04423
P	2.35401	-0.34615	0.05688
C	3.53115	0.98971	-0.63659
C	4.98664	1.00069	-0.10830
C	5.75153	2.23268	-0.64342
C	5.72393	2.30502	-2.18055
C	4.27996	2.26386	-2.71184
C	3.51842	1.03055	-2.18325
Ir	-0.00168	-0.00085	-0.13988
P	-2.38768	-0.22930	-0.10161
C	-3.35655	1.19559	-0.92797
C	-4.86909	1.30719	-0.62412
C	-5.45269	2.60141	-1.23453
C	-5.20042	2.67647	-2.75140
C	-3.70422	2.51740	-3.07808
C	-3.11854	1.23177	-2.45640
C	-3.05414	-0.28021	1.67596
C	-2.45472	-1.44447	2.49998
C	-3.05874	-1.49081	3.91944
C	-2.87084	-0.15330	4.65806
C	-3.44016	1.01858	3.83812
C	-2.84257	1.06205	2.41495
C	-3.08530	-1.80127	-0.95609
C	-4.44618	-2.29281	-0.40014
C	-5.01780	-3.43665	-1.26662
C	-4.02870	-4.60995	-1.37492
C	-2.66389	-4.13139	-1.90084
C	-2.08827	-2.97970	-1.04867
C	2.78946	-2.03301	-0.70999

C	2.18317	-2.23616	-2.11931
C	2.35373	-3.69900	-2.58208
C	3.83111	-4.13438	-2.54538
C	4.44510	-3.91023	-1.15129
C	4.27809	-2.44625	-0.68622
B	0.13197	2.75081	-0.99918
N	0.15468	4.13558	-0.12655
C	-1.13116	4.32551	0.62127
C	0.32998	5.27741	-1.08891
C	1.29130	4.14512	0.85111
H	0.34826	6.23301	-0.53887
H	1.27304	5.13741	-1.63506
H	-0.50482	5.26845	-1.80329
H	-1.10651	5.27315	1.18505
H	-1.95935	4.34270	-0.10098
H	-1.26836	3.48167	1.31231
H	-0.82732	2.81682	-1.73387
H	-0.02284	-1.56689	0.06162
H	-0.05520	0.06922	1.39652
H	1.20051	2.66864	-1.55969
H	-0.03610	1.85874	-0.08625
H	-4.14376	-0.45204	1.57694
H	-1.35792	-1.30859	2.56915
H	-2.61323	-2.41116	1.99063
H	-4.13978	-1.72246	3.84866
H	-2.59993	-2.31707	4.49128
H	-3.34852	-0.19211	5.65288
H	-1.78984	0.01657	4.83598
H	-3.25283	1.97925	4.35118
H	-4.54046	0.91410	3.76393
H	-1.75380	1.26408	2.47887
H	-3.29139	1.89806	1.84808
H	-3.25693	-1.44422	-1.99152
H	-4.30997	-2.66672	0.63233
H	-5.17786	-1.46954	-0.34325
H	-5.97900	-3.77540	-0.84045
H	-5.24301	-3.04867	-2.27974
H	-4.43793	-5.39881	-2.03045
H	-3.89618	-5.06966	-0.37548
H	-2.77744	-3.78287	-2.94683
H	-1.94278	-4.96793	-1.92693
H	-1.13172	-2.63444	-1.47789
H	-1.85496	-3.35380	-0.03245
H	-2.85114	2.08554	-0.50203
H	-5.39980	0.44168	-1.06315
H	-5.06740	1.28457	0.46196
H	-6.53428	2.65925	-1.01788
H	-4.98818	3.47767	-0.73854
H	-5.58422	3.62879	-3.15833
H	-5.77018	1.87023	-3.25398
H	-3.14481	3.39116	-2.68726
H	-3.54468	2.50870	-4.17113
H	-2.04031	1.15844	-2.68203
H	-3.60721	0.35828	-2.93019
H	2.23595	-2.71522	-0.03220
H	1.11064	-1.96075	-2.10813
H	2.67722	-1.56670	-2.84686
H	1.76063	-4.35998	-1.91925
H	1.94022	-3.81962	-3.59940
H	3.92487	-5.19476	-2.83907
H	4.40230	-3.55050	-3.29410
H	5.51626	-4.17975	-1.15143
H	3.95289	-4.58103	-0.41957
H	4.71081	-2.32165	0.32269
H	4.85477	-1.78912	-1.36460
H	3.03462	1.91755	-0.28657
H	5.01381	1.00866	0.99495
H	5.51060	0.08239	-0.43019
H	5.29329	3.15180	-0.22497
H	6.79224	2.20960	-0.27382
H	6.28903	1.44759	-2.59619
H	6.23903	3.21687	-2.53123
H	4.27162	2.26175	-3.81648
H	3.74279	3.18118	-2.39635
H	4.00593	0.11882	-2.57725
H	2.48153	1.03271	-2.56277
H	4.00325	-0.71441	1.81895
H	1.58185	0.98447	2.66747
H	3.15961	1.62949	2.16590
H	4.27539	0.53224	4.10959
H	2.96471	1.58794	4.66282
H	1.44656	-0.37454	4.94512
H	2.94144	-0.64673	5.85729
H	2.26046	-2.70086	4.54092
H	3.84454	-2.09034	4.03640
H	2.47058	-2.67789	2.05379
H	1.15943	-1.61027	2.58454
H	0.17835	-0.12638	-3.79602
H	0.12948	0.57108	-3.51854
H	1.29343	5.08843	1.42262
H	1.17949	3.29119	1.53412
H	2.23438	4.04490	0.29573

Int2$_{Ir}$

BP86 Energy = -1732.72536749
Enthalpy 0K= -1731.596759
Enthalpy 298K= -1731.542849
Free Energy 298K= -1731.685306
Nimag=0 (11.6247cm-1)
SCF PCM(DCM) = -1732.76800489
D3 Correction = -0.2267680

Ir	-0.00579	-0.02165	-0.27476
C	0.14053	5.31470	-1.05181
C	-1.21033	4.24813	0.68081
H	0.13766	6.25392	-0.47391
H	1.06728	5.23345	-1.63648
H	-0.71956	5.28835	-1.73501
H	-1.20612	5.17802	1.27399
H	-2.06494	4.25178	-0.01027
H	-1.28472	3.37792	1.34825
H	-0.91389	2.83731	-1.74764
H	-0.00254	-1.58995	-0.11183

H	-0.04622	0.00891	1.31783
P	-2.39369	-0.28174	-0.11244
P	2.35929	-0.32592	0.03016
B	0.06377	2.78323	-1.03771
H	1.12089	2.76664	-1.62573
H	-0.03548	1.84321	-0.15488
N	0.05322	4.13926	-0.11832
C	-3.01139	-0.36002	1.67789
C	-3.08944	-1.84971	-0.97066
C	2.88724	-0.36875	1.85675
C	2.90149	-2.04553	-0.59571
C	-3.38605	1.15088	-0.89959
C	3.47332	1.02128	-0.73567
H	-4.10336	-0.52600	1.59400
C	-2.40159	-1.54220	2.46740
H	-1.30348	-1.41328	2.51085
H	-2.58329	-2.49887	1.94703
C	-2.97246	-1.60887	3.90027
H	-4.05609	-1.83429	3.85240
H	-2.50372	-2.44692	4.44626
C	-2.76026	-0.28544	4.65686
H	-3.21346	-0.33952	5.66241
H	-1.67455	-0.12243	4.81018
C	-3.34522	0.90152	3.87074
H	-3.14252	1.85290	4.39512
H	-4.44732	0.80125	3.82100
C	-2.77911	0.96774	2.43534
H	-1.68876	1.16202	2.47758
H	-3.23905	1.81442	1.89356
H	-3.25516	-1.48812	-2.00597
C	-4.45443	-2.33286	-0.41625
H	-4.31897	-2.71342	0.61391
H	-5.17973	-1.50474	-0.35321
C	-5.03687	-3.46728	-1.28792
H	-6.00108	-3.79843	-0.86265
H	-5.25886	-3.07239	-2.29907
C	-4.05917	-4.64930	-1.40171
H	-4.47504	-5.43025	-2.06247
H	-3.93242	-5.11611	-0.40486
C	-2.68954	-4.18016	-1.92285
H	-2.79775	-3.82534	-2.96731
H	-1.97546	-5.02257	-1.95188
C	-2.10365	-3.03811	-1.06416
H	-1.14351	-2.70310	-1.49129
H	-1.87884	-3.41924	-0.04888
H	-2.86001	2.03540	-0.48857
C	-4.88458	1.26632	-0.52984
H	-5.43881	0.40901	-0.95514
H	-5.03668	1.23323	0.56309
C	-5.48770	2.56937	-1.10092
H	-6.55772	2.63027	-0.83365
H	-4.99617	3.43883	-0.61914
C	-5.30495	2.65616	-2.62665
H	-5.70195	3.61360	-3.00807
H	-5.90094	1.85676	-3.10936
C	-3.82593	2.49376	-3.02071
H	-3.24534	3.36158	-2.64859
H	-3.71456	2.49273	-4.11970
C	-3.21658	1.20068	-2.43705
H	-2.14958	1.13376	-2.71387
H	-3.72796	0.33238	-2.89612
H	2.35365	-2.70307	0.11025
C	2.39850	-2.41388	-2.01213
H	1.31458	-2.22375	-2.09098
H	2.89517	-1.77859	-2.76900
C	2.69337	-3.89718	-2.32744
H	2.10246	-4.53549	-1.64067
H	2.34762	-4.13275	-3.34989
C	4.18794	-4.23084	-2.17209
H	4.36292	-5.30509	-2.35862
H	4.76767	-3.68102	-2.93981
C	4.69938	-3.84039	-0.77417
H	5.78383	-4.03208	-0.68873
H	4.20736	-4.47414	-0.01003
C	4.41128	-2.35526	-0.46136
H	4.78488	-2.10817	0.54814
H	4.97776	-1.72679	-1.17459
H	2.93163	1.94084	-0.43583
C	4.92458	1.13253	-0.20670
H	4.94601	1.19661	0.89484
H	5.49715	0.22855	-0.48155
C	5.62781	2.37318	-0.80250
H	5.12085	3.28841	-0.43475
H	6.66612	2.42256	-0.42883
C	5.60514	2.36190	-2.34118
H	6.21475	1.51292	-2.70850
H	6.07582	3.27837	-2.73902
C	4.16769	2.22165	-2.87304
H	4.16500	2.16010	-3.97594
H	3.58409	3.12595	-2.60799
C	3.46375	0.98193	-2.28222
H	3.99170	0.07369	-2.62955
H	2.42831	0.92117	-2.66345
H	3.98583	-0.51016	1.82977
C	2.59274	0.96992	2.57184
H	1.49806	1.14159	2.55410
H	3.06130	1.81214	2.03040
C	3.08605	0.95276	4.03476
H	4.19094	0.87280	4.04523
H	2.83877	1.91320	4.52226
C	2.48189	-0.22506	4.81914
H	1.38625	-0.08177	4.90779
H	2.87946	-0.24491	5.84916
C	2.76472	-1.56059	4.10931
H	2.28745	-2.39693	4.65042
H	3.85441	-1.75955	4.12585
C	2.27372	-1.54920	2.64505
H	2.52621	-2.51365	2.17100
H	1.17043	-1.46294	2.62301
H	-0.39502	-0.10834	-2.01696
H	0.47556	-0.05174	-1.99549
C	1.22358	4.17534	0.81712
H	1.17182	3.30323	1.48354
H	2.14875	4.12711	0.22573

H 1.20800 5.10506 1.41038

$TS3_{Ir}$

BP86 Energy = -1732.71485140
Enthalpy 0K= -1731.588736
Enthalpy 298K= -1731.535162
Free Energy 298K= -1731.677100
Nimag=1 (-309.6754cm-1)
SCF PCM(DCM) = -1732.75777522
D3 Correction = -0.2250520

