Supporting information for

The Quest for Stable σ-Methane Complexes: Computational and Experimental Studies

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Figure S1. ORTEP diagram of **1-RhI** (50 % probability ellipsoids). Selected bond distances (Å): Rh1-N1 1.998(2) , Rh1-I1 2.6438(2), Rh1-P1 2.2572(6), Rh1-P2 2.2532(6).

Figure S2. ORTEP diagram of **1-RhMe** (50 % probability ellipsoids). Selected bond distances (Å): Rh1-N1 2.0437(15), Rh1-C33 2.1696(9), Rh1-P1 2.2425(2), Rh1-P2 2.2308(19).

Table S1: X-Ray crystal structure determination of **1-IrMe**, **1-RhI**, **1-RhMe**, and **2-PdMe**$^+$

Compound reference	**1-IrMe**	**1-RhI**	**1-RhMe**	**2-PdMe**$^+$
Chemical formula	$C_{33}H_{49}IrN_2O_2P_2$	$C_{71}H_{99}I_2N_4O_4P_4Rh_2$	$C_{33}H_{49}N_2O_2P_2Rh$	$C_{55}H_{56}BCl_2F_{24}NO_2P_2Pd$
Formula Mass	759.88	1656.04	670.59	1469.06
Crystal system	Monoclinic	Triclinic	Monoclinic	Monoclinic
a/Å	11.1882(3)	11.1948(4)	11.1771(2)	13.7687(5)
b/Å	12.8593(3)	12.7179(5)	12.8681(3)	23.5697(9)
c/Å	23.2460(6)	14.3447(9)	23.2854(5)	19.7027(7)
α/°	90.00	100.145(2)	90.00	90.00
β/°	94.8910(10)	102.482(2)	94.7390(10)	98.591(2)
γ/°	90.00	110.4030(10)	90.00	90.00
Unit cell volume/Å^3	3332.28(15)	1796.98(15)	3337.64(12)	6322.3(4)
Temperature/K	100(2)	100(2)	100(2)	100(2)
Space group	*P2(1)/c*	$P\bar{1}$	*P2(1)/c*	*P2(1)/c*
No. of formula units per unit cell, *Z*	4	1	4	4
No. of reflections measured	22893	29205	49137	59378
No. of independent reflections	6154	6587	5872	11956
R_{int}	0.0303	0.0285	0.0289	0.0310
Final R_1 values ($I > 2\sigma(I)$)	0.0257	0.0274	0.0232	0.0463
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.0616	0.0699	0.0604	0.1241
Final R_1 values (all data)	0.0313	0.0280	0.0244	0.0502
Final $wR(F^2)$ values (all data)	0.0641	0.0704	0.0613	0.1273
Goodness of fit on F^2	1.028	1.060	1.065	1.034

2. Kinetics of decay of 1-Ir(H)(Me)$^+$

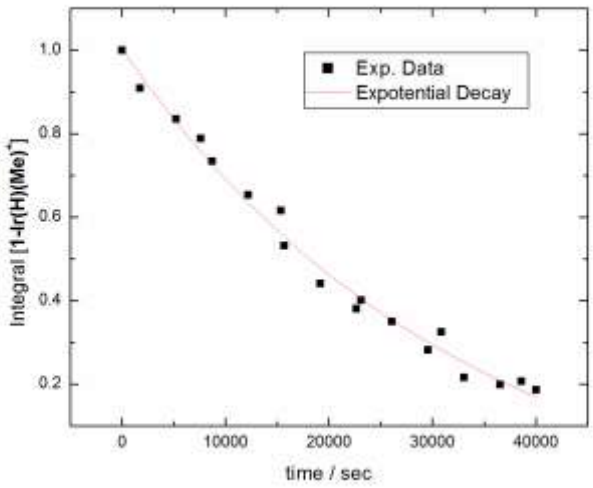

Figure S3. Kinetics of decay of **1-Ir(H)(Me)**$^+$ measured by $^{31}P\{^1H\}$ NMR spectroscopy at 292 K ($R^2 = 0.98919$).

3. Computational Results

Table S2. Calculated Electronic Energies, Enthalpies, and Free Energies in the Gas Phase (Hartrees) at 298.15 K[a,b]

Compund	E_{elec}	E_0	H	G
CH_4	-40.46186	-40.41661	-40.41280	-40.43393
$[Pd(I\text{-}H)]^{2+}$	-1366.39229	-1366.15843	-1366.13972	-1366.20441
$[Pd(I\text{-}H)(HMe)]^{2+}$	-1406.88981	-1406.60895	-1406.58695	-1406.65859
$[Pt(I\text{-}H)]^{2+}$	-1357.86945	-1357.63523	-1357.61662	-1357.68119
$[Pt(I\text{-}H)(HMe)]^{2+}$	-1398.37669	-1398.09505	-1398.07350	-1398.14402
$[Ir(I\text{-}NMe_2)]^{+}$	-1477.08033	-1476.77161	-1476.74865	-1476.82278
$[Ir(I\text{-}NMe_2)(H)(Me)]^{+}$	-1517.58297	-1517.22953	-1517.20369	-1517.28355
$[Ir(I\text{-}NMe_2)(HMe)]^{+}$	-1517.57718	-1517.22146	-1517.19572	-1517.27507
$[Ir(I\text{-}H)]^{+}$	-1343.24708	-1343.01213	-1342.99378	-1343.05753
$[Ir(I\text{-}H)(H)(Me)]^{+}$	-1383.75069	-1383.47082	-1383.44965	-1383.51895
$[Ir(I\text{-}H)(HMe)]^{+}$	-1383.74496	-1383.46292	-1383.44179	-1383.51081
$[Ir(I\text{-}CF_3)]^{+}$	-1679.96268	-1679.72307	-1679.70092	-1679.77524
$[Ir(I\text{-}CF_3)(H)(Me)]^{+}$	-1720.46641	-1720.18182	-1720.15688	-1720.23669
$[Ir(I\text{-}CF_3)(HMe)]^{+}$	-1720.46103	-1720.17432	-1720.14939	-1720.22885
$[Ir(I\text{-}NMe_3)]^{2+}$	-1516.59734	-1516.24698	-1516.22398	-1516.29686
$[Ir(I\text{-}NMe_3)(H)(Me)]^{2+}$	-1557.10153	-1556.70609	-1556.68032	-1556.75855
$[Ir(I\text{-}NMe_3)(HMe)]^{2+}$	-1557.09961	-1556.70210	-1556.67632	-1556.75442
$[Ir(II)]^{+}$	-2532.93798	-2532.79446	-2532.76723	-2532.85745
$[Ir(II)(H)(Me)]^{+}$	-2573.44328	-2573.25437	-2573.22457	-2573.31803
$[Ir(II)(HMe)]^{+}$	-2573.44370	-2573.25305	-2573.22309	-2573.31757
$[Ir(III)]^{+}$	-1359.25500	-1359.03218	-1359.01396	-1359.07746
$[Ir(III)(H)(Me)]^{+}$	-1399.75778	-1399.49000	-1399.46897	-1399.53799
$[Ir(III)(HMe)]^{+}$	-1399.75344	-1399.48350	-1399.46248	-1399.53130
$[Ir(III\text{-}H)]^{2+}$	-1359.51012	-1359.27430	-1359.25591	-1359.31952
$[Ir\ (III\text{-}H)(H)(Me)]^{2+}$	-1400.01314	-1399.73214	-1399.71102	-1399.77985
$[Ir\ (III\text{-}H)(HMe)]^{2+}$	-1400.01688	-1399.73458	-1399.71320	-1399.78273
$[Rh(I\text{-}NMe_2)]^{+}$	-1483.27219	-1482.96363	-1482.94063	-1483.01449
$[Rh(I\text{-}NMe_2)(H)(Me)]^{+}$	-1523.74552	-1523.39261	-1523.36675	-1523.44623
$[Rh(I\text{-}NMe_2)(HMe)]^{+}$	-1523.76197	-1523.40636	-1523.38032	-1523.46014
$[Rh(I\text{-}H)]^{+}$	-1349.43915	-1349.20436	-1349.18596	-1349.24946
$[Rh(I\text{-}H)(H)(Me)]^{+}$	-1389.91283	-1389.63354	-1389.61233	-1389.68129
$[Rh(I\text{-}H)(HMe)]^{+}$	-1389.92980	-1389.64808	-1389.62657	-1389.69629
$[Rh(I\text{-}CF_3)]^{+}$	-1686.15488	-1685.91542	-1685.89323	-1685.96725
$[Rh(I\text{-}CF_3)(H)(Me)]^{+}$	-1726.62851	-1726.34450	-1726.31952	-1726.39900
$[Rh(I\text{-}CF_3)(HMe)]^{+}$	-1726.64589	-1726.35955	-1726.33423	-1726.41452
$[Rh(I\text{-}NMe_3)]^{2+}$	-1522.79051	-1522.44029	-1522.41725	-1522.48983
$[Rh(I\text{-}NMe_3)(H)(Me)]^{2+}$	-1563.26378	-1562.86890	-1562.84309	-1562.92097
$[Rh(I\text{-}NMe_3)(HMe)]^{2+}$	-1563.28557	-1562.88843	-1562.86132	-1562.94314
$[Rh(II)]^{+}$	-2539.13219	-2538.98882	-2538.96157	-2539.05140
$[Rh\ (II)(H)(Me)]^{+}$	-2579.60638	-2579.41818	-2579.38830	-2579.48170
$[Rh(II)(HMe)]^{+}$	-2579.62946	-2579.43896	-2579.40877	-2579.50355
$[Rh(III)]^{+}$	-1365.44699	-1365.22433	-1365.20606	-1365.26932
$[Rh(III)(H)(Me)]^{+}$	-1405.91959	-1405.65241	-1405.63134	-1405.70002
$[Rh(III)(HMe)]^{+}$	-1405.93813	-1405.66878	-1405.64725	-1405.71731

