Supporting Information for "***Transition State Charge-Transfer Reveals Electrophilic, Ambiphilic, and Nucleophilic Carbon-Hydrogen Bond Activation***"

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Explanation of Truncated ligands.
For **4-IrOH**, **8-Ir**, and **12-Re**, truncated acac ligands were used (1,3-propanedialate). For **9-W** and **11Sc**, Cp rather than Cp* was utilized. The PNP* ligand was truncated as PMe_2 rather than PBu_2.

Referece 6c. QChem 3.1.0.2-serial ALMO version Full Reference
Y. Shao, L. Fusti-Molnar, Y. Jung, J. Kussmann, C. Ochsenfeld, S. T. Brown, A. T. B. Gilbert, L. V. Slipchenko,S. V. Levchenko, D. P. O'Neill, R. A. DiStasio Jr., R. C. Lochan, T. Wang, G. J. O. Beran, N. A. Besley, J. M. Herbert, C. Y. Lin, T. Van Voorhis, S. H. Chien, A. Sodt, R. P. Steele, V. A. Rassolov, P. E. Maslen, P. P. Korambath, R. D. Adamson, B. Austin, J. Baker, E. F. C. Byrd, H. Dachsel, R. J. Doerksen, A. Dreuw, B. D. Dunietz, A. D. Dutoi, T. R. Furlani, S. R. Gwaltney, A. Heyden, S. Hirata, C.-P. Hsu, G. Kedziora, R. Z. Khaliullin, P. Klunzinger, A. M. Lee, M. S. Lee, W. Liang, I. Lotan, N. Nair, B. Peters, E. I. Proynov, P. A. Pieniazek, Y. M. Rhee, J. Ritchie, E. Rosta, C. D. Sherrill, A. C. Simmonett, J. E. Subotnik, H. L. Woodcock III, W. Zhang, A. T. Bell, A. K. Chakraborty, D. M. Chipman, F. J. Keil, A. Warshel, W. J. Hehre, H. F. Schaefer III, J. Kong, A. I. Krylov, P. M. W. Gill, M. Head-Gordon, Q-Chem, Version 3.1, Q-Chem, Inc., Pittsburgh, PA (2007).

Additional authors for Version 3.1:
Z. Gan, Y. Zhao, N. E. Schultz, D. Truhlar, E. Epifanovsky and M. Oana.

Table S1. B3LYP/6-31++G(d,p)[LANL2DZ] Transition State Absolutely Localized Molecular Orbital Energy Decomposition Analysis results (kcal/mol). Compare with Table 1 in text.

TS	[a] E_{CT1}	[b] E_{CT2}	E_{FRZ}	E_{POL}	[c] E_{SE}	[d] E_{HO}	[e] E
1-Pt	**-40**	**-71**	57	-31	1	-2	-85
2-Pt	**-36**	**-55**	52	-20	1	-3	-62
3-Au	**-21**	**-51**	74	-44	2	5	-36
4-IrOH	**-25**	**-39**	90	-46	2	-1	-19
5-Ru	**-56**	**-68**	84	-48	2	1	-86
6-$RuNH_2$	**-27**	**-26**	86	-42	1	-2	-10
7-RuOH	**-31**	**-27**	90	-47	1	-2	-16
8-Ir	**-74**	**-66**	83	-44	1	3	-97
9-W	**-44**	**-36**	71	-31	1	-2	-42
11-Sc	**-39**	**-23**	70	-36	2	-3	-29

Table S2. Comparison of **1-Pt** and unprotonated **1-Pt**. B3LYP/6-31G(d,p)[LANL2DZ]. (kcal/mol).

TS	E_{CT1}	E_{CT2}	E_{FRZ}	E_{POL}	E_{SE}	E_{HO}	E
1-Pt	**-41**	**-70**	53	-27	3	-1	-83
no proton	**-52**	**-60**	62	-27	3	-1	-74

Protonation shifts the CT energy in favor of more electrophlic character. However, as shown in the table above, the total CT interaction energy for both TSs, E_{CT} sum to -111 kcal/mol. Therefore, the difference that make up the changes in total interaction energy is due to the E_{FRZ} term, and likely differences in electrostatics, since it is unlikely that exchange repulsions or correlation energies change significantly.