Ir	0.00499	0.01509	0.01855
C	-0.29462	-5.28375	-0.94903
C	1.24419	-4.26661	0.65283
H	-0.27648	-6.21596	-0.36073
H	-1.26638	-5.17117	-1.44912
H	0.50205	-5.29940	-1.70573
H	1.24657	-5.19238	1.25193
H	2.03687	-4.31186	-0.10711
H	1.41211	-3.39820	1.30442
H	0.84030	-2.83898	-1.73236
H	0.04166	0.92986	1.33352
H	0.02513	-0.52748	1.58370
P	2.40567	0.26271	-0.07764
P	-2.39136	0.32443	0.04152
B	-0.10414	-2.77749	-0.98495
H	-1.18972	-2.72083	-1.50072
H	0.09134	-1.80523	-0.12808
N	-0.07650	-4.10484	-0.03864
C	3.28716	0.10453	1.59755
C	3.00428	1.93997	-0.79653
C	-3.15093	0.32185	1.78817
C	-2.80742	2.08396	-0.57723
C	3.24050	-1.05090	-1.18665
C	-3.42913	-0.96911	-0.89815
H	4.35694	0.27891	1.36957
C	2.83371	1.17329	2.61974
H	1.75566	1.03719	2.83120
H	2.94769	2.18960	2.20446
C	3.62842	1.05675	3.93859
H	4.69403	1.28848	3.74372
H	3.26954	1.81716	4.65484
C	3.51502	-0.35298	4.54568
H	4.12693	-0.42801	5.46178
H	2.46580	-0.53512	4.85315
C	3.94050	-1.42833	3.52997
H	3.80523	-2.43942	3.95497
H	5.02180	-1.32276	3.31388
C	3.14924	-1.30789	2.20907
H	2.07554	-1.50190	2.40604
H	3.49505	-2.07896	1.49663
H	2.96262	1.74497	-1.88721
C	4.46913	2.29607	-0.42885
H	4.53228	2.51675	0.65385
H	5.14945	1.45004	-0.61727
C	4.95576	3.53522	-1.21188
H	5.99691	3.76510	-0.92310
H	4.97491	3.29832	-2.29398
C	4.04403	4.74894	-0.96722
H	4.37927	5.61133	-1.56995
H	4.12244	5.05763	0.09399
C	2.57987	4.40600	-1.29237
H	2.48101	4.21701	-2.37977
H	1.91968	5.26124	-1.06202
C	2.09193	3.15913	-0.52238
H	1.05202	2.93642	-0.81768
H	2.07150	3.38143	0.56212
H	2.76560	-1.98156	-0.81738
C	4.77444	-1.22149	-1.06857
H	5.28106	-0.32199	-1.46413
H	5.09262	-1.33041	-0.01681
C	5.24891	-2.44239	-1.88826
H	6.34463	-2.54679	-1.79510
H	4.80953	-3.36452	-1.45657
C	4.83923	-2.32079	-3.36688
H	5.15200	-3.21926	-3.92797
H	5.37653	-1.46556	-3.82217
C	3.32218	-2.10131	-3.50686
H	2.78550	-3.01084	-3.17092
H	3.04772	-1.95140	-4.56631
C	2.83353	-0.89756	-2.67219
H	1.73880	-0.78969	-2.76178
H	3.28543	0.02544	-3.08537
H	-2.21171	2.68966	0.13807
C	-2.28497	2.43058	-1.99277
H	-1.23733	2.10890	-2.11428
H	-2.87297	1.88200	-2.75103
C	-2.41960	3.94462	-2.26273
H	-1.76823	4.49964	-1.55811
H	-2.04975	4.17336	-3.27827
C	-3.87405	4.42194	-2.09871
H	-3.94116	5.51430	-2.24648
H	-4.49931	3.96009	-2.88822
C	-4.43374	4.03501	-0.71813
H	-5.49691	4.32312	-0.63523
H	-3.89456	4.59771	0.06974
C	-4.28667	2.52109	-0.44346
H	-4.69204	2.28712	0.55634
H	-4.90060	1.96306	-1.17552
H	-2.98252	-1.91454	-0.52826
C	-4.94610	-1.01182	-0.59068
H	-5.13733	-1.07031	0.49476
H	-5.42694	-0.08257	-0.94732
C	-5.60686	-2.22169	-1.28973
H	-5.20244	-3.15644	-0.85109
H	-6.69077	-2.22280	-1.07677
C	-5.35236	-2.21920	-2.80763
H	-5.86378	-1.34734	-3.26107
H	-5.79685	-3.11728	-3.27212
C	-3.84669	-2.14034	-3.11800
H	-3.67693	-2.08271	-4.20798
H	-3.34805	-3.06813	-2.77207
C	-3.18961	-0.92792	-2.42603

H	-3.63555	-0.00409	-2.83905
H	-2.10890	-0.89261	-2.64777
H	-4.23289	0.49198	1.62244
C	-2.98547	-1.04346	2.49306
H	-1.90338	-1.24023	2.62840
H	-3.38599	-1.85948	1.86380
C	-3.68247	-1.05639	3.87075
H	-4.77568	-0.95136	3.72553
H	-3.52567	-2.03544	4.35868
C	-3.17476	0.08446	4.77027
H	-2.10687	-0.08788	5.01216
H	-3.71715	0.08499	5.73213
C	-3.32444	1.44675	4.07036
H	-2.91206	2.25458	4.70074
H	-4.40037	1.67355	3.93566
C	-2.62760	1.46236	2.69175
H	-2.78091	2.44643	2.21531
H	-1.53608	1.34373	2.83563
H	-0.00700	1.54535	-0.37842
H	-0.02819	0.09525	-1.62950
C	-1.16712	-4.07527	0.98979
H	-1.01917	-3.20030	1.63774
H	-2.13414	-3.98648	0.47525
H	-1.14622	-4.99995	1.59014

(c) M-H/B-H exchange at $[ML_2(H)_2(\eta^2-H_3B{\cdot}NMe_3)]^+$

(i) M = Rh, L = PMe_3

$TS4'_{Rh}$

BP86 Energy = -565.503196644
Enthalpy 0K= -565.116687
Enthalpy 298K= -565.090654
Free Energy 298K= -565.171828
Nimag=1 (-752.8587cm-1)
SCF PCM(DCM) = -565.555443466
D3 Correction = -0.061276840

C	3.48675	-0.32966	-1.25147
P	2.29887	-1.02209	0.01158
Rh	-0.02756	-0.45291	-0.05321
P	-2.27765	-1.03909	0.01754
C	-2.52201	-2.84217	-0.36788
C	3.16643	-0.69470	1.62709
C	2.53967	-2.85533	-0.21253
B	-0.65134	1.53012	0.53857
N	-0.00065	2.92710	0.01674
C	-0.36184	3.95168	1.06589
C	-0.60172	3.34761	-1.29653
C	-3.14772	-0.83083	1.64554
C	-3.41916	-0.20980	-1.19823
H	0.07259	0.56620	-1.35437
H	4.48202	-0.79091	-1.14106
H	3.10254	-0.53659	-2.26259
H	3.58732	0.75968	-1.12738
H	3.61040	-3.11517	-0.17165
H	1.99503	-3.38489	0.58329
H	2.12548	-3.16276	-1.18508
H	4.19837	-1.08161	1.60109
H	3.19102	0.38763	1.82790
H	2.60625	-1.18781	2.43601
H	-0.05760	-1.58805	1.14708
H	-1.69296	3.40993	-1.18360
H	-0.19727	4.32825	-1.59411
H	-0.35386	2.59498	-2.05928
C	1.49303	2.88521	-0.11540
H	0.06712	3.64229	2.02975
H	0.04303	4.93397	0.77277
H	-1.45577	4.00591	1.15239
H	-0.04852	1.13187	1.53706
H	-0.05391	-0.53986	-1.62723
H	-1.84282	1.73870	0.57127
H	-4.44164	-0.61116	-1.10761
H	-3.43669	0.87364	-1.00691
H	-3.04860	-0.38689	-2.22009
H	-4.19985	-1.14895	1.56638
H	-2.63047	-1.44036	2.40198
H	-3.10522	0.22509	1.95268
H	-3.59499	-3.09588	-0.36347
H	-2.09674	-3.06555	-1.35828
H	-1.99299	-3.44360	0.38630
H	1.86947	3.87869	-0.40825
H	1.92552	2.59006	0.85118
H	1.75637	2.13956	-0.87733

$Int4'_{Rh}$

BP86 Energy = -565.519270615
Enthalpy 0K= -565.128403
Enthalpy 298K= -565.102416
Free Energy 298K= -565.183039
Nimag=0 (22.2634cm-1)
SCF PCM(DCM) =
D3 Correction =

C	3.51452	-0.55045	-1.16141
P	2.20444	-1.08733	0.05588
Rh	-0.06635	-0.52699	-0.22477
P	-2.38312	-0.77257	0.05942
C	-2.91019	-2.43011	-0.61416
C	2.99229	-0.73030	1.69995
C	2.31759	-2.94623	-0.06303
B	-0.04834	1.37244	0.87721
N	0.27790	2.75942	0.03196
C	0.28121	3.85474	1.06872
C	-0.76995	3.08996	-0.98852
C	-2.98645	-0.81720	1.81482
C	-3.57952	0.39898	-0.75748
H	0.37613	0.04758	-1.84674
H	4.47477	-1.04345	-0.93721
H	3.19923	-0.82199	-2.18131
H	3.65646	0.53987	-1.11247

H	3.36062	-3.27646	0.07320
H	1.68513	-3.39943	0.71534
H	1.96082	-3.28034	-1.05000
H	4.00956	-1.15159	1.74084
H	3.03546	0.35671	1.86455
H	2.37121	-1.17234	2.49371
H	-0.08415	-1.08193	1.24678
H	-1.74378	3.15008	-0.48335
H	-0.53983	4.05539	-1.46873
H	-0.80121	2.29823	-1.74882
C	1.62163	2.73718	-0.63020
H	1.06294	3.64123	1.81032
H	0.47450	4.82514	0.58134
H	-0.69661	3.87221	1.56961
H	0.84688	1.28201	1.69074
H	-0.47609	0.08697	-1.83974
H	-1.17207	1.54414	1.31054
H	-4.61792	0.07871	-0.57250
H	-3.43960	1.40922	-0.34389
H	-3.39474	0.42431	-1.84278
H	-4.07829	-0.96156	1.84928
H	-2.48525	-1.64326	2.34180
H	-2.72024	0.12839	2.31099
H	-3.98526	-2.59358	-0.43262
H	-2.71537	-2.47305	-1.69711
H	-2.33487	-3.22693	-0.11782
H	1.83443	3.71564	-1.09206
H	2.38248	2.51245	0.13087
H	1.63000	1.95299	-1.39939

(ii) M = Ir, L = PMe_3

TS4'$_{Ir}$

BP86 Energy = -559.362092864
Enthalpy 0K= -558.974057
Enthalpy 298K= -558.948199
Free Energy 298K= -559.028949
Nimag=1 (-587.3868cm-1)
SCF PCM(DCM) = -559.414745703
D3 Correction = -0.065114830

C	3.44551	-0.47996	-1.29960
P	2.25667	-1.02775	0.02777
Ir	-0.06364	-0.46332	-0.05913
P	-2.39330	-0.71720	0.03353
C	-2.85411	-2.46473	-0.40508
C	3.15267	-0.63565	1.60988
C	2.39864	-2.88280	-0.07503
B	-0.39959	1.58646	0.66380
N	0.27606	2.92849	0.02064
C	0.07123	4.00999	1.05287
C	-0.41619	3.34120	-1.24817
C	-3.18923	-0.46893	1.69087
C	-3.43795	0.29613	-1.12389
H	0.09538	0.58016	-1.35011
H	4.41522	-0.99061	-1.18178
H	3.02329	-0.72691	-2.28613
H	3.61172	0.60662	-1.24711
H	3.45582	-3.19089	-0.02236
H	1.83799	-3.33223	0.75808
H	1.96508	-3.23434	-1.02404
H	4.16919	-1.06139	1.59804
H	3.21796	0.45479	1.74602
H	2.58148	-1.05870	2.45008
H	-0.14819	-1.39122	1.33813
H	-1.48289	3.49557	-1.03481
H	0.02932	4.27365	-1.63056
H	-0.30298	2.54069	-1.99380
C	1.74468	2.79502	-0.24412
H	0.58669	3.72140	1.97974
H	0.48009	4.96103	0.67425
H	-1.00431	4.11507	1.25154
H	0.22098	1.28479	1.67524
H	-0.18791	-0.63637	-1.63835
H	-1.57479	1.87214	0.75597
H	-4.50218	0.02810	-1.02444
H	-3.31083	1.36367	-0.88949
H	-3.11095	0.11403	-2.15947
H	-4.27475	-0.64770	1.62917
H	-2.73471	-1.17151	2.40560
H	-3.00289	0.55844	2.03738
H	-3.94728	-2.59769	-0.35420
H	-2.50576	-2.69444	-1.42373
H	-2.36584	-3.15327	0.30095
H	2.15211	3.75704	-0.59552
H	2.24547	2.49574	0.68767
H	1.89212	2.02074	-1.00845

Int4'$_{Ir}$

BP86 Energy = -559.370142525
Enthalpy 0K= -558.979221
Enthalpy 298K= -558.953274
Free Energy 298K= -559.034353
Nimag=0 (18.2951cm-1)
SCF PCM(DCM) = -559.425032655
D3 Correction = -0.066674130

C	3.56737	0.38710	-0.79084
P	2.37226	-0.73537	0.08900
Ir	0.04010	-0.46272	-0.16732
P	-2.25581	-0.97124	0.08741
C	-2.44193	-2.81426	-0.11898
C	2.98544	-0.71962	1.83934
C	2.85865	-2.42381	-0.52954
B	0.02447	1.46102	0.89902
N	-0.20921	2.86987	0.04057
C	-0.21491	3.96404	1.07681
C	-1.52091	2.90361	-0.68106
C	-3.00608	-0.65141	1.75400
C	-3.53506	-0.31313	-1.09691
H	0.47559	0.16071	-1.75016
H	4.60422	0.05690	-0.61591