$[Rh(III\text{-}H)]^{2+}$	-1365.70234	-1365.46666	-1365.44823	-1365.51153
$[Rh(III\text{-}H)(H)(Me)]^{2+}$	-1406.17435	-1405.89388	-1405.87270	-1405.94119
$[Rh(III\text{-}H)(HMe)]^{2+}$	-1406.19952	-1405.91695	-1405.89543	-1405.96494
$[Ir(I\text{-}H)(HMe)]^{+}$ Transition state for Oxidative addition	-1383.73877	-1383.45958	-1383.43876	-1383.50738
$[Ir(III)(HMe)]^{+}$ Transition state for Oxidative addition	-1399.74532	-1399.47836	-1399.45763	-1399.52609

Cartesian coordinates (Å) for the Optimized Structures and Transition States in the Gas Phase and Total Electronic Energy.

CH_4 -40.4618564419 Hartrees

C	0.00000	0.00000	0.00000
H	0.63014	0.63014	0.63014
H	-0.63014	-0.63014	0.63014
H	-0.63014	0.63014	-0.63014
H	0.63014	-0.63014	-0.63014

$[Pd(I\text{-}H)]^{2+}$ -1366.39228922 Hartrees

Pd	-0.00000	-1.03839	0.00001
P	-2.31209	-0.71712	0.00003
P	2.31209	-0.71712	-0.00003
C	-1.17620	1.64514	-0.00021
C	1.17619	1.64514	0.00017
C	-1.20886	3.02703	-0.00020
C	1.20886	3.02703	0.00017
C	-0.00000	3.71410	-0.00001
H	-2.16887	3.52979	-0.00034
H	2.16887	3.52979	0.00030
H	-0.00000	4.79987	-0.00001
O	2.32295	0.95445	0.00038
O	-2.32296	0.95445	-0.00046
C	3.26641	-1.15985	1.46191
H	3.40677	-2.24601	1.48794
H	4.24982	-0.67840	1.41361
H	2.75123	-0.84369	2.37226
C	3.26614	-1.15924	-1.46234
H	4.24933	-0.67732	-1.41428
H	3.40701	-2.24533	-1.48851
H	2.75054	-0.84324	-2.37251
C	-3.26610	-1.15920	1.46239
H	-4.24952	-0.67778	1.41409
H	-3.40643	-2.24534	1.48893
H	-2.75072	-0.84263	2.37249
C	-3.26644	-1.15991	-1.46187
H	-3.40725	-2.24601	-1.48757
H	-4.24965	-0.67803	-1.41378
H	-2.75107	-0.84423	-2.37228
N	-0.00000	0.95652	-0.00002

$[Pd(I\text{-}H)(HMe)]^{2+}$ -1406.88981273 Hartrees

Pd	0.00001	-0.85948	0.00772
P	2.30283	-0.52237	0.02932
P	-2.30282	-0.52245	0.02932
C	1.17060	1.84162	-0.02711

C	-1.17067	1.84158	-0.02710
C	1.20880	3.22325	-0.04555
C	-1.20893	3.22321	-0.04554
C	-0.00007	3.91053	-0.05514
H	2.16815	3.72650	-0.05137
H	-2.16830	3.72642	-0.05135
H	-0.00010	4.99612	-0.06933
O	-2.31870	1.14765	-0.01785
O	2.31864	1.14774	-0.01787
C	-3.30482	-0.98897	-1.39473
H	-3.46172	-2.07268	-1.39193
H	-4.27915	-0.49219	-1.33059
H	-2.81187	-0.70058	-2.32626
C	-3.23680	-0.91614	1.52052
H	-4.21746	-0.42998	1.47561
H	-3.38295	-1.99961	1.58394
H	-2.70292	-0.57545	2.41096
C	3.30488	-0.98886	-1.39469
H	4.27919	-0.49204	-1.33053
H	3.46183	-2.07256	-1.39189
H	2.81195	-0.70050	-2.32624
C	3.23679	-0.91601	1.52054
H	3.38298	-1.99947	1.58399
H	4.21744	-0.42982	1.47565
H	2.70289	-0.57533	2.41097
N	-0.00003	1.14947	-0.01945
C	0.00016	-3.23916	-0.18944
H	-0.89991	-3.84972	-0.11869
H	-0.00027	-2.74131	-1.17418
H	0.90074	-3.84899	-0.11902
H	-0.00003	-2.61619	0.75672

$[Pt(I-H)]^{2+}$ -1357.86945243 Hartrees

Pt	0.00000	-0.85286	0.00001
P	-2.31436	-0.56599	0.00009
P	2.31436	-0.56599	-0.00008
C	-1.18355	1.80079	-0.00007
C	1.18355	1.80079	0.00001
C	-1.20901	3.18198	-0.00009
C	1.20901	3.18198	-0.00001
C	0.00000	3.86861	-0.00006
H	-2.16929	3.68459	-0.00012
H	2.16929	3.68459	0.00001
H	0.00000	4.95438	-0.00007
O	2.32686	1.11017	0.00008
O	-2.32686	1.11017	-0.00013
C	3.26757	-1.00629	1.46160
H	3.39380	-2.09419	1.49468
H	4.25693	-0.53882	1.40915
H	2.75462	-0.67946	2.36927
C	3.26737	-1.00606	-1.46196
H	4.25663	-0.53837	-1.40970
H	3.39384	-2.09393	-1.49507
H	2.75418	-0.67934	-2.36953
C	-3.26733	-1.00602	1.46201
H	-4.25671	-0.53856	1.40964
H	-3.39355	-2.09391	1.49532
H	-2.75424	-0.67902	2.36954
C	-3.26761	-1.00633	-1.46155
H	-3.39408	-2.09421	-1.49445
H	-4.25687	-0.53864	-1.40919
H	-2.75459	-0.67976	-2.36926