Table S3. Comparison of B3LYP, BP86, and M06 $\Delta E_{CT2\text{-}CT1}$ values. (6-31G(d,p)/LANL2DZ; kcal/mol).

TS	B3LYP	BP86	M06
1-Pt	-30	-38	-30
2-Pt	-28	-	-20
5-Ru	-12	13	13
6-RuNH$_2$	3	-3	4
7-Ir	4	8	5
8-RuOH	6	-1	6
9-W	12	17	11
10-IrPNP	13	20	11
11-Sc	23	27	21

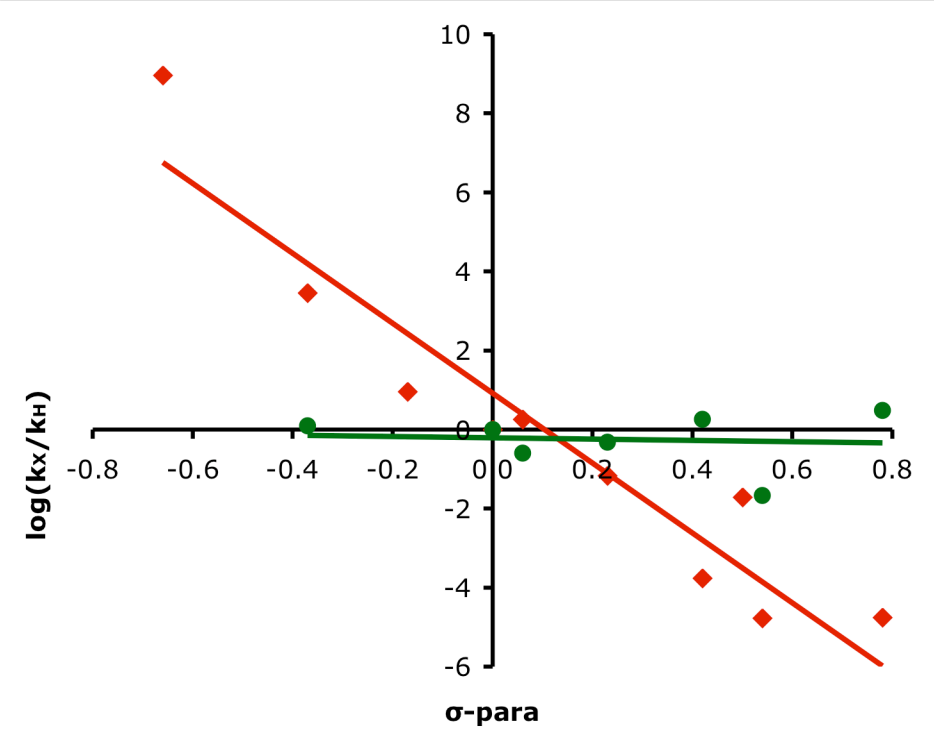

Figure 14. Hammett correlations for $(HS_2O_8)Au$ (red) and $(acac)_2IrOH$ (green) TSs with para substituted toluenes (sigma para values of NO_2 = 0.8, CF_3 = 0.5, CHO = 0.4, Cl = 0.2, F = 0.1, Me = -0.2, OH = -0.4, NH_2 = -0.7). The final free energies used to compare relative rates to toluene were computed with B3LYP/LACV3P**++ single point electronic energies with LACVP* geometries and free energy corrections, including solvation effects from implicit H_2SO_4 or water. Red line: y = -8.8x + 0.9; R^2 = 0.9. Green line: y = -0.2x - 0.2; R^2 = 0.0.

It should be noted that for the Hammett plot of (PCP)Ir in Figure 4 contains NO_2 CHO, H, OH, and NH_2 substituted toluenes. Inclusion of F and CF_3 substituents significantly deteriorated correlation. It is likely that an alternative sigma para scale might be more appropriate. However, for consistency, we have utilized the same sigma values for all Hammett correlation plots. Below in Table S4 are the ALMO-EDA results for the (PCP)Ir reaction with substituted toluenes corresponding to the Hammett plot. For toluene, E_{CT1} = -52 kcal/mol while the reverse E_{CT2} = -24 kcal/mol. As expected from the Hammett plot, E_{CT1} increases to -56 and -60 kcal/mol for NO_2 and CHO substitution, respectively. E_{CT2} also decreases slightly too. For OH and NH_2 substitution, again as expected, E_{CT1} decreases to -49 kcal/mol for NH_2 and stays the same for OH. E_{CT2} is unaffected.