H	3.35959	0.37542	-1.87219
H	3.45148	1.41362	-0.41215
H	3.93324	-2.59974	-0.35778
H	2.27638	-3.19033	0.00474
H	2.64598	-2.50166	-1.60707
H	4.07492	-0.88016	1.87263
H	2.73584	0.24922	2.29766
H	2.47422	-1.51579	2.40136
H	0.05605	-1.05876	1.32703
H	-2.32367	2.71192	0.04533
H	-1.67247	3.88992	-1.15058
H	-1.52913	2.12132	-1.45238
C	0.89541	3.15573	-0.93061
H	0.73874	3.94117	1.62207
H	-0.34644	4.94187	0.58376
H	-1.03730	3.78222	1.78206
H	1.12649	1.61272	1.39760
H	-0.42710	0.14626	-1.74642
H	-0.91487	1.42650	1.67079
H	-4.51677	-0.77320	-0.89830
H	-3.62575	0.77799	-0.98796
H	-3.22961	-0.54450	-2.12951
H	-4.04812	-1.00776	1.78408
H	-2.40917	-1.17457	2.51629
H	-2.97323	0.42646	1.97208
H	-3.49472	-3.11050	0.01931
H	-2.11296	-3.11188	-1.12692
H	-1.81641	-3.32843	0.62644
H	0.72275	4.12381	-1.42956
H	1.84527	3.18848	-0.37913
H	0.93668	2.35527	-1.68167

(iii) M = Rh, L = PCy_3

$TS4_{Rh}$

BP86 Energy = -1737.63882678
Enthalpy 0K= -1736.531789
Enthalpy 298K= -1736.479011
Free Energy 298K= -1736.619255
Nimag=1 (-559.3130cm-1)
SCF PCM(DCM) = -1737.68137763
D3 Correction = -0.22185070

B	-0.17952	-2.57425	0.25184
C	-1.81412	-3.96647	-1.28124
C	-0.23462	-5.09196	0.18837
C	0.56191	-3.99361	-1.83888
C	-2.47838	2.24627	-0.13788
C	-2.08612	3.00463	1.14968
C	-2.28690	4.52817	0.98785
C	-1.51389	5.08394	-0.22021
C	-1.89180	4.32780	-1.50522
C	-1.69271	2.80508	-1.34756
C	-3.14635	-0.07055	1.65286
C	-2.12120	-0.03672	2.81338
C	-2.80947	-0.24829	4.17792
C	-3.60459	-1.56515	4.20922
C	-4.60544	-1.62970	3.04251
C	-3.91658	-1.41315	1.67610
C	-3.54092	-0.31118	-1.31761
C	-4.95087	0.32448	-1.25955
C	-5.93081	-0.44161	-2.17693
C	-5.41818	-0.50088	-3.62765
C	-3.99112	-1.07706	-3.69691
C	-3.02272	-0.30490	-2.77434
C	2.69750	1.70016	-0.81106
C	4.17665	2.13532	-0.70161
C	4.37875	3.53489	-1.32412
C	3.88970	3.58251	-2.78327
C	2.42274	3.12536	-2.89734
C	2.21422	1.72564	-2.28159
C	2.62414	0.47609	1.92970
C	2.01449	1.79139	2.45907
C	2.40427	2.02874	3.93571
C	2.00702	0.84115	4.82998
C	2.60436	-0.47378	4.29856
C	2.21559	-0.71759	2.82520
C	3.46502	-1.29122	-0.32640
C	4.84804	-1.23846	0.37002
C	5.67853	-2.49993	0.03972
C	5.83679	-2.70882	-1.47581
C	4.46416	-2.74476	-2.17069
C	3.64106	-1.47855	-1.85075
H	-3.56090	2.41071	-0.30839
H	0.03897	0.87633	0.63643
H	0.85141	-1.08286	-1.46587
H	-3.88160	0.74732	1.80348
H	-3.63113	-1.37378	-1.01113
H	2.08166	2.44322	-0.26298
H	3.72651	0.58246	1.95860
H	2.92655	-2.18092	0.06143
H	-1.55944	0.91212	2.81570
H	-1.37640	-0.83690	2.64194
H	-2.05089	-0.23402	4.98115
H	-3.49352	0.59997	4.37944
H	2.34373	2.65295	1.85147
H	-2.90063	-2.41785	4.13579
H	-4.13225	-1.67565	5.17299
H	2.27376	-1.32882	4.91502
H	-5.38131	-0.85089	3.18091
H	-5.13572	-2.59900	3.03695
H	-3.20545	-2.24128	1.49058
H	-4.67862	-1.45383	0.87952
H	-5.34259	0.35234	-0.22704
H	-4.89292	1.37464	-1.60438
H	-6.06295	-1.47088	-1.78777
H	-6.92569	0.03637	-2.13772
H	-5.41624	0.52126	-4.05472
H	-6.10482	-1.09860	-4.25267
H	-4.01363	-2.14379	-3.39323
H	-3.61550	-1.05501	-4.73560
H	-2.94476	0.73667	-3.13880
H	-2.00358	-0.73006	-2.82537

H	-1.10058	-2.58731	1.03937
H	-0.84592	-1.55515	-1.14919
H	0.94004	-2.73925	0.68984
H	-1.96607	-3.11390	-1.95867
H	-2.53555	-3.90867	-0.45394
H	-1.95312	-4.90909	-1.83642
H	4.51372	2.13978	0.35062
H	4.81592	1.40902	-1.23868
H	3.82181	4.28151	-0.72400
H	5.44480	3.81709	-1.26242
H	4.52681	2.92155	-3.40374
H	4.00634	4.60157	-3.19230
H	2.10044	3.11904	-3.95397
H	1.77116	3.85317	-2.37354
H	2.77581	0.98245	-2.87671
H	1.14950	1.42808	-2.33202
H	0.91120	1.74063	2.37490
H	-0.41232	-6.02185	-0.37679
H	-0.94283	-5.01832	1.02556
H	0.79103	-5.07838	0.58131
H	3.49874	2.18711	4.00117
H	1.93269	2.96126	4.29382
H	2.33256	1.01935	5.87005
H	0.90234	0.75640	4.85605
H	3.70853	-0.43534	4.38375
H	2.67488	-1.65609	2.46530
H	1.12069	-0.85888	2.74443
H	5.40325	-0.34121	0.03944
H	4.73926	-1.16108	1.46471
H	6.66685	-2.42418	0.52685
H	5.17977	-3.38540	0.48203
H	6.39651	-3.63859	-1.67992
H	6.43797	-1.88121	-1.90100
H	3.90867	-3.64237	-1.82998
H	4.58201	-2.84509	-3.26452
H	2.65673	-1.52350	-2.35451
H	4.17108	-0.60264	-2.27015
H	1.57669	-3.93863	-1.42016
H	0.40620	-3.14648	-2.52084
H	0.43062	-4.94482	-2.38126
H	-2.67866	2.65192	2.01114
H	-1.02185	2.79996	1.38234
H	-3.36695	4.73899	0.86004
H	-1.97788	5.03864	1.91745
H	-0.42546	4.97785	-0.03919
H	-1.70796	6.16474	-0.33698
H	-1.29648	4.69103	-2.36202
H	-2.95213	4.53221	-1.75299
H	-1.98492	2.29318	-2.27999
H	-0.61667	2.58712	-1.19530
Rh	-0.04306	-0.42697	-0.34754
N	-0.42661	-3.90220	-0.71564
P	-2.30795	0.34976	-0.01765
P	2.23135	0.10677	0.10694

Int4$_{Rh}$

BP86 Energy = -1737.65390279
Enthalpy 0K= -1736.544052
Enthalpy 298K= -1736.491167
Free Energy 298K= -1736.629981
Nimag=0 (13.1420cm-1)
SCF PCM(DCM) = -1737.69700573
D3 Correction = -0.224785110

B	-0.07487	-2.39907	-0.12849
C	-1.75424	-3.08444	-2.05899
C	-0.43809	-4.76970	-0.89906
C	0.63085	-3.30331	-2.51259
C	-2.41443	2.11424	0.32545
C	-2.31349	2.53468	1.80879
C	-2.39661	4.07015	1.95467
C	-1.30784	4.78027	1.13118
C	-1.36786	4.35250	-0.34545
C	-1.30734	2.81771	-0.49896
C	-3.29369	-0.57993	1.45328
C	-2.40232	-0.75381	2.70650
C	-3.22662	-1.27277	3.90490
C	-3.93600	-2.59748	3.57407
C	-4.78893	-2.46278	2.30058
C	-3.95943	-1.93637	1.10818
C	-3.65643	0.05935	-1.43790
C	-5.07709	0.57769	-1.09970
C	-6.06900	0.24738	-2.23804
C	-5.59476	0.81421	-3.58769
C	-4.16712	0.34200	-3.91912
C	-3.18363	0.67199	-2.77501
C	2.78632	1.77997	-0.34020
C	4.26514	2.13960	-0.06099
C	4.51222	3.65165	-0.25751
C	4.09391	4.11406	-1.66456
C	2.62936	3.74085	-1.95837
C	2.37330	2.23031	-1.76346
C	2.70562	-0.11900	1.95493
C	2.05773	0.99906	2.80331
C	2.46901	0.88513	4.28842
C	2.14461	-0.50208	4.86959
C	2.78085	-1.61613	4.02020
C	2.35773	-1.50805	2.53993
C	3.49297	-1.24091	-0.71073
C	4.88639	-1.39596	-0.05169
C	5.68497	-2.53708	-0.72190
C	5.82064	-2.33122	-2.24057
C	4.44070	-2.15261	-2.89857
C	3.64651	-1.00880	-2.23188
H	-3.39942	2.45487	-0.05026
H	-0.13247	-0.23917	1.18836
H	0.47874	-0.27725	-2.06150
H	-4.10036	0.14258	1.69668
H	-3.72723	-1.03707	-1.58208
H	2.16064	2.36226	0.36830
H	3.80445	0.01581	1.99966
H	2.95030	-2.19796	-0.56850
H	-1.90577	0.19163	2.97664

H	-1.59804	-1.47438	2.46870
H	-2.56502	-1.39657	4.78087
H	-3.98073	-0.51167	4.18813
H	2.33975	1.99800	2.42602
H	-3.17613	-3.38960	3.42264
H	-4.56327	-2.92257	4.42282
H	2.50240	-2.61085	4.41190
H	-5.62819	-1.76469	2.49084
H	-5.24571	-3.43265	2.03307
H	-3.16572	-2.66969	0.86782
H	-4.61093	-1.85687	0.22105
H	-5.44606	0.15372	-0.15016
H	-5.04899	1.67595	-0.96390
H	-6.17805	-0.85265	-2.31639
H	-7.06828	0.64182	-1.98177
H	-5.61084	1.92111	-3.54505
H	-6.29140	0.52283	-4.39328
H	-4.17294	-0.75354	-4.08856
H	-3.81394	0.80324	-4.85868
H	-3.11315	1.77216	-2.67265
H	-2.16799	0.31668	-3.03454
H	-0.95875	-2.65064	0.66353
H	-0.38024	-0.22484	-2.12085
H	1.04577	-2.74921	0.18495
H	-1.75016	-2.06723	-2.47337
H	-2.52213	-3.15414	-1.27591
H	-1.96691	-3.81441	-2.85852
H	4.56143	1.84146	0.96005
H	4.91586	1.57870	-0.75850
H	3.93608	4.21540	0.50281
H	5.57744	3.87901	-0.07410
H	4.75093	3.63526	-2.41741
H	4.24040	5.20343	-1.77020
H	2.35287	4.03443	-2.98694
H	1.96483	4.31069	-1.27829
H	2.94999	1.66819	-2.52037
H	1.30754	2.00258	-1.94516
H	0.95563	0.92135	2.71799
H	-0.63314	-5.48475	-1.71645
H	-1.22456	-4.84376	-0.13586
H	0.53513	-4.98246	-0.43525
H	3.55708	1.07387	4.37759
H	1.96697	1.67878	4.87039
H	2.49028	-0.56914	5.91633
H	1.04560	-0.64244	4.89134
H	3.88455	-1.54878	4.09311
H	2.83188	-2.31516	1.95331
H	1.26581	-1.66421	2.45448
H	5.45503	-0.45257	-0.14515
H	4.79474	-1.60659	1.02682
H	6.68091	-2.61357	-0.25057
H	5.17244	-3.50005	-0.52574
H	6.35758	-3.18077	-2.69813
H	6.43537	-1.43050	-2.43567
H	3.87020	-3.09933	-2.80957
H	4.54730	-1.95147	-3.97969
H	2.65777	-0.89434	-2.71479
H	4.19102	-0.06139	-2.40446
H	1.60582	-3.53357	-2.06137
H	0.65850	-2.29128	-2.93661
H	0.40559	-4.03137	-3.31001
H	-3.11351	2.06581	2.40710
H	-1.34875	2.18510	2.22558
H	-3.39483	4.41377	1.61869
H	-2.31588	4.34287	3.02197
H	-0.31212	4.52560	1.54624
H	-1.41198	5.87612	1.21788
H	-0.54804	4.81762	-0.92204
H	-2.31170	4.71840	-0.79619
H	-1.37495	2.54667	-1.56686
H	-0.32031	2.45019	-0.13908
Rh	-0.05656	-0.23216	-0.38259
N	-0.41852	-3.36654	-1.44590
P	-2.37598	0.22786	-0.01872
P	2.27594	-0.00831	0.10344