N	0.00000	1.11545	-0.00002

$[Pt(I\text{-}H)(HMe)]^{2+}$ -1398.37669090 Hartrees

Pt	-0.00001	-0.72440	0.01231
P	2.30277	-0.39719	0.04200
P	-2.30278	-0.39705	0.04200
C	1.17427	1.97021	-0.03939
C	-1.17413	1.97029	-0.03939
C	1.20938	3.35096	-0.07002
C	-1.20916	3.35104	-0.07002
C	0.00013	4.03770	-0.08627
H	2.16849	3.85461	-0.07916
H	-2.16824	3.85474	-0.07916
H	0.00017	5.12311	-0.11000
O	-2.31964	1.27471	-0.02063
O	2.31973	1.27456	-0.02063
C	-3.31552	-0.87284	-1.37013
H	-3.46479	-1.95767	-1.36325
H	-4.29286	-0.38382	-1.29883
H	-2.83160	-0.58369	-2.30603
C	-3.22461	-0.77583	1.54317
H	-4.20870	-0.29735	1.50051
H	-3.36280	-1.85944	1.62170
H	-2.68359	-0.42151	2.42379
C	3.31548	-0.87304	-1.37013
H	4.29285	-0.38408	-1.29883
H	3.46468	-1.95788	-1.36325
H	2.83158	-0.58386	-2.30603
C	3.22458	-0.77603	1.54317
H	3.36270	-1.85964	1.62170
H	4.20869	-0.29761	1.50050
H	2.68358	-0.42168	2.42379
N	0.00005	1.27945	-0.02795
C	-0.00024	-3.09443	-0.30505
H	-0.90196	-3.68949	-0.16034
H	0.00027	-2.68446	-1.32239
H	0.90073	-3.69050	-0.15987
H	-0.00006	-2.42094	0.64484

$[Ir(I\text{-}NMe_2)]^{+}$ -1477.08033005 Hartrees

Ir	1.51070	0.00000	-0.00003
P	1.20505	-2.24618	-0.00001
P	1.20505	2.24618	0.00016
C	-1.16531	-1.16132	-0.00014
C	-1.16531	1.16132	-0.00003
C	-2.53747	-1.20558	-0.00017
C	-2.53747	1.20558	-0.00005
C	-3.27754	0.00000	-0.00013
H	-3.00406	-2.18007	-0.00030
H	-3.00406	2.18007	0.00007
O	-0.48467	2.31825	0.00006
O	-0.48467	-2.31825	-0.00020
C	1.59495	3.29076	1.43254
H	2.67795	3.44413	1.47563
H	1.09917	4.26231	1.35133
H	1.27982	2.78833	2.34933
C	1.59509	3.29122	-1.43183
H	1.09906	4.26263	-1.35046
H	2.67806	3.44486	-1.47460
H	1.28029	2.78899	-2.34885
C	1.59490	-3.29085	1.43231

H	1.09913	-4.26240	1.35102
H	2.67789	-3.44421	1.47544
H	1.27971	-2.78848	2.34912
C	1.59515	-3.29114	-1.43206
H	2.67812	-3.44478	-1.47479
H	1.09910	-4.26254	-1.35077
H	1.28039	-2.78884	-2.34906
N	-0.44829	0.00000	-0.00007
N	-4.62554	0.00000	-0.00017
C	-5.35454	1.25555	-0.00054
H	-5.12579	1.85110	-0.89191
H	-6.42339	1.04731	-0.00128
H	-5.12695	1.85103	0.89119
C	-5.35454	-1.25555	0.00017
H	-5.12689	-1.85104	-0.89153
H	-5.12585	-1.85109	0.89157
H	-6.42339	-1.04731	0.00084

$[Ir(I\text{-}NMe_2)(H)(Me)]^+$ -1517.58296775 Hartrees

Ir	-1.42550	0.00000	-0.03291
P	-1.03606	-2.24423	0.03385
P	-1.03604	2.24423	0.03380
C	1.37308	-1.15686	-0.02526
C	1.37310	1.15685	-0.02528
C	2.74632	-1.21426	-0.01563
C	2.74633	1.21423	-0.01565
C	3.47972	-0.00002	-0.01974
H	3.22303	-2.18349	0.00225
H	3.22306	2.18346	0.00220
O	0.65964	2.30458	-0.00691
O	0.65962	-2.30459	-0.00687
C	-1.44152	3.34224	-1.35343
H	-2.52424	3.50106	-1.37039
H	-0.93489	4.30542	-1.24702
H	-1.14399	2.87869	-2.29700
C	-1.39593	3.22003	1.51729
H	-0.91803	4.20195	1.46584
H	-2.48016	3.34642	1.59675
H	-1.04450	2.68471	2.40190
C	-1.44155	-3.34225	-1.35336
H	-0.93494	-4.30544	-1.24694
H	-2.52427	-3.50105	-1.37033
H	-1.14401	-2.87872	-2.29695
C	-1.39596	-3.21999	1.51735
H	-2.48019	-3.34637	1.59682
H	-0.91806	-4.20192	1.46591
H	-1.04453	-2.68466	2.40195
N	0.67904	-0.00001	-0.05091
C	-3.49763	0.00001	-0.16400
H	-3.98578	0.87885	0.27070
H	-3.74794	-0.00006	-1.24089
H	-3.98579	-0.87877	0.27081
H	-1.47555	0.00002	1.49407
N	4.82923	-0.00001	-0.01946
C	5.55943	-1.25451	-0.00923
H	5.32071	-1.86295	-0.88909
H	6.62801	-1.04548	-0.02661
H	5.34379	-1.83854	0.89327
C	5.55939	1.25451	-0.00878
H	5.32062	1.86327	-0.88839
H	5.34377	1.83819	0.89395
H	6.62798	1.04551	-0.02627

$[Ir(I\text{-}NMe_2)(HMe)]^+$ -1517.57718194 Hartrees

Ir	1.37428	0.00000	0.00284
P	1.02595	2.23666	0.03682
P	1.02595	-2.23666	0.03684
C	-1.35036	1.15665	-0.00701
C	-1.35036	-1.15665	-0.00702
C	-2.72315	1.20693	-0.01596
C	-2.72315	-1.20694	-0.01597
C	-3.46166	-0.00001	-0.02357
H	-3.19197	2.18020	-0.01392
H	-3.19196	-2.18021	-0.01395
O	-0.66343	-2.31250	0.00690
O	-0.66343	2.31250	0.00694
C	1.43096	-3.32261	-1.36238
H	2.51350	-3.48216	-1.38885
H	0.92988	-4.28947	-1.26164
H	1.12702	-2.84608	-2.29671
C	1.38953	-3.25113	1.49872
H	0.89350	-4.22346	1.43075
H	2.47120	-3.40472	1.56566
H	1.05772	-2.72786	2.39778
C	1.43091	3.32258	-1.36245
H	0.92985	4.28945	-1.26171
H	2.51344	3.48211	-1.38898
H	1.12692	2.84602	-2.29675
C	1.38957	3.25118	1.49865
H	2.47124	3.40479	1.56553
H	0.89351	4.22350	1.43068
H	1.05781	2.72794	2.39775
N	-0.63462	0.00000	-0.00834
C	3.71903	-0.00001	-0.28102
H	4.32279	-0.89633	-0.14143
H	3.29686	0.00026	-1.29439
H	4.32325	0.89596	-0.14111
H	3.02191	-0.00004	0.66949
N	-4.81083	-0.00001	-0.03398
C	-5.53965	1.25505	-0.03461
H	-5.30145	1.85607	-0.91986
H	-6.60851	1.04703	-0.04825
H	-5.32187	1.84627	0.86259
C	-5.53965	-1.25507	-0.03483
H	-5.30148	-1.85590	-0.92022
H	-5.32182	-1.84647	0.86223
H	-6.60851	-1.04705	-0.04837