Table S4. B3LYP ALMO-EDA results for (PCP)Ir insertion into the benzylic CH bond of para substituted toluenes (X group). Hammett plot is shown in Figure 4 of the text. (kcal/mol).[a]

TS	E_{CT1}	E_{CT2}	E_{FRZ}	E_{POL}	E_{SE}	E_{HO}	E
X = NO_2	**-56**	**-21**	57	-19	3	5	-31
X = CHO	**-60**	**-21**	55	-20	4	7	-35
X = H	**-52**	**-24**	57	-19	4	3	-31
X = OH	**-52**	**-24**	57	-20	4	3	-33
X = NH_2	**-49**	**-24**	57	-19	4	2	-30

a) 6-31G(d,p)/LANL2DZ basis set.

Table S5. B3LYP ALMO-EDA results now given in text. (kcal/mol).

TS	E_{CT1}	E_{CT2}	E_{FRZ}	E_{POL}	E_{SE}	E_{HO}	E
Cp(PH_3)IrMe-CH_4 TS[a]	**-36**	**-48**	62	-29	1	-3	-52
Au(SO4)[a]	**-39**	**-45**	44	-21	1	-1	-61
Cis-(H_2O)$PtCl_2$-CH4 TS[a]	**-48**	**-49**	70	-26	1	-2	-53
PCPIr-CH_4 TS[b]	**-56**	**-26**	58	-22	2	4	-39
$PtCl_3$-CH_4 TS[a]	**-43**	**-48**	69	-21	1	-2	-44

a) 6-311++G(d,p)/LANL2DZ basis set.b) 6-31G(d,p)/LANL2DZ basis set.

Cartesian Coordinates and Absolute Energies (au) of TS Decompositions

1-Pt: E = -1147.3989109142

2 1

Pt	1.513030	0.015145	1.511772
N	3.535138	-0.181326	2.375224
N	1.730749	-2.094547	1.637854
N	5.055753	-1.802576	3.074041
N	3.291848	-3.761648	2.353282
Cl	1.578730	2.314806	1.577738
C	3.865471	-1.458639	2.543796
C	2.913122	-2.512611	2.155217
C	5.960102	-0.871926	3.457350
C	5.642149	0.469124	3.295740
C	4.398495	0.788545	2.741981
C	2.424260	-4.727876	2.014793
C	1.172561	-4.409693	1.479706
C	0.854698	-3.063231	1.302730
H	6.895300	-1.231808	3.876023
H	6.340505	1.244400	3.592568
H	4.060270	1.810389	2.579982
H	2.738950	-5.754825	2.177949
H	0.461017	-5.182283	1.207651
H	-0.099720	-2.751137	0.895215
H	5.232624	-2.809920	3.172275

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0 1

C	0.031066	0.148642	-0.070959
H	-0.030417	0.074837	1.654318
H	0.770015	0.133245	-0.875143
H	-0.641581	-0.706448	-0.106334
H	-0.498517	1.097454	-0.029464

1-Pt-unprotonated: E = -1147.1698498888

1 1

Pt	1.537489	0.004383	1.528441
N	3.498922	-0.182223	2.372703
N	1.747225	-2.072816	1.644255
N	5.080237	-1.815315	3.051263
N	3.253341	-3.783821	2.312089
Cl	1.551003	2.329603	1.571697
C	3.909596	-1.460732	2.551808
C	2.933455	-2.512331	2.151382
C	5.912038	-0.825793	3.405252
C	5.576799	0.521984	3.262726
C	4.327988	0.815290	2.727802
C	2.348000	-4.702943	1.959893

C	1.100311	-4.351946	1.442309
C	0.833238	-2.997856	1.296380
H	6.872378	-1.128620	3.814815
H	6.256610	1.314044	3.554540
H	3.960232	1.824471	2.571220
H	2.633383	-5.742364	2.100143
H	0.363445	-5.096134	1.163434
H	-0.108963	-2.636791	0.903241