(iv) M = Ir, L = PCy_3

$TS4_{Ir}$

BP86 Energy = -1731.49353862
Enthalpy 0K= -1730.386466
Enthalpy 298K= -1730.333327
Free Energy 298K= -1730.474795
Nimag=1 (-628.2872cm-1)
SCF PCM(DCM) = -1731.53679894
D3 Correction = -0.226112170

B	0.24521	-2.46582	-0.14775
C	-1.97452	-3.35647	-1.25463
C	-0.21584	-4.89481	-0.56435
C	0.09188	-3.50456	-2.54275
C	-2.45580	2.19154	0.43855
C	-1.96120	2.58678	1.84916
C	-2.10075	4.10735	2.08229
C	-1.36404	4.92156	1.00497
C	-1.84103	4.52562	-0.40297
C	-1.70893	3.00676	-0.64266
C	-3.39359	-0.37593	1.58052
C	-2.46583	-0.78891	2.74888
C	-3.27624	-1.18843	3.99966
C	-4.28025	-2.31232	3.69056
C	-5.19046	-1.92482	2.51287
C	-4.37664	-1.52668	1.26080
C	-3.59096	0.08575	-1.39355
C	-4.87849	0.94242	-1.31618
C	-5.87757	0.53346	-2.42100
C	-5.24170	0.63526	-3.81924
C	-3.93595	-0.17715	-3.89981
C	-2.94163	0.22767	-2.78934
C	2.62399	1.86824	0.00409
C	3.95578	2.38994	0.59929
C	3.97646	3.93522	0.61336
C	3.74383	4.52498	-0.78860

C	2.43995	3.98698	-1.40463
C	2.41625	2.44387	-1.41826
C	3.06179	-0.49938	1.77708
C	2.38757	0.22135	2.96762
C	3.13166	-0.07469	4.28798
C	3.22280	-1.58753	4.55581
C	3.85884	-2.32270	3.36266
C	3.11487	-2.02249	2.04248
C	3.43991	-0.92207	-1.14830
C	4.94874	-0.58975	-1.05834
C	5.77173	-1.54687	-1.94938
C	5.29208	-1.51382	-3.41153
C	3.78247	-1.80234	-3.50887
C	2.96141	-0.84663	-2.61612
H	-3.53539	2.43581	0.38281
H	0.00620	0.21188	1.44482
H	0.09856	0.29156	-1.62128
H	-4.00011	0.49408	1.90696
H	-3.89539	-0.97563	-1.28783
H	1.79880	2.25316	0.63862
H	4.10608	-0.13407	1.70529
H	3.31050	-1.97534	-0.82586
H	-1.76010	0.02067	2.99620
H	-1.84200	-1.64258	2.42002
H	-2.58464	-1.49523	4.80459
H	-3.82286	-0.30221	4.37880
H	2.33963	1.31236	2.80043
H	-3.72630	-3.23825	3.43651
H	-4.88703	-2.54638	4.58295
H	3.87009	-3.41318	3.54001
H	-5.83153	-1.07118	2.80874
H	-5.87473	-2.75378	2.25757
H	-3.81057	-2.41145	0.90910
H	-5.07401	-1.25085	0.45205
H	-5.35713	0.85953	-0.32340
H	-4.61670	2.00901	-1.45296
H	-6.21358	-0.50726	-2.24169
H	-6.77954	1.16777	-2.35844
H	-5.02337	1.69788	-4.04380
H	-5.95384	0.29327	-4.59068
H	-4.17106	-1.25626	-3.80029
H	-3.46127	-0.04971	-4.88924
H	-2.62597	1.27533	-2.95369
H	-2.02271	-0.38227	-2.85496
H	-0.30779	-2.56510	0.94018
H	-0.21129	-0.91556	-1.68193
H	1.41087	-2.77585	-0.24301
H	-2.17989	-2.36364	-1.67528
H	-2.40073	-3.41760	-0.24388
H	-2.41318	-4.13953	-1.89533
H	4.11162	2.01670	1.62528
H	4.80594	2.02349	-0.00440
H	3.18883	4.30095	1.30189
H	4.93901	4.28514	1.02710
H	4.59508	4.25594	-1.44479
H	3.72131	5.62812	-0.74288
H	2.30887	4.36909	-2.43300
H	1.57593	4.35794	-0.81766
H	3.22685	2.08471	-2.08036
H	1.46551	2.08065	-1.84998
H	1.34082	-0.12721	3.04671
H	-0.67485	-5.67588	-1.19287
H	-0.63875	-4.93086	0.44947
H	0.87126	-5.04486	-0.50993
H	4.15277	0.35283	4.23823
H	2.61971	0.43716	5.12247
H	3.79892	-1.78138	5.47785
H	2.20458	-1.98836	4.73078
H	4.91759	-2.01173	3.26181
H	3.61255	-2.55469	1.21248
H	2.08408	-2.41791	2.10185
H	5.11764	0.44867	-1.40091
H	5.31267	-0.64602	-0.01753
H	6.84218	-1.28178	-1.88716
H	5.68099	-2.57793	-1.55360
H	5.86195	-2.23839	-4.01958
H	5.49835	-0.51373	-3.84125
H	3.59324	-2.84904	-3.19326
H	3.44007	-1.72249	-4.55648
H	1.88661	-1.08729	-2.67951
H	3.07622	0.18454	-2.99790
H	1.17846	-3.65212	-2.47195
H	-0.11367	-2.52319	-2.99437
H	-0.35902	-4.29863	-3.16034
H	-2.52696	2.04905	2.62909
H	-0.90085	2.28895	1.96105
H	-3.17463	4.37998	2.07605
H	-1.72156	4.35957	3.08873
H	-0.27413	4.73607	1.08826
H	-1.51080	6.00336	1.17121
H	-1.27373	5.07310	-1.17698
H	-2.90181	4.82083	-0.52682
H	-2.08105	2.75725	-1.65146
H	-0.63763	2.71948	-0.62454
Ir	-0.05453	-0.28900	-0.14523
N	-0.49325	-3.53956	-1.16143
P	-2.39215	0.31183	0.08485
P	2.30707	-0.01910	0.09378

Int4$_{Ir}$

BP86 Energy = -1731.50478790
Enthalpy 0K= -1730.394489
Enthalpy 298K= -1730.341746
Free Energy 298K= -1730.480391
Nimag=0 (15.7720cm-1)
SCF PCM(DCM) = -1731.54822142
D3 Correction = -0.229233020

B	-0.07004	-2.38453	0.02777
C	-1.74965	-3.18186	-1.87044
C	-0.42757	-4.80138	-0.62963
C	0.63328	-3.41242	-2.31377
C	-2.43503	2.15681	0.27508

C	-2.34015	2.62909	1.74356
C	-2.42944	4.16828	1.83559
C	-1.34030	4.85311	0.99155
C	-1.39511	4.37524	-0.46975
C	-1.32986	2.83647	-0.57200
C	-3.31372	-0.49759	1.49103
C	-2.43882	-0.62101	2.76217
C	-3.28084	-1.09225	3.96782
C	-3.98399	-2.43032	3.68033
C	-4.81746	-2.34875	2.38957
C	-3.97031	-1.86876	1.18993
C	-3.63132	0.02156	-1.43360
C	-5.06139	0.54238	-1.14156
C	-6.03139	0.14976	-2.27901
C	-5.54044	0.65822	-3.64588
C	-4.10264	0.18720	-3.93176
C	-3.14193	0.58012	-2.78821
C	2.80328	1.77685	-0.41173
C	4.28892	2.13520	-0.17066
C	4.54582	3.63395	-0.44173
C	4.10917	4.03397	-1.86223
C	2.63711	3.66045	-2.11611
C	2.37181	2.16264	-1.84824
C	2.73531	0.00001	1.97963
C	2.11801	1.17308	2.77548
C	2.55016	1.13044	4.25844
C	2.21240	-0.21826	4.91731
C	2.81906	-1.38607	4.12003
C	2.37569	-1.35095	2.64215
C	3.48513	-1.26500	-0.63509
C	4.88015	-1.40263	0.02480
C	5.66680	-2.57804	-0.59845
C	5.79849	-2.43864	-2.12489
C	4.41709	-2.27943	-2.78461
C	3.63329	-1.10199	-2.16576
H	-3.42187	2.47658	-0.11402
H	-0.13300	-0.11352	1.28961
H	0.50124	-0.37551	-1.95683
H	-4.12534	0.23178	1.69486
H	-3.69041	-1.08077	-1.53076
H	2.19286	2.39771	0.27686
H	3.83661	0.11965	2.00244
H	2.93216	-2.20752	-0.44487
H	-1.94566	0.33412	3.00229
H	-1.63223	-1.35032	2.56338
H	-2.63200	-1.17982	4.85757
H	-4.03954	-0.32134	4.20930
H	2.41256	2.14527	2.34209
H	-3.22121	-3.22665	3.57264
H	-4.62391	-2.72161	4.53189
H	2.53130	-2.35391	4.56817
H	-5.66106	-1.64588	2.53858
H	-5.26792	-3.32974	2.15389
H	-3.16990	-2.60747	0.99330
H	-4.60757	-1.82800	0.28997
H	-5.44247	0.16037	-0.17910
H	-5.04415	1.64608	-1.05753
H	-6.12859	-0.95377	-2.30766
H	-7.03835	0.54546	-2.05722
H	-5.56880	1.76564	-3.65543
H	-6.22057	0.32176	-4.44798
H	-4.09376	-0.91483	-4.05130
H	-3.73828	0.60926	-4.88533
H	-3.08645	1.68445	-2.73360
H	-2.11846	0.22563	-3.01474
H	-0.95440	-2.61852	0.82950
H	-0.41789	-0.34230	-2.01521
H	1.04628	-2.74312	0.35864
H	-1.74852	-2.18619	-2.33423
H	-2.51823	-3.21578	-1.08564
H	-1.96037	-3.95036	-2.63375
H	4.59760	1.88350	0.85918
H	4.92467	1.53569	-0.84967
H	3.98662	4.23775	0.30024
H	5.61567	3.85974	-0.28558
H	4.75049	3.51497	-2.60185
H	4.26283	5.11592	-2.02071
H	2.34702	3.90868	-3.15281
H	1.98776	4.26687	-1.45318
H	2.93224	1.56148	-2.58716
H	1.30155	1.93369	-1.99985
H	1.01402	1.11183	2.70988
H	-0.62011	-5.55777	-1.40956
H	-1.21301	-4.84035	0.13728
H	0.54653	-4.98648	-0.15587
H	3.64240	1.30514	4.32165
H	2.07004	1.96232	4.80436
H	2.57232	-0.23507	5.96126
H	1.11179	-0.33930	4.96179
H	3.92462	-1.33250	4.17412
H	2.83007	-2.19453	2.09244
H	1.28102	-1.49603	2.57950
H	5.45658	-0.46908	-0.11117
H	4.79075	-1.56640	1.11154
H	6.66367	-2.64232	-0.12732
H	5.14700	-3.52727	-0.35943
H	6.32789	-3.31083	-2.54722
H	6.41851	-1.55140	-2.36078
H	3.84083	-3.21739	-2.65238
H	4.52019	-2.12605	-3.87384
H	2.64326	-1.00310	-2.64912
H	4.18325	-0.16690	-2.38247
H	1.60891	-3.62320	-1.85447
H	0.66088	-2.41949	-2.78150
H	0.40774	-4.17435	-3.07904
H	-3.14069	2.17836	2.35487
H	-1.37564	2.29746	2.17512
H	-3.42774	4.49628	1.48460
H	-2.35337	4.47794	2.89308
H	-0.34510	4.61587	1.41793
H	-1.44796	5.95096	1.04042
H	-0.57525	4.82288	-1.05990
H	-2.33894	4.72254	-0.93505
H	-1.39488	2.52919	-1.62975

H	-0.34141	2.48420	-0.19920
Ir	-0.05549	-0.22331	-0.31272
N	-0.41387	-3.42815	-1.24452
P	-2.38435	0.26098	0.00130
P	2.29138	0.01814	0.12979

(d) M-H/B-H exchange at $[ML_2(H)_2(\eta^2-H_3B{\cdot}NMe_3)]^+$: alternative higher energy pathways via $Int3_M$ (see Figures S-5 and S-6)

(i) M = Rh, L = PMe_3

TS to $Int3'_{Rh}$

BP86 Energy = -565.507321100
Enthalpy 0K= -565.118470
Enthalpy 298K= -565.093392
Free Energy 298K= -565.171120
Nimag=1 (-428.9171cm-1)
SCF PCM(DCM) = -565.559902622
D3 Correction = -0.062291890