$[Ir(I\text{-}H)]^+$ -1343.24708111 Hartrees

Ir	0.00021	-0.87006	-0.00027
P	2.25152	-0.58051	0.00016
P	-2.25170	-0.58104	0.00017
C	1.16909	1.79021	0.00016
C	-1.16936	1.78996	0.00000
C	1.20235	3.17451	-0.00018
C	-1.20281	3.17431	0.00003
C	-0.00029	3.86683	-0.00005
H	2.16507	3.66965	-0.00009
H	-2.16561	3.66928	-0.00001
H	-0.00051	4.95176	-0.00013
O	-2.32120	1.11160	-0.00023
O	2.32100	1.11210	0.00102
C	-3.29135	-0.97145	-1.43384

H	-3.44241	-2.05483	-1.47763
H	-4.26425	-0.47835	-1.35227
H	-2.78966	-0.65409	-2.35030
C	-3.29062	-0.97076	1.43490
H	-4.26266	-0.47578	1.35453
H	-3.44380	-2.05389	1.47796
H	-2.78748	-0.65519	2.35118
C	3.29086	-0.97037	-1.43422
H	4.26388	-0.47754	-1.35266
H	3.44188	-2.05379	-1.47813
H	2.78895	-0.65320	-2.35062
C	3.29064	-0.97161	1.43434
H	3.44313	-2.05488	1.47643
H	4.26300	-0.47724	1.35416
H	2.78791	-0.65651	2.35100
N	-0.00004	1.08755	-0.00011

$[Ir(I-H)(H)(Me)]^+$ -1383.75069036 Hartrees

Ir	-0.00000	-0.79570	-0.02759
P	2.24919	-0.41969	0.03003
P	-2.24919	-0.41969	0.03003
C	1.16490	1.99306	-0.02892
C	-1.16490	1.99306	-0.02892
C	1.21150	3.37920	-0.02865
C	-1.21148	3.37920	-0.02866
C	0.00001	4.06277	-0.03227
H	2.16771	3.88653	-0.02020
H	-2.16770	3.88652	-0.02020
H	0.00000	5.14812	-0.03134
O	-2.30603	1.28004	-0.01013
O	2.30603	1.28004	-0.01013
C	-3.33405	-0.82299	-1.36659
H	-3.49265	-1.90582	-1.38578
H	-4.29839	-0.31732	-1.26584
H	-2.86442	-0.52397	-2.30669
C	-3.23267	-0.77565	1.50794
H	-4.21286	-0.29491	1.44979
H	-3.36352	-1.85955	1.58601
H	-2.70247	-0.42649	2.39654
C	3.33405	-0.82301	-1.36659
H	4.29839	-0.31733	-1.26585
H	3.49265	-1.90583	-1.38578
H	2.86442	-0.52397	-2.30669
C	3.23267	-0.77567	1.50794
H	3.36353	-1.85956	1.58600
H	4.21286	-0.29493	1.44979
H	2.70247	-0.42650	2.39654
N	0.00000	1.31785	-0.04529
C	0.00000	-2.86329	-0.14182
H	-0.87962	-3.34961	0.29232
H	0.00002	-3.11283	-1.21960
H	0.87962	-3.34960	0.29235
H	-0.00000	-0.77886	1.50052

$[Ir(I-H)(HMe)]^+$ -1383.74495646 Hartrees

Ir	-0.00001	-0.74352	0.00448
P	2.24171	-0.41072	0.03443
P	-2.24172	-0.41068	0.03443
C	1.16435	1.96595	-0.02811
C	-1.16432	1.96597	-0.02811
C	1.20400	3.35056	-0.05107

C	-1.20394	3.35058	-0.05106
C	0.00004	4.04175	-0.06397
H	2.16550	3.84771	-0.05615
H	-2.16543	3.84775	-0.05615
H	0.00005	5.12665	-0.08153
O	-2.31505	1.28109	-0.00815
O	2.31507	1.28105	-0.00815
C	-3.32181	-0.82576	-1.36463
H	-3.48106	-1.90856	-1.38350
H	-4.28924	-0.32485	-1.26851
H	-2.84443	-0.52795	-2.30053
C	-3.25296	-0.76295	1.49968
H	-4.22532	-0.26749	1.42791
H	-3.40728	-1.84412	1.57393
H	-2.73000	-0.42484	2.39660
C	3.32180	-0.82582	-1.36463
H	4.28924	-0.32492	-1.26852
H	3.48103	-1.90862	-1.38350
H	2.84442	-0.52800	-2.30052
C	3.25295	-0.76301	1.49968
H	3.40725	-1.84417	1.57393
H	4.22532	-0.26756	1.42792
H	2.72999	-0.42489	2.39660
N	0.00001	1.26506	-0.02135
C	-0.00006	-3.09143	-0.22750
H	-0.89744	-3.69502	-0.09668
H	-0.00009	-2.65635	-1.23827
H	0.89732	-3.69502	-0.09673
H	-0.00000	-2.39503	0.71386

$[Ir(I\text{-}CF_3)]^+$ -1679.96267613 Hartrees

Ir	1.66973	-0.00003	0.00606
P	1.38316	-2.25353	0.00161
P	1.38327	2.25350	0.00161
C	-0.98730	-1.16944	-0.02154
C	-0.98723	1.16951	-0.02153
C	-2.37099	-1.20387	-0.03761
C	-2.37094	1.20402	-0.03759
C	-3.05961	0.00010	-0.04267
H	-2.87455	-2.16197	-0.05294
H	-2.87446	2.16213	-0.05290
O	-0.31198	2.32014	-0.01739
O	-0.31209	-2.32009	-0.01741
C	1.75430	3.29275	1.44023
H	2.83687	3.44602	1.49607
H	1.26044	4.26476	1.35279
H	1.42773	2.79054	2.35320
C	1.78653	3.28993	-1.43033
H	1.29086	4.26211	-1.35604
H	2.87009	3.44315	-1.46206
H	1.48065	2.78578	-2.34935
C	1.75413	-3.29279	1.44025
H	1.26024	-4.26478	1.35281
H	2.83669	-3.44610	1.49610
H	1.42757	-2.79057	2.35320
C	1.78639	-3.28999	-1.43032
H	2.86994	-3.44327	-1.46203
H	1.29067	-4.26215	-1.35603
H	1.48055	-2.78584	-2.34935
N	-0.28492	0.00002	-0.01230
C	-4.57083	0.00006	0.00345
F	-5.06603	1.08486	-0.59593