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0 1

C	0.084569	0.102738	-0.058000
H	-0.001825	0.044121	1.697369
H	0.811793	0.038511	-0.870839
H	-0.621043	-0.726515	-0.088690
H	-0.422534	1.064513	-0.059538

2-Pt: E = -1156.5496317793

Pt	-1.498411	2.096189	2.746966
Cl	-0.778472	1.648518	4.953466
Cl	-2.077957	2.768419	0.555144
O	-1.034442	4.161012	3.143182
H	-0.327370	4.221591	3.805666
H	-0.763777	4.604552	2.323112

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0 1

C	-1.319026	0.026702	2.158330
H	-2.442337	0.856374	2.692964
H	-1.167808	-0.599824	3.034293
H	-2.061686	-0.376570	1.468277
H	-0.388274	0.199093	1.616472

2-Pt-cis-water TS: E = -1156.5375946830

0 1

Pt	0.018170	2.155841	0.168122
Cl	1.416418	2.040868	1.999859
Cl	0.385966	4.467846	-0.270780
O	-1.304990	2.419579	-1.554325
H	-1.241274	3.401183	-1.581089
H	-0.843937	2.112714	-2.351349

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0 1

C	0.127009	-0.002618	-0.024955
H	-0.817850	0.998245	0.794945
H	0.177098	-0.580968	0.897256
H	-0.649010	-0.375868	-0.693538
H	1.109479	-0.006324	-0.500838

3-Au: E = -1574.5123522304

Au	-0.752156	-1.864906	1.859711
S	-0.235307	0.225404	0.120932
O	-0.491141	0.116850	1.746339
O	1.136782	0.629776	-0.122277
O	-0.408372	-1.371548	-0.091001
O	-1.339041	0.944004	-0.488440
O	-1.011044	-3.930235	1.583396
S	-0.525161	-4.896377	2.682662
O	0.365438	-5.927765	2.197752
O	-1.889608	-5.582392	3.227943
O	-0.074497	-4.069165	3.854871
H	-2.040211	-6.401919	2.724923

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0 1

C	-1.258055	-1.676780	4.054369
H	-0.786796	-0.701241	4.156820
H	-0.604574	-2.806966	3.796817
H	-1.092633	-2.198322	5.012709
H	-2.339124	-1.620923	3.925773

4-IrOH: E = -906.8773604543

Ir1	0.2027371143	0.0775061700	0.0882566957
O2	0.9282617775	-0.5935255486	1.9216997229
C3	1.0896574730	-1.7498652679	-1.9997180364
O4	1.1813657936	-1.5073482341	-0.7532140406
H5	1.6919811430	-2.6041732097	-2.3308273573
C6	-0.3184522634	2.8229439633	0.9275697741
O7	-0.7650325314	1.6282997555	1.0142450529
H8	-0.9452836136	3.5675848230	1.4318862355
C9	1.7766193115	2.4926600289	-0.3840378061
C10	0.8408237924	3.2815866941	0.2987173230
H11	2.6489453842	3.0036739019	-0.8090847115
H12	1.0400291700	4.3461153065	0.3505582286
O13	1.7646241183	1.2360313626	-0.5830069842
C14	-0.5024759787	0.0150440689	-2.7520487350
C15	0.3291415180	-1.0865901799	-2.9712978050
H16	-1.0445140167	0.4159293580	-3.6170976581
H17	0.3899707188	-1.4643446393	-3.9858854404
O18	-0.7341437459	0.6360542348	-1.6614205170
C19	-1.4362182559	-1.3107138371	0.9217295053
H20	-0.3035880616	-1.0326556121	1.5508103732
H21	0.7707700451	0.1192261129	2.5600432645
H22	-1.9531532266	-1.0488133597	-0.0053210799
H23	-1.3016829399	-2.3958382934	0.9216180056