C	-3.03116	-0.84104	1.51093
P	-2.00256	-1.34324	0.03386
C	-3.17032	-1.15328	-1.41389
C	-2.03022	-3.19839	0.24513
Rh	0.23625	-0.58106	-0.16900
B	0.24502	1.51930	-0.25481
N	-0.89823	2.65522	0.00072
C	-1.01191	2.92664	1.47700
H	0.58447	-2.23249	0.07260
C	-0.43086	3.91632	-0.68704
H	-3.98646	-1.39087	1.51762
H	-2.46244	-1.08557	2.42166
H	-3.24554	0.23828	1.51592
H	-3.06667	-3.55590	0.35739
H	-1.57482	-3.67552	-0.63623
H	-1.45016	-3.47383	1.13926
H	-4.12009	-1.67555	-1.21208
H	-3.37863	-0.09465	-1.62477
H	-2.69533	-1.59637	-2.30336
P	2.57787	-0.35438	0.04505
H	0.52594	-2.18117	-0.84001
H	-0.01555	3.17851	1.86684
H	-1.70541	3.76593	1.65076
H	-1.37582	2.01888	1.97726
H	-0.29939	3.70858	-1.75876
H	-1.18253	4.71064	-0.54820
H	0.53017	4.22622	-0.25612
H	0.11277	1.00000	-1.41192
H	0.11281	-0.02031	1.30718
H	1.27778	2.10504	-0.01589
C	3.45059	0.51610	-1.34924
C	3.21907	0.48374	1.57448
C	3.45114	-1.99881	0.09899
H	4.32103	0.49450	1.57568
H	2.84072	1.51564	1.61297
H	2.85356	-0.06335	2.45702
H	4.53678	0.54635	-1.16402
H	3.25418	-0.02477	-2.28808
H	3.06290	1.54119	-1.44267
H	4.53983	-1.85214	0.18678
H	3.09135	-2.57666	0.96427
H	3.23382	-2.56192	-0.82178
C	-2.24707	2.31036	-0.54948
H	-2.15171	2.11986	-1.62788
H	-2.61318	1.40828	-0.04765
H	-2.94842	3.14247	-0.37494

$Int3'_{Rh}$

BP86 Energy = -565.512155822
Enthalpy 0K= -565.122537
Enthalpy 298K= -565.096795
Free Energy 298K= -565.175839
Nimag=0 (29.2561cm-1)
SCF PCM(DCM) = -565.564498606
D3 Correction = -0.062186860

C	-2.93644	-0.86890	1.59329
P	-1.98658	-1.32948	0.05109
Rh	0.24479	-0.55198	-0.22760
P	2.57108	-0.32327	0.06337
C	3.44605	-1.96755	0.08944
C	-3.25679	-1.16623	-1.31309
C	-1.95106	-3.18768	0.24188
B	0.22553	1.48586	-0.21041
N	-0.93048	2.62496	-0.00063
C	-0.47679	3.88195	-0.70266
C	-1.03256	2.90003	1.47601
C	3.50692	0.61010	-1.24707
C	3.13631	0.45367	1.65368
H	0.64061	-2.36320	-0.67188
H	-3.87128	-1.44952	1.65576
H	-2.30477	-1.09614	2.46609
H	-3.18589	0.20279	1.61623
H	-2.96584	-3.57408	0.43080
H	-1.55638	-3.64675	-0.67758
H	-1.29379	-3.45620	1.08287
H	-4.17104	-1.72564	-1.05484
H	-3.51971	-0.11464	-1.49655
H	-2.82859	-1.58172	-2.23898
H	0.47806	-2.00747	-1.38886
H	-0.04011	3.18717	1.85149
H	-1.75048	3.71731	1.65480
H	-1.35936	1.98270	1.98484
C	-2.27998	2.26408	-0.53712
H	-0.35567	3.66627	-1.77431
H	-1.23070	4.67430	-0.56402
H	0.48706	4.20033	-0.28447
H	0.09981	0.94023	-1.40086
H	0.33554	-1.18549	1.20613
H	1.24500	2.11030	0.00020

H	4.23686	0.47531	1.70500
H	2.74528	1.47962	1.71865
H	2.73746	-0.13206	2.49601
H	4.58211	0.64163	-1.00666
H	3.36314	0.10813	-2.21656
H	3.11627	1.63611	-1.31785
H	4.52669	-1.82781	0.25471
H	3.03078	-2.58836	0.89822
H	3.29147	-2.48399	-0.87070
H	-2.98012	3.10164	-0.38538
H	-2.18818	2.04087	-1.60957
H	-2.64565	1.37808	-0.00739

TS5′$_{Rh}$

BP86 Energy = -565.496065011
Enthalpy 0K= -565.108579
Enthalpy 298K= -565.083408
Free Energy 298K= -565.160696
Nimag=1 (-130.2805cm-1)
SCF PCM(DCM) = -565.550176762
D3 Correction = -0.063549090

C	-2.98061	-0.65631	1.57891
P	-2.06611	-1.22372	0.05663
Rh	0.18770	-0.53883	-0.19122
P	2.52651	-0.43948	0.06304
C	3.35485	-2.03223	-0.42978
C	-3.31154	-0.99804	-1.31811
C	-2.13774	-3.07478	0.27324
B	0.20140	1.32936	0.38506
N	-0.74142	2.60551	0.01336
C	0.12432	3.53032	-0.81102
C	-1.10955	3.29531	1.30468
C	3.46652	0.82417	-0.92932
C	3.14655	-0.17591	1.79390
H	0.49432	-2.29059	-0.85126
H	-3.95193	-1.17065	1.66131
H	-2.36139	-0.88835	2.45876
H	-3.15653	0.43030	1.55252
H	-3.17793	-3.40438	0.42989
H	-1.73602	-3.56793	-0.62563
H	-1.52121	-3.35912	1.13884
H	-4.25719	-1.50614	-1.06719
H	-3.51581	0.06568	-1.50542
H	-2.89659	-1.43729	-2.23883
H	0.35873	-1.82920	-1.51635
H	-0.19164	3.56886	1.84276
H	-1.69974	4.19846	1.08221
H	-1.70397	2.60608	1.92242
C	-1.99190	2.32098	-0.76423
H	0.39319	3.01788	-1.74617
H	-0.43926	4.45089	-1.03333
H	1.03247	3.77678	-0.24348
H	0.03608	0.41510	-1.54635
H	0.28488	-1.36658	1.22277
H	1.07988	1.84535	1.05033

H	4.24758	-0.13317	1.81020
H	2.73746	0.76323	2.19576
H	2.79380	-1.00835	2.42110
H	4.55230	0.72062	-0.77051
H	3.23353	0.68677	-1.99644
H	3.15388	1.83495	-0.62483
H	4.44229	-1.96610	-0.26335
H	2.94258	-2.85646	0.17222
H	3.16280	-2.23454	-1.49486
H	-2.48153	3.27125	-1.03118
H	-1.72149	1.75244	-1.66375
H	-2.66836	1.72314	-0.14076

Int5′$_{Rh}$

BP86 Energy = -565.496481455
Enthalpy 0K= -565.108071
Enthalpy 298K= -565.082409
Free Energy 298K= -565.161636
Nimag=0 (22.3159cm-1)
SCF PCM(DCM) = -565.551215664
D3 Correction = -0.064351870

C	-3.10249	-0.37037	1.46350
P	-2.14865	-1.11267	0.04520
Rh	0.14425	-0.57681	-0.13980
P	2.49018	-0.52103	0.05100
C	3.25270	-2.14839	-0.43721
C	-3.28442	-0.89242	-1.41834
C	-2.35327	-2.93282	0.38893
B	0.16015	1.24747	0.56359
N	-0.57000	2.59774	0.01296
C	0.52824	3.36715	-0.68372
C	-1.06126	3.40209	1.19172
C	3.44159	0.68674	-0.99916
C	3.18253	-0.24754	1.75283
H	0.38155	-2.38216	-0.60210
H	-4.10805	-0.81667	1.52999
H	-2.54738	-0.56537	2.39367
H	-3.20747	0.71854	1.33661
H	-3.41905	-3.18345	0.51725
H	-1.94499	-3.51560	-0.45138
H	-1.79602	-3.18908	1.30232
H	-4.28503	-1.29980	-1.19897
H	-3.37729	0.16937	-1.68851
H	-2.85129	-1.42849	-2.27715
H	0.27795	-1.99982	-1.32487
H	-0.21724	3.61677	1.86112
H	-1.50876	4.34262	0.83286
H	-1.81762	2.81741	1.73584
C	-1.69927	2.40999	-0.95870
H	0.85926	2.78930	-1.55847
H	0.13577	4.34656	-1.00218
H	1.36518	3.51402	0.01444
H	0.04665	0.15375	-1.62532
H	0.20124	-1.21945	1.37740
H	0.85992	1.65648	1.46788

H	4.28424	-0.25577	1.72873
H	2.83199	0.71708	2.14934
H	2.81525	-1.04915	2.41101
H	4.52700	0.52339	-0.89840
H	3.14288	0.55750	-2.05077
H	3.20582	1.71589	-0.68701
H	4.34671	-2.10986	-0.30956
H	2.83936	-2.94809	0.19630
H	3.01683	-2.36497	-1.49051
H	-2.00527	3.39093	-1.35631
H	-1.35717	1.74201	-1.76078
H	-2.54594	1.95013	-0.43223

TS6'$_{Rh}$

BP86 Energy = -565.485849722
Enthalpy 0K= -565.099585
Enthalpy 298K= -565.074030
Free Energy 298K= -565.154342
Nimag=1 (-714.3545cm-1)
SCF PCM(DCM) = -565.540190513
D3 Correction = -0.06217300

C	-3.40834	0.90975	-0.73449
P	-2.50594	-0.53304	0.02360
Rh	-0.15854	-0.52894	-0.07413
P	2.05644	-1.31634	0.02464
C	2.18042	-3.08039	0.59487
C	-3.28991	-1.98288	-0.83095
C	-3.19737	-0.60951	1.74390
B	-0.12217	1.42482	0.55460
N	0.67817	2.73605	0.01104
C	1.40451	3.33367	1.19260
C	-0.36612	3.71183	-0.47514
C	2.98416	-1.35064	-1.58912
C	3.24741	-0.47215	1.18658
H	-0.45730	-2.11764	0.16311
H	-4.49944	0.76511	-0.67273
H	-3.13813	1.83288	-0.19814
H	-3.11400	1.00583	-1.79134
H	-4.29923	-0.62420	1.72478
H	-2.82050	-1.51991	2.23391
H	-2.84730	0.26501	2.31367
H	-4.38862	-1.93299	-0.75654
H	-2.98885	-1.98287	-1.88978
H	-2.92347	-2.90972	-0.36496
H	-1.05537	3.94342	0.34861
H	0.12835	4.63358	-0.82158
H	-0.91820	3.25430	-1.30960
C	1.66179	2.49698	-1.09807
H	2.13027	2.60039	1.57442
H	1.93338	4.24646	0.87483
H	0.67691	3.57312	1.97999
H	0.03422	0.21266	-1.50929
H	-0.14656	-0.56897	1.53913
H	-0.80993	1.89602	1.43840
H	4.21147	-1.00640	1.21066
H	3.42761	0.56641	0.86720
H	2.80845	-0.46333	2.19622
H	3.98835	-1.78453	-1.45415
H	2.41472	-1.96037	-2.30743
H	3.07778	-0.33207	-1.99589
H	3.23239	-3.40728	0.63952
H	1.71946	-3.16427	1.59074
H	1.61808	-3.71809	-0.10352
H	2.13939	3.44997	-1.37767
H	2.41909	1.78172	-0.75307
H	1.13229	2.06629	-1.95812
H	-0.24400	-1.07392	-1.61085

Int6'$_{Rh}$

BP86 Energy = -565.493883776
Enthalpy 0K= -565.104518
Enthalpy 298K= -565.078840
Free Energy 298K= -565.159671
Nimag=0 (21.9329cm-1)
SCF PCM(DCM) = -565.547621096
D3 Correction = -0.060873080

C	3.52883	0.33755	-0.43996
P	2.28425	-0.99334	-0.03562
Rh	0.00001	-0.48275	0.09606
P	-2.28420	-0.99343	-0.03563
C	-2.66097	-2.27835	-1.32193
C	2.98849	-1.72775	1.52203
C	2.66115	-2.27761	-1.32253
B	0.00031	1.40529	-0.70313
N	-0.00007	2.89995	-0.02051
C	-1.22659	3.61914	-0.52331
C	1.22677	3.61933	-0.52224
C	-2.98862	-1.72707	1.52230
C	-3.52870	0.33727	-0.44082
H	0.00004	-2.13441	0.33620
H	4.54484	-0.08418	-0.51670
H	3.25815	0.80632	-1.39898
H	3.52079	1.10082	0.35454
H	3.73447	-2.52817	-1.31997
H	2.06381	-3.17607	-1.10853
H	2.37315	-1.89254	-2.31267
H	4.04908	-1.99412	1.38239
H	2.90166	-1.00232	2.34620
H	2.40998	-2.62704	1.78148
H	1.20383	3.64603	-1.62034
H	1.24340	4.64509	-0.11930
H	2.12182	3.07677	-0.18477
C	-0.00072	2.93363	1.47959
H	-2.12184	3.07650	-0.18653
H	-1.24366	4.64493	-0.12047
H	-1.20275	3.64575	-1.62139
H	-0.00025	0.25992	1.71063
H	0.00003	-0.79522	-1.43186
H	0.00093	1.68500	-1.88681
H	-4.54470	-0.08448	-0.51755