F	-4.98678	-0.00119	1.27302
F	-5.06598	-1.08362	-0.59801

$[Ir(I\text{-}CF_3)(H)(Me)]^+$ -1720.46640695 Hartrees

Ir	-1.58952	0.00000	-0.02464
P	-1.21555	-2.25070	0.02848
P	-1.21554	2.25070	0.02848
C	1.19721	-1.16509	-0.04274
C	1.19721	1.16509	-0.04274
C	2.58313	-1.21278	-0.05244
C	2.58314	1.21277	-0.05244
C	3.26307	-0.00000	-0.05803
H	3.09840	-2.16456	-0.05713
H	3.09841	2.16455	-0.05712
O	0.48755	2.30472	-0.02200
O	0.48755	-2.30472	-0.02201
C	-1.62287	3.33288	-1.36834
H	-2.70563	3.49290	-1.38222
H	-1.11562	4.29679	-1.27140
H	-1.32933	2.86133	-2.30920
C	-1.55774	3.23648	1.50748
H	-1.07399	4.21490	1.44477
H	-2.64074	3.37149	1.59160
H	-1.20545	2.70629	2.39485
C	-1.62289	-3.33288	-1.36834
H	-1.11565	-4.29679	-1.27140
H	-2.70565	-3.49288	-1.38221
H	-1.32934	-2.86133	-2.30920
C	-1.55774	-3.23647	1.50749
H	-2.64074	-3.37148	1.59162
H	-1.07399	-4.21490	1.44477
H	-1.20544	-2.70629	2.39486
N	0.52288	-0.00000	-0.05385
C	-3.65690	-0.00001	-0.12340
H	-4.13962	0.87984	0.31388
H	-3.91268	-0.00012	-1.19970
H	-4.13961	-0.87977	0.31406
H	-1.55677	0.00000	1.50338
C	4.77512	-0.00000	-0.00360
F	5.18370	0.00003	1.26860
F	5.27522	1.08387	-0.60099
F	5.27522	-1.08391	-0.60093

$[Ir(I\text{-}CF_3)(HMe)]^+$ -1720.46103049 Hartrees

Ir	-1.53338	0.00003	0.00530
P	-1.20362	-2.24353	0.03109
P	-1.20354	2.24360	0.03110
C	1.17278	-1.16459	-0.02491
C	1.17281	1.16457	-0.02503
C	2.55699	-1.20534	-0.04743
C	2.55702	1.20528	-0.04755
C	3.24446	-0.00004	-0.05714
H	3.06235	-2.16227	-0.06167
H	3.06241	2.16219	-0.06188
O	0.49108	2.31408	-0.00864
O	0.49101	-2.31407	-0.00835
C	-1.61329	3.31745	-1.37354
H	-2.69584	3.47842	-1.39468
H	-1.11118	4.28455	-1.28028
H	-1.31479	2.83582	-2.30704
C	-1.55438	3.25956	1.49265

H	-1.05584	4.23015	1.41823
H	-2.63522	3.41775	1.56409
H	-1.21965	2.73876	2.39211
C	-1.61321	-3.31723	-1.37371
H	-1.11121	-4.28439	-1.28046
H	-2.69577	-3.47809	-1.39506
H	-1.31449	-2.83555	-2.30712
C	-1.55469	-3.25964	1.49249
H	-2.63553	-3.41789	1.56371
H	-1.05609	-4.23020	1.41805
H	-1.22013	-2.73893	2.39206
N	0.47212	0.00000	-0.01753
C	-3.88086	-0.00021	-0.21605
H	-4.48502	0.89717	-0.08865
H	-3.44097	0.00015	-1.22560
H	-4.48408	-0.89826	-0.08887
H	-3.18681	0.00007	0.72469
C	4.75540	-0.00006	-0.01682
F	5.17776	0.00008	1.25114
F	5.24975	-1.08428	-0.61887
F	5.24977	1.08402	-0.61911

$[Ir(I\text{-}NMe_3)]^{2+}$ -1516.59733564 Hartrees

Ir	-1.69679	-0.00008	0.00161
P	-1.42585	2.26151	0.00008
P	-1.42549	-2.26163	0.00009
C	0.95276	1.16722	-0.01187
C	0.95296	-1.16697	-0.01192
C	2.34457	1.20300	-0.02417
C	2.34475	-1.20250	-0.02425
C	3.03546	0.00031	-0.03901
H	2.80385	2.18116	-0.02978
H	2.80426	-2.18056	-0.02979
O	0.29441	-2.31239	-0.00658
O	0.29405	2.31254	-0.00654
C	-1.79221	-3.29456	1.43990
H	-2.87544	-3.45130	1.48602
H	-1.29958	-4.26770	1.35710
H	-1.47899	-2.79041	2.35648
C	-1.80367	-3.29314	-1.43780
H	-1.31079	-4.26654	-1.35975
H	-2.88729	-3.44934	-1.47587
H	-1.49717	-2.78818	-2.35622
C	-1.79277	3.29441	1.43987
H	-1.30028	4.26762	1.35707
H	-2.87602	3.45099	1.48595
H	-1.47950	2.79032	2.35646
C	-1.80413	3.29296	-1.43784
H	-2.88777	3.44900	-1.47594
H	-1.31139	4.26643	-1.35978
H	-1.49753	2.78803	-2.35624
N	0.24846	0.00008	-0.00751
N	4.52789	0.00018	-0.00106
C	5.10309	-1.21068	-0.68619
H	4.71445	-1.26439	-1.70337
H	6.18740	-1.10116	-0.70261
H	4.85112	-2.10939	-0.12675
C	5.10361	1.21286	-0.68246
H	4.71530	1.26973	-1.69959
H	4.85182	2.10998	-0.12038
H	6.18789	1.10305	-0.69889
C	4.96589	-0.00205	1.44273

H	4.57411	0.89046	1.93077
H	4.57387	-0.89591	1.92811
H	6.05682	-0.00226	1.47304

$[Ir(I\text{-}NMe_3)(H)(Me)]^{2+}$ -1557.10153373 Hartrees

Ir	-1.62035	0.00000	-0.02651
P	-1.26193	-2.25677	0.02582
P	-1.26192	2.25678	0.02582
C	1.16474	-1.16376	-0.03604
C	1.16475	1.16374	-0.03604
C	2.55974	-1.21219	-0.03941
C	2.55975	1.21216	-0.03941
C	3.24040	-0.00001	-0.05331
H	3.03150	-2.18416	-0.03277
H	3.03152	2.18413	-0.03277
O	0.47151	2.29585	-0.01343
O	0.47150	-2.29586	-0.01343
C	-1.63824	3.33409	-1.37943
H	-2.72024	3.50339	-1.39955
H	-1.12821	4.29647	-1.28085
H	-1.34756	2.85771	-2.31874
C	-1.58960	3.24634	1.50196
H	-1.10080	4.22225	1.43800
H	-2.67246	3.39268	1.57820
H	-1.25273	2.71594	2.39515
C	-1.63827	-3.33408	-1.37943
H	-1.12826	-4.29647	-1.28085
H	-2.72027	-3.50337	-1.39954
H	-1.34759	-2.85771	-2.31874
C	-1.58962	-3.24633	1.50196
H	-2.67249	-3.39266	1.57821
H	-1.10083	-4.22225	1.43800
H	-1.25275	-2.71593	2.39516
N	0.49334	-0.00001	-0.05501
C	-3.68277	0.00001	-0.11596
H	-4.16376	0.88017	0.32021
H	-3.93078	-0.00003	-1.19428
H	-4.16377	-0.88013	0.32027
H	-1.58220	0.00001	1.50257
N	4.73595	-0.00001	-0.00708
C	5.31753	-1.21104	-0.68655
H	4.93336	-1.26877	-1.70515
H	6.40152	-1.09804	-0.69887
H	5.06671	-2.10941	-0.12628
C	5.31750	1.21107	-0.68650
H	4.93333	1.26882	-1.70511
H	5.06664	2.10941	-0.12620
H	6.40149	1.09810	-0.69882
C	5.16421	-0.00003	1.43905
H	4.76915	0.89311	1.92328
H	4.76917	-0.89319	1.92325
H	6.25490	-0.00002	1.47679