H24	-2.0898707420	-0.9794365720	1.7345607512

5-Ru: E = -990.0968141236

0 1

Ru	0.597923	-0.115794	0.277977
N	0.682832	-0.525202	-1.877311
C	0.553828	0.276098	2.098692
C	1.188873	-2.226295	0.681900
N	0.182158	1.945310	-0.341467
N	2.687178	0.493947	0.028617
N	3.032047	1.224034	-1.062921
N	1.315981	0.361478	-2.686952
N	0.874059	2.468685	-1.385731
B	1.964599	1.639259	-2.102259
H	2.468195	2.285108	-2.979517
O	0.531845	0.524647	3.231192
H	2.039853	-2.107355	1.354328
H	1.525786	-2.620614	-0.277493
H	0.520362	-2.962850	1.145865
C	4.359026	1.482498	-1.036546
H	4.819734	2.056536	-1.827012
C	4.896812	0.905918	0.104240
H	5.925455	0.925110	0.430636
C	0.241933	-1.521461	-2.656155
H	-0.299515	-2.350636	-2.223257
C	0.590199	-1.283679	-3.994060
H	0.376231	-1.899382	-4.854257
C	0.456441	3.733225	-1.620310
H	0.896461	4.315534	-2.416488
C	-0.535890	4.046100	-0.703651
H	-1.079062	4.974206	-0.611036
C	3.802753	0.298361	0.739505
H	3.766998	-0.259424	1.664636
C	1.271892	-0.075768	-3.964910
H	1.726484	0.501921	-4.756211
C	-0.668894	2.887957	0.077871
H	-1.325408	2.694143	0.914410

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0 1

H	-0.219327	-1.466136	0.524339
C	-1.569514	-0.642315	0.275670
H	-1.856431	-0.818496	-0.762182
H	-1.986911	-1.442202	0.899347
H	-2.011947	0.293283	0.621250

6-RuNH_2: E = -1006.1547764977

0 1

Ru	-0.097506	-0.005873	-0.073317
N	-0.053663	0.001502	2.107207
C	-0.179243	0.021642	-1.936208
N	-1.540879	1.526699	0.137819
N	-1.762660	-1.375271	0.148093
N	-2.692567	-1.108288	1.101453
N	-1.231822	0.071301	2.776604
N	-2.513475	1.398516	1.077190
B	-2.563868	0.149043	1.990782
H	-3.491311	0.223578	2.747933
O	-0.234884	0.058548	-3.094582
N	1.700385	1.123998	-0.029123
H	1.908732	1.677782	-0.852300
C	-3.641347	-2.071845	1.095151
H	-4.467920	-2.029585	1.789002
C	-3.324802	-2.993164	0.109540
H	-3.872961	-3.882119	-0.162267
C	0.919363	-0.036697	3.024417
H	1.953060	-0.095053	2.714466
C	0.370348	0.008441	4.314800
H	0.893626	-0.008015	5.258528
C	-3.300455	2.497874	1.063416
H	-4.131772	2.582416	1.747602
C	-2.831993	3.363368	0.087048
H	-3.233622	4.326791	-0.187169
C	-2.135821	-2.508223	-0.456854
H	-1.540676	-2.913000	-1.263164
C	-0.999497	0.076628	4.107473
H	-1.821259	0.128166	4.806535
C	-1.722718	2.706024	-0.465746
H	-1.057982	3.015996	-1.258825
H	1.742598	1.711299	0.797430

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0 1

C	1.694802	-1.588583	-0.076796
H	1.843600	-0.251912	-0.040189
H	0.842557	-2.274893	-0.069372
H	2.274909	-1.811730	0.825534
H	2.288263	-1.811331	-0.968552

7-Ir: E = -718.2813730924

0 1

Ir	0.000000	0.000000	0.416503
O	-0.199340	2.045004	0.426169
O	1.358283	0.022906	-1.268708

O	-1.358283	-0.022906	-1.268708
O	0.199340	-2.045004	0.426169
C	-1.828787	-0.107282	1.520014
C	0.359591	2.775543	-0.458097
C	1.203039	2.416980	-1.513193
C	1.632663	1.122582	-1.840013
C	-1.632663	-1.122582	-1.840013
C	-1.203039	-2.416980	-1.513193
C	-0.359591	-2.775543	-0.458097
H	1.561249	3.223973	-2.142829
H	-1.561249	-3.223973	-2.142829
H	-1.903793	-1.030372	2.098158
H	-1.965536	0.761164	2.166662
H	-2.582253	-0.089810	0.731296
H	0.131253	3.842798	-0.348916
H	2.305848	1.037883	-2.705567
H	-2.305848	-1.037883	-2.705567
H	-0.131253	-3.842798	-0.348916