H	-3.52081	1.10091	0.35334
H	-3.25782	0.80560	-1.40000
H	-4.04917	-1.99356	1.38265
H	-2.41010	-2.62620	1.78230
H	-2.90194	-1.00121	2.34612
H	-3.73432	-2.52880	-1.31945
H	-2.37274	-1.89383	-2.31222
H	-2.06376	-3.17675	-1.10734
H	-0.00103	3.97957	1.82764
H	-0.89618	2.41565	1.84921
H	0.89460	2.41594	1.84998
H	0.00004	-0.58340	1.86882

TS7′$_{Rh}$

BP86 Energy = -565.490044808
Enthalpy 0K= -565.101663
Enthalpy 298K= -565.076181
Free Energy 298K= -565.157017
Nimag=1 (-332.0793cm-1)
SCF PCM(DCM) = -565.543745623
D3 Correction = -0.06081725

C	3.50833	0.31235	-0.59235
P	2.28192	-0.98033	-0.04037
Rh	0.01378	-0.42059	0.13429
P	-2.22573	-1.08581	-0.04071
C	-2.46608	-2.48028	-1.24269
C	3.05527	-1.61705	1.52700
C	2.58808	-2.35198	-1.25357
B	-0.02025	1.44332	-0.70562
N	-0.08161	2.94161	-0.03220
C	-1.30425	3.63116	-0.58181
C	1.14765	3.68568	-0.48745
C	-2.97505	-1.74328	1.52982
C	-3.50839	0.14456	-0.60850
H	0.05152	-2.04085	0.58131
H	4.51796	-0.11951	-0.69311
H	3.18783	0.72156	-1.56301
H	3.54005	1.12527	0.15040
H	3.65842	-2.61393	-1.27933
H	1.99305	-3.22700	-0.95365
H	2.26212	-2.02986	-2.25430
H	4.10004	-1.92062	1.34892
H	3.03293	-0.83084	2.29816
H	2.47141	-2.47838	1.88424
H	1.16602	3.71130	-1.58568
H	1.12916	4.71179	-0.08524
H	2.03993	3.16078	-0.11568
C	-0.14047	2.97341	1.46663
H	-2.19806	3.06460	-0.28181
H	-1.36427	4.65517	-0.17834
H	-1.23798	3.66051	-1.67803
H	-0.41577	0.02551	1.82303
H	0.02263	-0.78123	-1.38048
H	0.00591	1.71703	-1.89166
H	-4.49738	-0.33333	-0.70654
H	-3.57892	0.96343	0.12506
H	-3.20439	0.55689	-1.58322
H	-4.00396	-2.09628	1.35060
H	-2.35376	-2.57364	1.89714
H	-2.99225	-0.94999	2.29385
H	-3.52395	-2.78857	-1.27114
H	-2.14910	-2.15334	-2.24473
H	-1.83531	-3.32600	-0.93195
H	-0.18466	4.01805	1.81558
H	-1.03328	2.42755	1.79996
H	0.75427	2.48081	1.87003
H	0.41862	0.04637	1.82366

(ii) M = Ir, L = PMe$_3$

TS to Int3′$_{Ir}$

BP86 Energy = -559.363698790
Enthalpy 0K= -558.974904
Enthalpy 298K= -558.949905
Free Energy 298K= -559.028193
Nimag=1 (-648.8338cm-1)
SCF PCM(DCM) = -559.416133277
D3 Correction = -0.064549440

C	-3.05577	-0.84568	1.53540
P	-2.02465	-1.29768	0.04635
C	-3.18631	-1.09453	-1.39993
C	-2.00570	-3.15392	0.21191
Ir	0.21258	-0.48556	-0.10478
B	0.15912	1.59673	-0.10946
N	-1.00528	2.73952	0.00264
C	-1.11004	3.08953	1.46465
H	0.59554	-2.13504	-0.10515
C	-0.57161	3.96507	-0.76406
H	-4.00812	-1.40040	1.52680
H	-2.48441	-1.11375	2.43777
H	-3.27311	0.23219	1.57394
H	-3.03049	-3.54413	0.32201
H	-1.54184	-3.59449	-0.68387
H	-1.40899	-3.43281	1.09366
H	-4.11668	-1.65921	-1.22535
H	-3.43494	-0.03813	-1.57295
H	-2.68677	-1.48630	-2.29975
P	2.56492	-0.20599	0.05516
H	0.46283	-1.80432	-1.14228
H	-0.11872	3.39707	1.82730
H	-1.82837	3.91510	1.59793
H	-1.43740	2.19884	2.01840
H	-0.44389	3.69528	-1.82263
H	-1.33843	4.75143	-0.66951
H	0.38586	4.32111	-0.36196
H	0.02290	0.91886	-1.29348
H	0.22990	-0.80894	1.46759
H	1.17433	2.25612	-0.01697
C	3.38981	0.71240	-1.33388
C	3.18574	0.63068	1.59117

C	3.46981	-1.82874	0.07330
H	4.28631	0.68442	1.58718
H	2.76642	1.64579	1.64776
H	2.84612	0.05724	2.46730
H	4.47841	0.76338	-1.17017
H	3.18438	0.18699	-2.27938
H	2.97977	1.73121	-1.39708
H	4.55598	-1.66501	0.16098
H	3.11984	-2.42954	0.92665
H	3.25718	-2.37582	-0.85806
C	-2.35014	2.33022	-0.50878
H	-2.26168	2.07267	-1.57384
H	-2.69067	1.45546	0.05528
H	-3.06713	3.15760	-0.38238

Int3′$_{Ir}$

BP86 Energy = -559.365554951
Enthalpy 0K= -558.975217
Enthalpy 298K= -558.949875
Free Energy 298K= -559.028508
Nimag=0 (29.8104cm-1)
SCF PCM(DCM) = -559.418058547
D3 Correction = -0.064777140

C	-2.97695	-0.84385	1.60497
P	-2.01463	-1.28460	0.06720
Ir	0.21836	-0.47456	-0.14316
P	2.56013	-0.18533	0.07866
C	3.47783	-1.80278	0.05378
C	-3.25640	-1.10514	-1.31725
C	-1.97398	-3.14320	0.22985
B	0.15069	1.56731	-0.10448
N	-1.02958	2.70178	0.00556
C	-0.59098	3.92611	-0.75966
C	-1.14969	3.05536	1.46453
C	3.43264	0.80099	-1.23337
C	3.11972	0.58133	1.67356
H	0.63070	-2.23465	-0.56915
H	-3.91265	-1.42430	1.65227
H	-2.35102	-1.08413	2.47834
H	-3.22323	0.22795	1.64184
H	-2.98979	-3.53901	0.39127
H	-1.55690	-3.58430	-0.68866
H	-1.33211	-3.42033	1.07974
H	-4.17070	-1.67583	-1.08617
H	-3.52467	-0.05367	-1.48994
H	-2.80481	-1.50350	-2.23943
H	0.46508	-1.82948	-1.31742
H	-0.16409	3.37254	1.83418
H	-1.87683	3.87429	1.59080
H	-1.47364	2.16382	2.01902
C	-2.36788	2.29058	-0.51950
H	-0.45874	3.65540	-1.81747
H	-1.35757	4.71316	-0.66880
H	0.36501	4.28156	-0.35353
H	0.06011	0.95503	-1.32822
H	0.33429	-1.21237	1.27615
H	1.15213	2.23892	0.04832
H	4.21950	0.63514	1.71474
H	2.69691	1.59314	1.75754
H	2.74627	-0.02932	2.50976
H	4.51234	0.85850	-1.02051
H	3.27632	0.31457	-2.20873
H	3.01147	1.81646	-1.27152
H	4.55810	-1.63697	0.19474
H	3.09861	-2.44794	0.86106
H	3.31199	-2.30555	-0.91172
H	-3.08163	3.12464	-0.42107
H	-2.26363	2.00983	-1.57716
H	-2.72542	1.43090	0.05690

TS5′$_{Ir}$

BP86 Energy = -559.361223404
Enthalpy 0K= -558.972672
Enthalpy 298K= -558.947582
Free Energy 298K= -559.026749
Nimag=1 (-586.3900cm-1)
SCF PCM(DCM) = -559.414881193
D3 Correction = -0.064110210

C	3.54481	0.27038	-0.24355
P	2.23908	-1.04430	-0.03202
Ir	-0.05007	-0.45098	0.04995
P	-2.40075	-0.71530	-0.03021
C	-2.99160	-1.48986	-1.60787
C	2.82799	-1.95774	1.47361
C	2.62794	-2.20415	-1.42633
B	-0.03427	1.47844	-0.70951
N	0.27542	2.93106	-0.01246
C	-0.94769	3.79348	-0.20160
C	1.42057	3.54305	-0.78200
C	-3.07039	-1.83666	1.28896
C	-3.49284	0.78537	0.12713
H	-0.16655	-2.12190	-0.00099
H	4.55023	-0.18122	-0.27371
H	3.36451	0.80676	-1.18864
H	3.50118	0.98015	0.59771
H	3.68856	-2.50253	-1.40348
H	1.98559	-3.09234	-1.33384
H	2.40077	-1.70670	-2.38133
H	3.87968	-2.26700	1.35993
H	2.72851	-1.30995	2.35845
H	2.19219	-2.84449	1.61555
H	1.15237	3.59625	-1.84622
H	1.62494	4.55375	-0.39304
H	2.31261	2.91333	-0.65557
C	0.62880	2.91389	1.44627
H	-1.78999	3.34322	0.34336
H	-0.75028	4.80257	0.19543
H	-1.18568	3.85105	-1.27283
H	-0.07287	-0.83254	1.67928
H	-0.06823	-0.69080	-1.55906

```
H  -0.29577  1.80705 -1.84814
H  -4.55777  0.50356  0.08354
H  -3.29281  1.28172  1.08988
H  -3.27062  1.48051 -0.69787
H  -4.15965 -1.96296  1.17709
H  -2.57019 -2.81335  1.21015
H  -2.84941 -1.40800  2.27872
H  -4.08313 -1.64021 -1.58533
H  -2.72127 -0.83823 -2.45262
H  -2.48287 -2.45690 -1.73550
H   0.84120  3.94113  1.78462
H  -0.21273  2.49752  2.01600
H   1.50890  2.27507  1.59486
H   0.03704  0.33883  1.51814
```

Int5′$_{Ir}$

```
BP86 Energy =  -559.362024505
Enthalpy 0K=  -558.972129
Enthalpy 298K=  -558.946630
Free Energy 298K=  -559.027694
Nimag=0 (17.3149cm-1)
SCF PCM(DCM) = -559.415918390
D3 Correction = -0.063783810

C   3.54320  0.48333 -0.25425
P   2.31509 -0.90163 -0.03611
Ir  0.00004 -0.43313  0.05242
P  -2.31497 -0.90197 -0.03611
C  -2.75554 -2.04511 -1.42882
C   2.96409 -1.77442  1.47064
C   2.75540 -2.04720 -1.42691
B  -0.00118  1.48243 -0.72396
N  -0.00030  2.96886 -0.01797
C  -1.22600  3.69621 -0.51005
C   1.22458  3.69574 -0.51282
C  -2.96309 -1.77763  1.46935
C  -3.54354  0.48307 -0.25107
H   0.00026 -2.11747  0.18316
H   4.57265  0.09142 -0.30157
H   3.31794  1.02040 -1.18886
H   3.46576  1.17849  0.59682
H   3.83003 -2.29065 -1.40653
H   2.15963 -2.96648 -1.32716
H   2.50115 -1.56653 -2.38380
H   4.03224 -2.01899  1.35153
H   2.83421 -1.13022  2.35445
H   2.38479 -2.69778  1.62015
H   1.20428  3.72743 -1.61094
H   1.23536  4.71991 -0.10560
H   2.12125  3.15618 -0.17543
C   0.00138  2.98435  1.48186
H  -2.12212  3.15683 -0.17088
H  -1.23566  4.72029 -0.10257
H  -1.20803  3.72815 -1.60820
H   0.00005 -0.60872  1.78712
H   0.00007 -0.73994 -1.51963
```