$[Ir(I\text{-}NMe_3)(HMe)]^{2+}$ -1557.09960677 Hartrees

Ir	-1.55960	0.00004	0.00265
P	-1.24655	-2.25079	0.02620
P	-1.24636	2.25085	0.02619
C	1.13781	-1.16236	-0.01728
C	1.13790	1.16221	-0.01726
C	2.53005	-1.20413	-0.03421
C	2.53016	1.20388	-0.03416

C	3.21979	-0.00014	-0.05262
H	2.99079	-2.18144	-0.03841
H	2.99099	2.18114	-0.03841
O	0.47305	2.30637	-0.00086
O	0.47286	-2.30646	-0.00088
C	-1.62882	3.31580	-1.38857
H	-2.71074	3.48353	-1.41648
H	-1.12610	4.28269	-1.29542
H	-1.33159	2.82867	-2.31963
C	-1.59076	3.26871	1.48382
H	-1.08977	4.23815	1.40982
H	-2.67161	3.43506	1.54443
H	-1.27165	2.74920	2.38969
C	-1.62912	-3.31572	-1.38854
H	-1.12649	-4.28265	-1.29539
H	-2.71106	-3.48337	-1.41643
H	-1.33187	-2.82862	-2.31962
C	-1.59101	-3.26861	1.48385
H	-2.67187	-3.43487	1.54447
H	-1.09010	-4.23810	1.40985
H	-1.27184	-2.74912	2.38970
N	0.43502	-0.00004	-0.01479
C	-3.90515	0.00005	-0.19118
H	-4.51021	0.89838	-0.07714
H	-3.45052	0.00006	-1.19749
H	-4.51001	-0.89842	-0.07712
H	-3.22469	0.00008	0.75153
N	4.71259	-0.00010	-0.01776
C	5.28667	-1.21059	-0.70299
H	4.89532	-1.26531	-1.71904
H	6.37097	-1.10122	-0.72187
H	5.03578	-2.10904	-0.14272
C	5.28634	1.21172	-0.70086
H	4.89502	1.26809	-1.71684
H	5.03509	2.10909	-0.13900
H	6.37067	1.10272	-0.71987
C	5.15409	-0.00123	1.42454
H	4.76253	0.89140	1.91251
H	4.76287	-0.89481	1.91103
H	6.24511	-0.00105	1.45273

$[Ir(II)]^+$ -2532.93798460 Hartrees

Ir	0.00000	-0.51624	-0.00025
P	-2.21686	-0.18922	-0.00007
P	2.21686	-0.18922	-0.00007
C	-1.16468	2.15704	-0.00022
C	1.16467	2.15704	-0.00022
C	-1.20397	3.53725	-0.00022
C	1.20396	3.53724	-0.00022
C	-0.00000	4.22982	-0.00022
H	-2.16735	4.03188	-0.00022
H	2.16735	4.03187	-0.00022
H	0.00000	5.31471	-0.00022
O	2.32404	1.46857	-0.00021
O	-2.32405	1.46857	-0.00021
C	3.30402	-0.62626	1.47800
C	3.30463	-0.62645	-1.47762
C	-3.30400	-0.62626	1.47801
C	-3.30464	-0.62646	-1.47761
N	0.00000	1.45154	-0.00019
F	4.50672	-0.08024	1.39965
F	2.69531	-0.19702	2.57907

F	3.41287	-1.95255	1.51461
F	4.50699	-0.07968	-1.39925
F	3.41426	-1.95270	-1.51344
F	2.69597	-0.19820	-2.57911
F	-3.41430	-1.95271	-1.51340
F	-2.69598	-0.19825	-2.57911
F	-4.50699	-0.07966	-1.39925
F	-4.50672	-0.08027	1.39965
F	-3.41282	-1.95254	1.51466
F	-2.69530	-0.19698	2.57908

$[Ir(II)(H)(Me)]^+$ -2573.44327984 Hartrees

Ir	0.00000	-0.51945	-0.04519
P	2.21075	-0.09764	0.01017
P	-2.21075	-0.09764	0.01017
C	1.15894	2.29296	-0.07434
C	-1.15894	2.29296	-0.07434
C	1.21334	3.67490	-0.07956
C	-1.21334	3.67490	-0.07956
C	0.00000	4.35853	-0.08688
H	2.16998	4.18198	-0.07161
H	-2.16998	4.18198	-0.07161
H	0.00000	5.44375	-0.09007
O	-2.30648	1.56455	-0.04808
O	2.30648	1.56455	-0.04808
C	-3.33074	-0.55982	-1.43281
C	-3.26093	-0.47335	1.52778
C	3.33074	-0.55982	-1.43281
C	3.26093	-0.47335	1.52778
N	0.00000	1.61683	-0.08942
C	0.00000	-2.58154	-0.11566
H	-0.88417	-3.04545	0.32815
H	-0.00001	-2.83283	-1.19258
H	0.88417	-3.04545	0.32814
H	0.00000	-0.47425	1.48497
F	-2.62709	0.00737	2.59504
F	-3.37103	-1.79350	1.63112
F	-4.46414	0.07237	1.44685
F	-3.57464	-1.86423	-1.36057
F	-2.65658	-0.29604	-2.55498
F	-4.46855	0.11228	-1.43651
F	2.65658	-0.29604	-2.55498
F	3.57464	-1.86423	-1.36057
F	3.37104	-1.79350	1.63112
F	4.46415	0.07237	1.44685
F	2.62709	0.00737	2.59504
F	4.46855	0.11228	-1.43651

$[Ir(II)(HMe)]^+$ -2573.44369502 Hartrees

Ir	0.00000	-0.45232	-0.04733
P	2.20141	-0.08039	0.00922
P	-2.20142	-0.08040	0.00921
C	1.15961	2.27071	-0.12039
C	-1.15962	2.27070	-0.12040
C	1.20554	3.65057	-0.16599
C	-1.20556	3.65056	-0.16600
C	-0.00001	4.34153	-0.19158
H	2.16747	4.14745	-0.17717
H	-2.16749	4.14744	-0.17719
H	-0.00001	5.42587	-0.22697
O	-2.31753	1.57391	-0.08495

O	2.31753	1.57392	-0.08491
C	-3.36293	-0.59788	-1.38130
C	-3.22002	-0.44029	1.55461
C	3.36293	-0.59786	-1.38130
C	3.22002	-0.44031	1.55461
N	-0.00000	1.56782	-0.10503
C	0.00002	-2.79124	-0.30248
H	-0.90147	-3.38771	-0.16824
H	-0.00002	-2.36495	-1.31698
H	0.90151	-3.38770	-0.16829
H	0.00002	-2.11100	0.65091
F	-3.55568	-1.91354	-1.26502
F	-2.76478	-0.34229	-2.54234
F	-4.52737	0.02784	-1.34109
F	-2.60018	0.10509	2.59656
F	-3.26426	-1.76415	1.70724
F	-4.45235	0.03788	1.47622
F	3.26429	-1.76418	1.70718
F	4.45234	0.03788	1.47623
F	2.60017	0.10502	2.59657
F	4.52738	0.02785	-1.34107
F	3.55566	-1.91352	-1.26506
F	2.76478	-0.34222	-2.54234