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0 1

C	1.828787	0.107282	1.520014
H	2.582253	0.089810	0.731296
H	1.903793	1.030372	2.098158
H	1.965536	-0.761164	2.166662
H	0.000000	0.000000	1.964117

8-RuOH: E = -1026.0264551946

0 1

Ru	0.001866	0.000635	0.000204
N	-0.003196	-0.002336	2.183540
C	0.062941	0.014005	-1.868793
N	2.027125	-0.596411	0.182877
N	0.735179	1.986586	0.159899
N	1.686886	2.255127	1.091816
N	1.067259	0.535802	2.820783
N	2.819358	0.014000	1.101356
B	2.240350	1.131048	2.000103
H	3.084768	1.562751	2.734126
O	0.120637	0.028640	-3.024682
O	-0.987240	-1.897664	-0.005740
H	-0.885755	-2.245039	0.891896
C	2.008645	3.567570	1.043655
H	2.752491	3.971954	1.714187
C	1.249773	4.171590	0.053470
H	1.263042	5.208054	-0.246854
C	-0.843829	-0.440961	3.129745

H	-1.780855	-0.903560	2.853756
C	-0.314995	-0.187028	4.403643
H	-0.754117	-0.418854	5.361795
C	4.046570	-0.553833	1.085008
H	4.819881	-0.203547	1.752778
C	4.054306	-1.557200	0.128083
H	4.876174	-2.202279	-0.142431
C	0.465708	3.134751	-0.473867
H	-0.265219	3.156829	-1.269343
C	0.899833	0.435831	4.157367
H	1.652580	0.814408	4.833204
C	2.758770	-1.545332	-0.411384
H	2.320656	-2.161068	-1.183499

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0 1

C	-2.332660	0.381187	0.027072
H	-1.743566	-0.863281	0.041374
H	-2.010950	1.427113	0.011786
H	-2.922707	0.262702	0.943044
H	-2.971586	0.230178	-0.848188

9-W: E = -782.5595094919

0 1

W	-0.257980	0.076191	0.141452
C	-1.628379	1.338288	0.800859
O	-2.412934	2.096343	1.209160
C	-1.479858	0.222932	-1.388729
O	-2.169254	0.325377	-2.327426
B	-1.072307	-1.960321	-0.539716
C	1.994794	0.056671	1.087684
C	2.009095	-0.721555	-0.103948
C	1.685076	0.140556	-1.192334
C	1.471834	1.455642	-0.669321
C	1.658867	1.395234	0.746395
H	2.188524	-0.311362	2.086703
H	2.218567	-1.779161	-0.178227
H	1.638344	-0.147266	-2.233198
H	1.247890	2.343255	-1.244319
H	1.577565	2.225230	1.435050
O	-0.253395	-2.804658	-1.273790
O	-2.346984	-2.470535	-0.399113
C	-2.457058	-3.654281	-1.205593
H	-2.935807	-4.447849	-0.623764
H	-3.087016	-3.430827	-2.074415
C	-1.002727	-3.988842	-1.605653
H	-0.597005	-4.835631	-1.038788

H	-0.891293	-4.201106	-2.673193

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0 1

C	-0.966676	-0.824575	2.308209
H	-2.049256	-0.808530	2.415306
H	-0.513609	-0.055742	2.931953
H	-0.586620	-1.796062	2.638531
H	-0.771012	-1.400003	0.921650