TS6′$_{Ir}$

```
BP86 Energy =  -559.356397386
Enthalpy 0K=  -558.967168
Enthalpy 298K=  -558.941837
Free Energy 298K=  -559.022899
Nimag=1 (-362.6594cm-1)
SCF PCM(DCM) = -559.410189652
D3 Correction = -0.063672650

C   3.52499  0.27436 -0.55826
P   2.26303 -1.00204 -0.05881
Ir -0.01140 -0.37877  0.10107
P  -2.31056 -0.90301 -0.05857
C  -2.63727 -2.23389 -1.30806
C   2.99087 -1.70364  1.49963
C   2.53327 -2.34574 -1.30800
B   0.02957  1.50512 -0.72582
N   0.07854  3.00452 -0.03786
C  -1.14531  3.74873 -0.50424
C   1.30466  3.70310 -0.56506
C  -3.06549 -1.57470  1.50022
C  -3.51880  0.42445 -0.55639
H  -0.04813 -2.02212  0.55890
H   4.52567 -0.17807 -0.65651
H   3.22711  0.71546 -1.52209
H   3.56396  1.06557  0.20711
H   3.59331 -2.64659 -1.32913
H   1.90247 -3.20615 -1.04082
H   2.23136 -1.98121 -2.30156
H   4.02811 -2.03553  1.32928
H   2.98018 -0.93733  2.29075
H   2.37410 -2.55478  1.82426
H   1.25641  3.73362 -1.66229
H   1.35156  4.72716 -0.15974
H   2.19751  3.14249 -0.25168
C   0.11643  3.02295  1.46094
H  -2.04161  3.22337 -0.14325
H  -1.13188  4.77462 -0.10107
H  -1.15205  3.77568 -1.60268
H  -0.43581  0.08915  1.76841
H  -0.02174 -0.78950 -1.43842
```

H	0.02082	1.79261	-1.90975
H	-4.53708	0.01299	-0.65385
H	-3.52494	1.21640	0.20910
H	-3.20420	0.85329	-1.52033
H	-4.11559	-1.86384	1.33075
H	-2.48376	-2.45042	1.82416
H	-3.02280	-0.80960	2.29142
H	-3.70892	-2.49037	-1.32850
H	-2.32127	-1.88192	-2.30176
H	-2.04257	-3.11980	-1.04153
H	0.15036	4.06431	1.82084
H	-0.78102	2.52175	1.84758
H	1.00721	2.47854	1.80225
H	0.43583	0.07031	1.76745

(iii) M = Rh, L = PCy_3

TS to $Int3_{Rh}$

BP86 Energy = -1737.63178020
Enthalpy 0K= -1736.524250
Enthalpy 298K= -1736.471770
Free Energy 298K= -1736.611756
Nimag=1 (-379.7953cm-1)
SCF PCM(DCM) = -1737.67489602
D3 Correction = -0.21674790

Rh	0.03068	-0.21061	-0.28711
C	0.30511	-4.44841	-1.90849
C	0.09957	-4.34064	0.52733
H	-0.15084	-5.45249	-1.90522
H	0.06680	-3.93294	-2.85000
H	1.39532	-4.52782	-1.80268
H	-0.34533	-5.34959	0.53331
H	1.19274	-4.41205	0.61073
H	-0.29219	-3.74784	1.36564
H	1.67564	-2.52449	-0.78173
H	-0.05064	1.45301	-0.75131
H	0.01796	1.40530	0.18370
P	2.39790	0.17852	-0.07577
P	-2.35886	0.12844	0.09513
B	0.51578	-2.19247	-0.79222
H	0.11766	-1.48266	-1.78144
H	0.05733	-0.94718	1.11519
N	-0.24477	-3.64141	-0.75909
C	3.39390	-0.63963	1.32884
C	2.72883	2.06825	0.10194
C	-2.99047	-0.32284	1.83723
C	-2.67488	2.03340	0.06210
C	3.29397	-0.31375	-1.69746
C	-3.64551	-0.66929	-1.07648
H	4.39740	-0.17618	1.23223
C	2.83613	-0.31489	2.73537
H	1.82289	-0.75421	2.82206
H	2.71707	0.77022	2.87825
C	3.75112	-0.87597	3.84651
H	4.72528	-0.34955	3.81047
H	3.31173	-0.64884	4.83437
C	3.98586	-2.38870	3.69443
H	4.69514	-2.74763	4.46100
H	3.03290	-2.92621	3.87246
C	4.49988	-2.72621	2.28374
H	4.60807	-3.81915	2.16069
H	5.51107	-2.29566	2.14428
C	3.55486	-2.17221	1.19560
H	2.55807	-2.63566	1.31347
H	3.91922	-2.45880	0.19429
H	2.28955	2.43785	-0.84800
C	4.22211	2.47814	0.12306
H	4.68292	2.14461	1.07318
H	4.78054	1.99001	-0.68982
C	4.37862	4.01102	-0.01025
H	5.45061	4.27429	0.03201
H	4.02045	4.31975	-1.01232
C	3.59205	4.77296	1.06949
H	3.66790	5.86198	0.90277
H	4.04414	4.57512	2.06136
C	2.11746	4.33179	1.09224
H	1.62208	4.64032	0.14992
H	1.57584	4.83472	1.91342
C	1.99867	2.80126	1.25487
H	0.93681	2.50541	1.32324
H	2.45679	2.52087	2.22090
H	2.84099	-1.30754	-1.88220
C	4.83007	-0.51294	-1.70419
H	5.34878	0.45304	-1.56980
H	5.15923	-1.16147	-0.87473
C	5.27681	-1.12020	-3.05381
H	6.37327	-1.25463	-3.05374
H	4.83669	-2.13180	-3.16168
C	4.84130	-0.24129	-4.24084
H	5.13775	-0.71092	-5.19547
H	5.37618	0.72767	-4.19012
C	3.32317	0.01698	-4.22080
H	2.78566	-0.93517	-4.40209
H	3.03613	0.70054	-5.03990
C	2.86220	0.60250	-2.86859
H	1.76424	0.73753	-2.86819
H	3.31057	1.60720	-2.74126
H	-1.80007	2.40484	0.63351
C	-2.58098	2.63071	-1.36238
H	-1.69022	2.24787	-1.89410
H	-3.46256	2.31049	-1.94997
C	-2.55024	4.17346	-1.31803
H	-1.62338	4.50271	-0.80723
H	-2.50103	4.57347	-2.34664
C	-3.77360	4.73878	-0.57462
H	-3.70807	5.83902	-0.50576
H	-4.68909	4.51565	-1.15746
C	-3.90230	4.12150	0.82904
H	-4.81258	4.49136	1.33378
H	-3.04541	4.44475	1.45318
C	-3.93563	2.57607	0.78022
H	-4.01204	2.18659	1.80926

H	-4.84832	2.25333	0.24937
H	-3.63361	-1.72792	-0.75087
C	-5.11048	-0.18934	-0.94501
H	-5.44466	-0.20847	0.10754
H	-5.18863	0.85883	-1.28774
C	-6.04614	-1.06318	-1.81043
H	-6.04165	-2.10013	-1.41895
H	-7.08468	-0.69919	-1.71594
C	-5.60886	-1.06890	-3.28656
H	-5.72860	-0.05062	-3.70605
H	-6.26560	-1.72969	-3.87934
C	-4.13870	-1.50472	-3.43259
H	-3.82109	-1.44900	-4.48928
H	-4.04666	-2.56920	-3.13292
C	-3.20071	-0.64376	-2.55894
H	-3.21825	0.39616	-2.93299
H	-2.15240	-0.98174	-2.65517
H	-4.02243	0.07833	1.87746
C	-3.06741	-1.83913	2.11387
H	-2.04664	-2.26619	2.03656
H	-3.69979	-2.34706	1.36223
C	-3.62758	-2.12885	3.52458
H	-4.67813	-1.78137	3.57262
H	-3.65218	-3.21995	3.69746
C	-2.80504	-1.42371	4.61733
H	-1.78554	-1.85777	4.64570
H	-3.25122	-1.60777	5.61050
C	-2.70569	0.08722	4.34325
H	-2.06685	0.57711	5.09964
H	-3.71039	0.54434	4.43949
C	-2.14752	0.37281	2.93273
H	-2.10240	1.46337	2.76438
H	-1.10585	0.00449	2.85987
C	-1.73123	-3.58874	-0.89719
H	-2.13748	-3.02756	-0.04874
H	-1.98322	-3.07892	-1.83655
H	-2.14369	-4.61152	-0.90284

TS7$_{Rh}$

BP86 Energy = -1737.62059441
Enthalpy 0K= -1736.513428
Enthalpy 298K= -1736.460861
Free Energy 298K= -1736.599648
Nimag=1 (-261.7145cm-1)
SCF PCM(DCM) = -1737.66377044
D3 Correction = -0.2251520

C	-2.80755	1.79138	-1.07552
C	-2.81582	0.49761	1.69907
C	3.39316	-0.39999	-1.60171
C	2.59124	2.00593	-0.06132
C	-3.58936	-1.07014	-0.78786
C	3.13486	-0.73542	1.35108
C	-2.22739	3.11156	-0.52414
C	-2.75404	4.32546	-1.32340
C	-2.47488	4.19280	-2.83095
C	-3.02783	2.86597	-3.38078
C	-2.48005	1.66345	-2.58248
C	-4.22006	1.12136	1.89091
C	-4.61716	1.14512	3.38423
C	-3.56696	1.87016	4.24352
C	-2.16954	1.25713	4.03928
C	-1.76394	1.24622	2.55020
C	-4.94474	-0.56081	-1.33825
C	-5.74790	-1.72355	-1.96648
C	-5.96817	-2.87707	-0.97268
C	-4.62934	-3.36752	-0.39111
C	-3.83702	-2.19967	0.23482
C	1.99206	2.67846	1.19421
C	2.00270	4.21531	1.05113
C	3.42263	4.74639	0.78351
C	4.05549	4.04837	-0.43311
C	4.03764	2.50859	-0.28937
C	4.66227	-0.52670	1.48705
C	5.24617	-1.44947	2.58065
C	4.54676	-1.24246	3.93578
C	3.02113	-1.40550	3.80465
C	2.44520	-0.48045	2.71120
C	3.47668	-1.92776	-1.79986
C	4.43994	-2.29886	-2.95002
C	4.06128	-1.59214	-4.26351
C	3.97428	-0.06894	-4.06430
C	2.99806	0.29597	-2.92484
P	-2.31196	0.21997	-0.11890
Rh	-0.03724	-0.44449	-0.38451
P	2.28106	0.11464	-0.13535
B	-0.00714	-2.46359	-0.69531
N	0.06703	-3.77143	0.29807
C	1.41959	-4.40244	0.09490
C	-0.11122	-3.47176	1.75812
C	-0.98017	-4.76852	-0.12879
H	-3.90852	1.83040	-0.95862
H	-2.85145	-0.54321	2.08191
H	4.40107	-0.03790	-1.31947
H	1.97534	2.33198	-0.92484
H	-3.02576	-1.50577	-1.63707
H	2.96648	-1.80495	1.10160
H	-1.12238	3.07078	-0.58211
H	-2.48385	3.23951	0.54103
H	-3.84617	4.41909	-1.16144
H	-2.30090	5.25105	-0.92544
H	-2.90959	5.04771	-3.37842
H	-1.38127	4.23060	-3.00618
H	-2.77143	2.75002	-4.44906
H	-4.13422	2.87254	-3.32212
H	-1.37949	1.63334	-2.70008
H	-2.87202	0.71904	-3.00326
H	-4.22279	2.15679	1.50040
H	-4.98205	0.56675	1.31709
H	-5.60741	1.62210	3.49414
H	-4.72995	0.10317	3.74485
H	-3.85300	1.83349	5.30957
H	-3.54007	2.94157	3.96257

H	-2.16652	0.21785	4.42608
H	-1.41405	1.81120	4.62497
H	-0.77456	0.77646	2.41924
H	-1.66412	2.28881	2.19589
H	-5.54324	-0.11017	-0.52426
H	-4.80039	0.22588	-2.09686
H	-6.71620	-1.34298	-2.33708
H	-5.20056	-2.10140	-2.85286
H	-6.50251	-3.71045	-1.46175
H	-6.61743	-2.53058	-0.14478
H	-4.02922	-3.82701	-1.20275
H	-4.80240	-4.15513	0.36518
H	-2.87258	-2.55365	0.64704
H	-4.41531	-1.80369	1.09153
H	0.96413	2.31444	1.36694
H	2.59451	2.40412	2.08111
H	1.33600	4.50527	0.21467
H	1.58219	4.67666	1.96281
H	3.40420	5.84007	0.63087
H	4.05310	4.56564	1.67664
H	5.09522	4.39134	-0.58023
H	3.50019	4.33054	-1.34967
H	4.49100	2.05688	-1.18805
H	4.67588	2.22191	0.56674
H	5.18299	-0.71125	0.53150
H	4.86388	0.52512	1.76185
H	5.13104	-2.50541	2.26303
H	6.33202	-1.27008	2.67358
H	4.77107	-0.22444	4.31028
H	4.94682	-1.94647	4.68666
H	2.52454	-1.19711	4.76928
H	2.78876	-2.46119	3.55361
H	2.60465	0.57004	3.01488
H	1.35206	-0.61377	2.61861
H	2.46286	-2.31526	-2.02615
H	3.81313	-2.42263	-0.87024
H	5.47092	-2.01218	-2.66382
H	4.44912	-3.39532	-3.08750
H	3.08101	-1.97123	-4.61534
H	4.79297	-1.83617	-5.05367
H	3.65446	0.42763	-4.99756
H	4.97969	0.33026	-3.82544
H	2.95860	1.39237	-2.80101
H	1.97912	-0.02417	-3.21898
H	-0.08222	1.21358	-0.19802
H	-0.45203	-0.18690	-2.12325
H	0.35183	-0.39494	-2.14284
H	-0.04432	-0.75097	1.14254
H	0.00118	-2.99900	-1.79403
H	1.48688	-5.32544	0.69437
H	1.54970	-4.63630	-0.97104
H	2.19656	-3.69441	0.41473
H	-1.09503	-3.00754	1.90805
H	0.66384	-2.76092	2.07088
H	-0.03660	-4.40576	2.33980
H	-0.80389	-5.04355	-1.17750
H	-1.97467	-4.31185	-0.03353
H	-0.92095	-5.66259	0.51373