$[Ir(III)]^+$ -1359.25500408 Hartrees

Ir	0.00004	-0.86795	-0.00007
P	2.25796	-0.57198	-0.00002
P	-2.25800	-0.57207	0.00006
C	1.16019	1.78502	0.00020
C	-1.16023	1.78497	-0.00011
C	1.13962	3.17654	0.00012
C	-1.13971	3.17649	-0.00012
H	2.07798	3.72189	0.00026
H	-2.07810	3.72180	-0.00026
O	-2.31871	1.12643	-0.00030
O	2.31869	1.12651	0.00052
C	-3.29542	-0.95703	-1.43574
H	-3.45119	-2.03982	-1.47958
H	-4.26628	-0.45983	-1.35459
H	-2.79189	-0.64151	-2.35187
C	-3.29499	-0.95647	1.43633
H	-4.26528	-0.45803	1.35592
H	-3.45211	-2.03909	1.47972
H	-2.79059	-0.64199	2.35234
C	3.29509	-0.95636	-1.43620
H	4.26595	-0.45915	-1.35511
H	3.45089	-2.03913	-1.48041
H	2.79135	-0.64058	-2.35213
C	3.29522	-0.95710	1.43585
H	3.45203	-2.03978	1.47885
H	4.26564	-0.45893	1.35535
H	2.79115	-0.64277	2.35208
N	-0.00001	1.07560	0.00004
N	-0.00006	3.85434	-0.00001

$[Ir(III)(H)(Me)]^+$ -1399.75778404 Hartrees

Ir	0.00000	-0.79369	-0.02686
P	2.25396	-0.41401	0.02839
P	-2.25396	-0.41402	0.02839
C	1.15765	1.98850	-0.02893
C	-1.15765	1.98850	-0.02893

C	1.14854	3.38314	-0.02687
C	-1.14855	3.38314	-0.02687
H	2.07856	3.94195	-0.01957
H	-2.07857	3.94194	-0.01957
O	-2.30347	1.29423	-0.01120
O	2.30346	1.29423	-0.01121
C	-3.33677	-0.80809	-1.37128
H	-3.50150	-1.89007	-1.39206
H	-4.29845	-0.29724	-1.27088
H	-2.86407	-0.51038	-2.31026
C	-3.23917	-0.76151	1.50616
H	-4.21669	-0.27559	1.44607
H	-3.37616	-1.84469	1.58503
H	-2.70819	-0.41444	2.39513
C	3.33677	-0.80809	-1.37128
H	4.29845	-0.29724	-1.27089
H	3.50150	-1.89006	-1.39207
H	2.86408	-0.51037	-2.31026
C	3.23917	-0.76150	1.50616
H	3.37616	-1.84468	1.58503
H	4.21669	-0.27558	1.44607
H	2.70820	-0.41443	2.39513
N	-0.00000	1.30908	-0.04554
C	0.00001	-2.86038	-0.13191
H	-0.88008	-3.34494	0.30260
H	0.00004	-3.11021	-1.20975
H	0.88007	-3.34493	0.30265
H	0.00000	-0.76479	1.50147
N	-0.00001	4.04955	-0.02954

$[Ir(III)(HMe)]^{+}$ -1399.75344070 Hartrees

Ir	0.00001	-0.74072	0.00423
P	2.24733	-0.40321	0.02933
P	-2.24732	-0.40328	0.02933
C	1.15568	1.96021	-0.02517
C	-1.15575	1.96018	-0.02517
C	1.14078	3.35214	-0.04407
C	-1.14089	3.35210	-0.04407
H	2.07757	3.89962	-0.04938
H	-2.07769	3.89956	-0.04938
O	-2.31255	1.29512	-0.00834
O	2.31251	1.29519	-0.00834
C	-3.32061	-0.80775	-1.37673
H	-3.48590	-1.88963	-1.39949
H	-4.28568	-0.30177	-1.28328
H	-2.83731	-0.50959	-2.30950
C	-3.26293	-0.75280	1.49103
H	-4.23196	-0.25115	1.41722
H	-3.42448	-1.83322	1.56161
H	-2.74109	-0.42014	2.39067
C	3.32063	-0.80766	-1.37674
H	4.28569	-0.30165	-1.28329
H	3.48595	-1.88953	-1.39950
H	2.83732	-0.50951	-2.30950
C	3.26295	-0.75270	1.49102
H	3.42452	-1.83312	1.56161
H	4.23197	-0.25103	1.41722
H	2.74110	-0.42006	2.39067
N	-0.00002	1.25245	-0.01948
C	0.00013	-3.09060	-0.19168
H	-0.89834	-3.69495	-0.07473
H	0.00012	-2.63621	-1.19703

H	0.89863	-3.69488	-0.07466
H	-0.00000	-2.40191	0.74653
N	-0.00006	4.02906	-0.05458

$[Ir(III-H)]^{2+}$ -1359.51012456 Hartrees

Ir	0.00000	-0.87072	-0.00005
P	2.28193	-0.62089	-0.00008
P	-2.28194	-0.62090	0.00009
C	1.17573	1.75095	0.00006
C	-1.17573	1.75095	0.00002
C	1.17867	3.14084	0.00006
C	-1.17867	3.14084	0.00005
H	2.09692	3.71406	0.00008
H	-2.09692	3.71406	0.00005
O	-2.31797	1.11039	-0.00002
O	2.31798	1.11039	0.00012
C	-3.29928	-0.98958	-1.44539
H	-3.45576	-2.07362	-1.48798
H	-4.27418	-0.49883	-1.36714
H	-2.79250	-0.67797	-2.36131
C	-3.29894	-0.98941	1.44587
H	-4.27348	-0.49785	1.36822
H	-3.45631	-2.07334	1.48802
H	-2.79155	-0.67862	2.36172
C	3.29902	-0.98937	-1.44580
H	4.27392	-0.49858	-1.36769
H	3.45556	-2.07340	-1.48852
H	2.79206	-0.67771	-2.36159
C	3.29916	-0.98963	1.44547
H	3.45635	-2.07359	1.48756
H	4.27377	-0.49823	1.36763
H	2.79201	-0.67876	2.36143
N	0.00000	1.04297	0.00001
N	0.00000	3.77569	0.00006
H	0.00000	4.79413	0.00007

$[Ir(III-H)(H)(Me)]^{2+}$ -1400.01314022 Hartrees

Ir	0.00000	-0.80425	-0.02516
P	2.27092	-0.47248	0.02588
P	-2.27092	-0.47248	0.02588
C	1.17328	1.95641	-0.02487
C	-1.17328	1.95641	-0.02487
C	1.18830	3.35428	-0.02158
C	-1.18831	3.35428	-0.02158
H	2.09582	3.94424	-0.01393
H	-2.09582	3.94424	-0.01393
O	-2.29828	1.28303	-0.00629
O	2.29828	1.28303	-0.00629
C	-3.33696	-0.82744	-1.38939
H	-3.51307	-1.90888	-1.41619
H	-4.29787	-0.31407	-1.29025
H	-2.85528	-0.53432	-2.32533
C	-3.25902	-0.78898	1.50173
H	-4.23236	-0.29484	1.43483
H	-3.41399	-1.87153	1.57523
H	-2.72912	-0.45777	2.39748
C	3.33696	-0.82744	-1.38939
H	4.29787	-0.31407	-1.29025
H	3.51307	-1.90888	-1.41619
H	2.85528	-0.53432	-2.32533
C	3.25902	-0.78898	1.50173

H	3.41399	-1.87153	1.57523
H	4.23236	-0.29484	1.43484
H	2.72912	-0.45777	2.39748
N	0.00000	1.29164	-0.04592
C	0.00000	-2.86189	-0.11347
H	-0.88135	-3.34503	0.31622
H	0.00000	-3.09304	-1.19646
H	0.88135	-3.34503	0.31622
H	0.00000	-0.77758	1.50589
N	0.00000	3.97339	-0.02426
H	0.00000	4.99278	-0.02295