10-IrPNP: E = -1312.7733786876

0 1

Ir	-0.080556	0.002703	-0.001656
N	-0.380963	0.025200	-2.070640
P	0.038249	-2.300613	-0.343012
P	0.013403	2.278245	-0.291182
C	-0.268380	-1.187334	-2.774403
C	-0.071306	-2.382028	-2.094339
H	-0.001949	-3.310891	-2.651399
C	-0.606730	1.191887	-2.754887
C	1.687767	3.007040	-0.578146
H	2.268136	2.965735	0.347544
H	2.204103	2.404539	-1.329722
H	1.627832	4.046195	-0.919220
C	-0.797755	3.558707	0.769416
H	-0.733364	4.556996	0.324040
H	-1.848656	3.295228	0.915783
H	-0.312393	3.580365	1.749509
C	1.595954	-3.141497	0.208457
H	2.452023	-2.588047	-0.183379
H	1.657220	-3.160689	1.301620
H	1.634897	-4.171170	-0.163685
C	-1.240462	-3.418603	0.407059
H	-2.233375	-3.056856	0.130121
H	-1.122651	-4.445511	0.043959
H	-1.156141	-3.419969	1.499010
C	-0.358007	-1.134483	-4.209817
C	-0.541433	0.048566	-4.865408
H	-0.260761	-2.067778	-4.755088
H	-0.594305	0.067925	-5.951252
C	-0.673082	1.252782	-4.130217
H	-0.853352	2.199932	-4.625217
C	-0.844240	2.437617	-1.928602
H	-1.915047	2.518478	-1.695972
H	-0.560902	3.339151	-2.481737

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0 1

C	-0.242561	-0.081841	2.252086
H	0.822889	-0.048271	1.353284
H	-1.330614	-0.144768	2.152726
H	0.108691	-0.963528	2.795267
H	0.012215	0.810530	2.828454

11-Sc: E = -514.0143478632

0 1

Sc	0.002817	0.185049	0.000010
C	-0.037533	2.114450	1.432155
C	1.611433	-1.746642	0.000045
C	1.906828	-0.968182	-1.146930
C	1.906624	-0.968303	1.147158
C	2.410352	0.285754	-0.707342
C	2.410228	0.285678	0.707792
C	-2.513402	0.441782	-0.000072
C	-2.182740	-0.322654	1.146619
C	-2.182624	-0.322350	-1.146933
C	-1.636161	-1.555546	0.710633
C	-1.636088	-1.555357	-0.711219
H	0.035175	1.361361	2.234692
H	0.805143	2.800650	1.569217
H	-0.969796	2.665842	1.593979
H	1.214954	-2.753874	-0.000045
H	1.789639	-1.283473	-2.177379
H	1.789257	-1.283703	2.177553
H	2.734812	1.098658	-1.343457
H	2.734575	1.098514	1.344049
H	-2.934208	1.439021	0.000039
H	-2.316507	-0.013104	2.176084
H	-2.316289	-0.012522	-2.176327
H	-1.293502	-2.361365	1.347783
H	-1.293363	-2.361006	-1.348549

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0 1

H	-0.028038	2.071554	0.000079
C	-0.037315	2.114559	-1.431999
H	0.035573	1.361534	-2.234578
H	0.805369	2.800791	-1.568858
H	-0.969567	2.665937	-1.593937

12-Re: E = -728.5801415013

0 1

Re	-1.272247	0.461425	-0.041352
C	-3.718508	0.165858	1.700902
H	-4.747114	-0.199018	1.807240

C	-1.216298	3.369159	-0.820340
H	-1.759098	4.282454	-1.091240
C	1.018056	2.371422	-0.409675
C	0.176832	3.438072	-0.751077
H	2.094150	2.571807	-0.349705
H	0.642949	4.395382	-0.955171
C	-1.850923	1.324503	2.831507
C	-3.147482	0.795815	2.805148
H	-1.522391	1.809453	3.760806
H	-3.751241	0.887622	3.700759
O	-0.993279	1.316466	1.895343
O	-3.209537	-0.051862	0.547419
O	-1.956294	2.351514	-0.590951
O	0.692889	1.164839	-0.162377
O	-0.577798	-1.236683	0.564754
H	0.388367	-1.269219	0.620174

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0 1

C	-2.279561	-0.439094	-1.845544
H	-1.769522	-0.733705	-2.764823
H	-2.723060	-1.322073	-1.385094
H	-3.050151	0.296795	-2.081288
H	-0.787245	0.205845	-1.581319