(iv) M = It, L = PCy_3

TS to $Int3_{Ir}$

BP86 Energy = -1731.48770983
Enthalpy 0K= -1730.379383
Enthalpy 298K= -1730.327158
Free Energy 298K= -1730.465735
Nimag=1 (-600.5987cm-1)
SCF PCM(DCM) = -1731.53088593
D3 Correction = -0.2208360

Ir	0.03831	-0.19018	-0.20902
C	0.27523	-4.45374	-1.70541
C	-0.00614	-4.36854	0.72583
H	-0.20621	-5.44522	-1.74497
H	0.09143	-3.91399	-2.64592
H	1.35734	-4.56451	-1.55556
H	-0.44489	-5.37974	0.69887
H	1.08327	-4.43525	0.85414
H	-0.43741	-3.79033	1.55517
H	1.63281	-2.59807	-0.54690
H	-0.05374	1.21029	-1.13892
H	0.01688	1.49240	-0.09244
P	2.42066	0.18305	-0.05947
P	-2.36346	0.16343	0.08488
B	0.48747	-2.21223	-0.48816
H	0.12029	-1.44049	-1.55758
H	0.03050	0.03941	1.37462
N	-0.30209	-3.65475	-0.56566
C	3.35583	-0.50184	1.45113
C	2.83767	2.06026	-0.09430
C	-3.07855	-0.24109	1.80867
C	-2.65915	2.06973	-0.00671
C	3.33142	-0.53065	-1.58635
C	-3.61118	-0.64858	-1.11584
H	4.40162	-0.17903	1.27242
C	2.88083	0.11558	2.78753
H	1.81923	-0.15539	2.95002
H	2.92307	1.21597	2.74962
C	3.73493	-0.38201	3.97462
H	4.77044	-0.00618	3.85637
H	3.35024	0.05633	4.91285
C	3.76037	-1.91732	4.06432
H	4.42193	-2.24417	4.88594
H	2.74507	-2.28675	4.31191
C	4.21267	-2.53481	2.72976
H	4.18004	-3.63836	2.78075
H	5.26934	-2.26349	2.53635
C	3.33665	-2.04404	1.55713
H	2.29136	-2.36722	1.71938
H	3.66942	-2.51414	0.61519
H	2.56501	2.31486	-1.13914
C	4.34350	2.37484	0.09628
H	4.63350	2.15695	1.14244

H	4.97080	1.73615	-0.54519
C	4.64696	3.85878	-0.21124
H	5.72195	4.05436	-0.04878
H	4.45242	4.05051	-1.28503
C	3.78877	4.80774	0.64174
H	3.98022	5.85803	0.35933
H	4.08161	4.71016	1.70575
C	2.29310	4.47539	0.49680
H	1.96587	4.68957	-0.54029
H	1.68723	5.12095	1.15772
C	2.00842	2.99318	0.82317
H	0.92751	2.79157	0.72906
H	2.26365	2.80850	1.88269
H	2.82292	-1.50934	-1.68492
C	4.84960	-0.82058	-1.49797
H	5.42088	0.12365	-1.43821
H	5.09931	-1.39814	-0.59158
C	5.31584	-1.59273	-2.75339
H	6.40101	-1.78777	-2.68567
H	4.82000	-2.58392	-2.77489
C	4.98501	-0.82541	-4.04661
H	5.29117	-1.41272	-4.93042
H	5.57588	0.11138	-4.07413
C	3.48640	-0.48032	-4.12565
H	2.89839	-1.41419	-4.22913
H	3.27531	0.12448	-5.02573
C	3.01007	0.27707	-2.86710
H	1.92553	0.48142	-2.93403
H	3.52341	1.25756	-2.82778
H	-1.77797	2.44408	0.55346
C	-2.56300	2.62999	-1.44695
H	-1.68065	2.22487	-1.97409
H	-3.45163	2.30812	-2.02269
C	-2.51266	4.17289	-1.44201
H	-1.58319	4.50380	-0.93733
H	-2.45577	4.54493	-2.48069
C	-3.73121	4.77170	-0.71778
H	-3.65292	5.87248	-0.67603
H	-4.64744	4.54472	-1.29795
C	-3.87074	4.19098	0.69999
H	-4.77947	4.58142	1.19190
H	-3.01324	4.52192	1.31917
C	-3.91772	2.64516	0.69147
H	-4.00404	2.28648	1.73040
H	-4.83089	2.31601	0.16445
H	-3.62370	-1.69977	-0.76848
C	-5.07374	-0.14878	-1.04046
H	-5.44262	-0.14664	0.00060
H	-5.12893	0.89434	-1.40229
C	-5.99180	-1.02720	-1.91997
H	-6.01433	-2.05613	-1.50841
H	-7.02783	-0.64804	-1.86710
C	-5.50624	-1.06865	-3.38029
H	-5.59759	-0.05765	-3.82381
H	-6.15240	-1.73254	-3.98117
C	-4.03836	-1.52710	-3.46804
H	-3.68523	-1.49877	-4.51447
H	-3.97112	-2.58587	-3.14268
C	-3.11826	-0.65880	-2.58289
H	-3.11101	0.37294	-2.97875
H	-2.07113	-1.00912	-2.63699
H	-4.10168	0.18304	1.78204
C	-3.20900	-1.74762	2.11874
H	-2.19612	-2.19833	2.12495
H	-3.80046	-2.26262	1.33933
C	-3.87664	-1.98333	3.49259
H	-4.92031	-1.61474	3.45191
H	-3.93740	-3.06802	3.69442
C	-3.12342	-1.26192	4.62406
H	-2.12023	-1.71740	4.74481
H	-3.64934	-1.40419	5.58450
C	-2.96473	0.23683	4.31340
H	-2.37188	0.73519	5.10094
H	-3.96101	0.72170	4.31771
C	-2.29272	0.46030	2.94175
H	-2.18794	1.54189	2.74584
H	-1.26514	0.04866	2.96609
C	-1.78149	-3.58286	-0.74965
H	-2.20562	-3.01333	0.08405
H	-1.99747	-3.07317	-1.69804
H	-2.20762	-4.59996	-0.76734

$TS7_{Ir}$

BP86 Energy = -1731.48637666
Enthalpy 0K= -1730.378079
Enthalpy 298K= -1730.325593
Free Energy 298K= -1730.465238
Nimag=1 (-299.5336cm-1)
SCF PCM(DCM) = -1731.52935180
D3 Correction = -0.2251520

C	-2.83012	1.82801	-1.02934
C	-2.87369	0.49454	1.72726
C	3.39967	-0.37895	-1.59401
C	2.63627	2.03391	-0.03735
C	-3.57625	-1.04903	-0.79736
C	3.18354	-0.71186	1.36328
C	-2.29220	3.15157	-0.44326
C	-2.82601	4.36553	-1.23754
C	-2.50749	4.26245	-2.73953
C	-3.01812	2.93284	-3.32256
C	-2.46280	1.73037	-2.52951
C	-4.29940	1.07499	1.89619
C	-4.72812	1.06690	3.38087
C	-3.71816	1.81072	4.27191
C	-2.29835	1.24456	4.08768
C	-1.86304	1.26751	2.60708
C	-4.92021	-0.54986	-1.38393
C	-5.69282	-1.71684	-2.04184
C	-5.92985	-2.87885	-1.06194
C	-4.60325	-3.35938	-0.44534
C	-3.84178	-2.18775	0.21098
C	2.06250	2.70538	1.23106

C	2.07657	4.24222	1.08964
C	3.49401	4.76770	0.79850
C	4.10372	4.06891	-0.42959
C	4.08134	2.52885	-0.28891
C	4.71601	-0.52155	1.46941
C	5.30875	-1.45221	2.55158
C	4.63792	-1.23822	3.92009
C	3.10808	-1.38005	3.81777
C	2.52475	-0.44504	2.73676
C	3.46984	-1.90794	-1.79013
C	4.41036	-2.28692	-2.95637
C	4.01417	-1.57962	-4.26434
C	3.94154	-0.05555	-4.06632
C	2.98716	0.31797	-2.91127
P	-2.33599	0.24986	-0.08489
Ir	-0.02609	-0.36804	-0.32500
P	2.31929	0.14601	-0.11090
B	-0.00631	-2.40443	-0.64048
N	0.06519	-3.70069	0.38137
C	1.42315	-4.32503	0.20286
C	-0.12995	-3.37037	1.83157
C	-0.96650	-4.71657	-0.03517
H	-3.93426	1.84402	-0.93996
H	-2.88609	-0.55068	2.09958
H	4.41409	-0.02210	-1.32941
H	2.00689	2.36444	-0.88894
H	-2.98193	-1.47221	-1.63151
H	2.99867	-1.77953	1.11935
H	-1.18589	3.13554	-0.47299
H	-2.57977	3.25772	0.61624
H	-3.92362	4.43279	-1.10128
H	-2.40339	5.29449	-0.81469
H	-2.94740	5.11626	-3.28456
H	-1.41109	4.32618	-2.88728
H	-2.73365	2.83897	-4.38588
H	-4.12550	2.91481	-3.29084
H	-1.35944	1.72615	-2.61909
H	-2.82362	0.78430	-2.97409
H	-4.32310	2.11506	1.51887
H	-5.03315	0.50696	1.29913
H	-5.73420	1.51292	3.47587
H	-4.81738	0.01712	3.72497
H	-4.02453	1.74917	5.33114
H	-3.71904	2.88656	4.00717
H	-2.26960	0.20069	4.46085
H	-1.57241	1.81403	4.69548
H	-0.85558	0.83519	2.48985
H	-1.79361	2.31748	2.26858
H	-5.54667	-0.10973	-0.58533
H	-4.76182	0.24230	-2.13395
H	-6.65376	-1.34356	-2.43804
H	-5.11618	-2.08350	-2.91418
H	-6.44109	-3.71436	-1.57160
H	-6.60641	-2.54451	-0.25110
H	-3.97485	-3.80717	-1.24180
H	-4.78965	-4.15365	0.30073
H	-2.88616	-2.53474	0.64786
H	-4.44825	-1.80370	1.05337
H	1.03719	2.34366	1.42195
H	2.68154	2.42802	2.10541
H	1.39654	4.53592	0.26535
H	1.67382	4.70382	2.00915
H	3.47777	5.86162	0.64740
H	4.13868	4.58323	1.68066
H	5.14238	4.40757	-0.59320
H	3.53462	4.35507	-1.33636
H	4.51680	2.07717	-1.19649
H	4.73282	2.23697	0.55545
H	5.21650	-0.71280	0.50451
H	4.93587	0.52772	1.74000
H	5.17446	-2.50620	2.23517
H	6.39830	-1.28639	2.62387
H	4.88324	-0.22412	4.29197
H	5.04275	-1.94911	4.66188
H	2.63291	-1.16559	4.79179
H	2.85537	-2.43173	3.57011
H	2.70960	0.60219	3.03692
H	1.42825	-0.55841	2.66780
H	2.44973	-2.28903	-1.99649
H	3.81988	-2.40297	-0.86575
H	5.44816	-2.00709	-2.68856
H	4.40942	-3.38356	-3.09218
H	3.02538	-1.95221	-4.59872
H	4.73049	-1.82997	-5.06651
H	3.60937	0.44198	-4.99473
H	4.95353	0.33705	-3.84509
H	2.95689	1.41477	-2.78831
H	1.96146	0.00379	-3.18827
H	-0.05482	1.31845	-0.16958
H	-0.46905	-0.14156	-2.04166
H	0.37700	-0.32208	-2.06290
H	-0.01844	-0.58948	1.25067
H	-0.00123	-2.96783	-1.72587
H	1.48900	-5.24146	0.81266
H	1.56830	-4.56969	-0.85885
H	2.19234	-3.60967	0.52481
H	-1.11949	-2.91233	1.96178
H	0.63403	-2.64380	2.13469
H	-0.05206	-4.28979	2.43574
H	-0.77988	-5.00635	-1.07818
H	-1.96740	-4.27171	0.04514
H	-0.90116	-5.59968	0.62192