Bergman's $[Cp(PH_3)IrMe\text{-}CH_4]^+$ TS: E = -825.2680399391

1 1

Ir	0.022090	-0.046992	-0.449965
P	-2.207512	0.166060	0.078108
C	-0.368504	1.599464	-1.804367
C	1.703960	-1.175461	0.735364
C	0.925472	-0.458542	1.672869
C	1.011706	0.948833	1.339363
C	1.897765	1.077216	0.222784
C	2.288788	-0.232077	-0.189201
H	0.513267	1.749050	-2.427591
H	-1.227860	1.414160	-2.450134
H	-0.549956	2.492004	-1.202592
H	2.183183	2.004266	-0.255347
H	2.964361	-0.469991	-0.999094
H	1.826259	-2.249800	0.698867
H	0.368525	-0.883484	2.496917
H	0.575102	1.764944	1.898680
H	-3.059478	-0.916592	-0.223459
H	-2.917028	1.235492	-0.503615
H	-2.506565	0.358402	1.440801

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0 1

C	-0.591584	-1.964656	-1.505140
H	-0.049800	-0.574014	-1.958085
H	0.242829	-2.459231	-2.001331
H	-0.885944	-2.541180	-0.628913
H	-1.435297	-1.877953	-2.189994

[$PtCl_3$-CH_4]$^-$ TS: E = -1540.4375572805

-1 1

Pt	0.004314	2.189067	0.114367
Cl	1.371154	1.977659	2.065939
Cl	-1.396745	2.277381	-1.822880
Cl	0.483304	4.519110	-0.045750

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0 1

C	0.101714	0.026546	-0.125141
H	-0.846269	0.980724	0.626859
H	0.351196	-0.514667	0.787549
H	-0.734912	-0.415217	-0.667058
H	0.975771	0.075430	-0.777442

Au(HSO_4) TS: E = -1575.8196923075

0 1

Au	-1.147312	-0.782331	2.752188
S	-0.555162	-2.154496	0.245802
O	-1.833962	-1.455728	0.572795
O	0.152148	-1.804364	-0.972258
O	0.320944	-1.945088	1.528882
O	-0.933233	-3.709918	0.252829
H	-0.095234	-4.234386	0.152024
O	2.198550	-5.309105	2.646220
S	2.450891	-4.616180	1.405186
O	2.689134	-3.058647	1.620902
H	1.800759	-2.575585	1.592984
O	3.928976	-5.040042	0.928788
O	1.538746	-4.799120	0.261616
H	4.077377	-4.700146	0.029595

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0 1

C	-2.541076	0.355123	3.917797
H	-2.377164	0.656088	4.952521
H	-3.395114	-0.320121	3.863897
H	-2.643268	1.237686	3.287110
H	-1.045581	-0.192479	4.205666

PCPIr-CH_4 TS: E = -1296.7394881671

0 1

Ir	-0.008291	0.003998	0.029011
C	-0.350862	-0.009400	-2.026832
P	0.059526	-2.270119	-0.296831
P	-0.021646	2.275358	-0.345037
C	-0.168434	-1.184553	-2.805152
C	-0.791377	1.155855	-2.712015
C	1.608267	3.038715	-0.764822
H	2.269166	2.992912	0.104895
H	2.063583	2.458036	-1.570374
H	1.497319	4.081721	-1.081254
C	-0.757966	3.531301	0.796284
H	-0.757495	4.532313	0.352279
H	-1.785099	3.244500	1.036111
H	-0.184998	3.558753	1.727856
C	1.334187	-3.355069	0.486496
H	2.324919	-2.929751	0.306325
H	1.169162	-3.391275	1.567366
H	1.299677	-4.374616	0.088301
C	-1.496580	-3.237277	-0.028822
H	-2.300893	-2.768143	-0.601117
H	-1.386532	-4.280054	-0.346140
H	-1.769317	-3.211109	1.029583
C	-0.430694	-1.193674	-4.178942
C	-0.860266	-0.032952	-4.822953
H	-0.287906	-2.106950	-4.753747
H	-1.056862	-0.042629	-5.892040
C	-1.032748	1.141090	-4.089886
H	-1.365430	2.047683	-4.593066
C	-1.006386	2.430849	-1.915666
H	-2.058387	2.533591	-1.616446
H	-0.748103	3.332871	-2.485115
C	0.367472	-2.430272	-2.125112
H	-0.054767	-3.355394	-2.538444
H	1.456453	-2.494382	-2.251165

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0 1

C	-0.137011	0.038380	2.290053
H	1.020784	0.009429	1.272784
H	-1.232771	0.009529	2.273209
H	0.224175	-0.822805	2.859483
H	0.180500	0.946954	2.808589