$[Ir(III-H)(HMe)]^{2+}$ -1400.01688346 Hartrees

Ir	0.00001	-0.74427	-0.00034
P	-2.27250	-0.45192	0.00008
P	2.27251	-0.45183	0.00008
C	-1.17000	1.92127	-0.00019
C	1.16992	1.92131	-0.00019
C	-1.17905	3.30914	0.00008
C	1.17892	3.30919	0.00008
H	-2.09701	3.88226	0.00018
H	2.09686	3.88234	0.00018
O	2.31304	1.27374	-0.00043
O	-2.31310	1.27365	-0.00043
C	3.29787	-0.81508	1.44348
H	3.47013	-1.89633	1.48537
H	4.26565	-0.31071	1.36497
H	2.79001	-0.50939	2.36082
C	3.29963	-0.81561	-1.44190
H	4.26705	-0.31068	-1.36256
H	3.47251	-1.89679	-1.48286
H	2.79272	-0.51076	-2.36004
C	-3.29786	-0.81519	1.44348
H	-4.26566	-0.31086	1.36495
H	-3.47010	-1.89645	1.48536
H	-2.79003	-0.50949	2.36082
C	-3.29960	-0.81573	-1.44191
H	-3.47243	-1.89692	-1.48287
H	-4.26704	-0.31085	-1.36257
H	-2.79269	-0.51085	-2.36004
N	-0.00003	1.21033	-0.00030
C	0.00014	-3.06193	0.00020
H	0.90176	-3.67197	-0.00008
H	0.00016	-2.47735	0.97078
H	-0.90139	-3.67211	0.00005
H	0.00003	-2.47719	-0.97043
N	-0.00008	3.94696	0.00019
H	-0.00010	4.96457	0.00039

$[Rh(I-NMe_2)]^{+}$ -1483.27218667 Hartrees

Rh	1.78107	0.00000	-0.00004
P	1.45344	-2.24290	-0.00009
P	1.45344	2.24290	0.00022
C	-0.91602	-1.15611	-0.00018
C	-0.91602	1.15611	0.00001
C	-2.28893	-1.20621	-0.00021
C	-2.28893	1.20621	-0.00001
C	-3.02840	0.00000	-0.00013
H	-2.75641	-2.18021	-0.00038
H	-2.75641	2.18021	0.00015
O	-0.23442	2.31497	0.00011

O	-0.23442	-2.31497	-0.00029
C	1.83977	3.29526	1.43022
H	2.92119	3.46037	1.46976
H	1.33373	4.26159	1.34840
H	1.53172	2.79533	2.35099
C	1.83990	3.29583	-1.42932
H	1.33355	4.26198	-1.34729
H	2.92129	3.46128	-1.46848
H	1.53226	2.79616	-2.35036
C	1.83971	-3.29543	1.42980
H	1.33369	-4.26175	1.34784
H	2.92113	-3.46053	1.46938
H	1.53160	-2.79562	2.35061
C	1.83997	-3.29566	-1.42974
H	2.92135	-3.46112	-1.46886
H	1.33360	-4.26182	-1.34785
H	1.53237	-2.79588	-2.35073
N	-0.19975	0.00000	-0.00008
N	-4.37665	0.00000	-0.00016
C	-5.10566	1.25538	-0.00100
H	-4.87687	1.85081	-0.89241
H	-6.17454	1.04717	-0.00172
H	-4.87810	1.85137	0.89037
C	-5.10566	-1.25538	0.00066
H	-4.87805	-1.85137	-0.89070
H	-4.87692	-1.85081	0.89209
H	-6.17454	-1.04717	0.00132

$[Rh(I\text{-}NMe_2)(H)(Me)]^+$ -1523.74552423 Hartrees

Rh	1.64259	0.00000	-0.06717
P	1.26679	2.23818	0.04561
P	1.26681	-2.23817	0.04562
C	-1.14244	1.15584	-0.03455
C	-1.14243	-1.15585	-0.03456
C	-2.51543	1.21506	-0.01961
C	-2.51541	-1.21508	-0.01962
C	-3.24844	-0.00001	-0.02507
H	-2.99268	2.18389	0.00416
H	-2.99266	-2.18391	0.00414
O	-0.42826	-2.30395	-0.01410
O	-0.42828	2.30396	-0.01409
C	1.68732	-3.36423	-1.31543
H	2.76941	-3.52814	-1.31366
H	1.17471	-4.32313	-1.19856
H	1.40679	-2.91692	-2.27192
C	1.61166	-3.18880	1.54979
H	1.13687	-4.17281	1.50968
H	2.69520	-3.31122	1.64451
H	1.24922	-2.63918	2.42114
C	1.68727	3.36427	-1.31542
H	1.17460	4.32314	-1.19855
H	2.76935	3.52825	-1.31363
H	1.40678	2.91696	-2.27192
C	1.61164	3.18881	1.54979
H	2.69517	3.31128	1.64448
H	1.13681	4.17280	1.50970
H	1.24924	2.63917	2.42115
N	-0.44893	0.00000	-0.06743
C	3.69064	-0.00001	-0.22564
H	4.18217	-0.88122	0.19680
H	3.87091	-0.00029	-1.31393
H	4.18215	0.88142	0.19635

H	1.93139	0.00001	1.40320
N	-4.59748	-0.00002	-0.02450
C	-5.32817	1.25441	-0.01224
H	-5.08502	1.86614	-0.88844
H	-6.39655	1.04506	-0.03605
H	-5.11706	1.83473	0.89369
C	-5.32816	-1.25445	-0.01223
H	-5.08502	-1.86618	-0.88843
H	-5.11705	-1.83476	0.89370
H	-6.39655	-1.04510	-0.03603

$[Rh(I\text{-}NMe_2)(HMe)]^+$ -1523.76196980 Hartrees

Rh	-1.59305	0.00001	0.00205
P	-1.24262	-2.23357	0.02204
P	-1.24260	2.23358	0.02209
C	1.13165	-1.15343	-0.00817
C	1.13166	1.15343	-0.00813
C	2.50503	-1.20696	-0.01206
C	2.50504	1.20695	-0.01202
C	3.24357	-0.00001	-0.01531
H	2.97377	-2.18029	-0.01075
H	2.97378	2.18028	-0.01068
O	0.44528	2.31111	-0.00228
O	0.44527	-2.31110	-0.00236
C	-1.64453	3.31040	-1.38626
H	-2.72615	3.47637	-1.41204
H	-1.13721	4.27503	-1.29455
H	-1.34563	2.82595	-2.31828
C	-1.60862	3.26798	1.47122
H	-1.10787	4.23726	1.39333
H	-2.68982	3.42750	1.53203
H	-1.28254	2.75724	2.37975
C	-1.64456	-3.31037	-1.38633
H	-1.13725	-4.27501	-1.29463
H	-2.72618	-3.47632	-1.41211
H	-1.34565	-2.82591	-2.31834
C	-1.60861	-3.26799	1.47115
H	-2.68981	-3.42752	1.53198
H	-1.10786	-4.23727	1.39324
H	-1.28251	-2.75728	2.37969
N	0.41632	0.00000	-0.00877
C	-3.96247	-0.00005	-0.15263
H	-4.57562	0.89735	-0.08272
H	-3.44353	-0.00021	-1.12925
H	-4.57569	-0.89738	-0.08245
H	-3.30200	0.00008	0.77407
N	4.59288	-0.00001	-0.01934
C	5.32163	-1.25501	-0.01688
H	5.08850	-1.85551	-0.90387
H	6.39060	-1.04704	-0.02429
H	5.09876	-1.84702	0.87856
C	5.32165	1.25498	-0.01747
H	5.08858	1.85503	-0.90478
H	5.09872	1.84745	0.87766
H	6.39061	1.04700	-0.02469

$[Rh(I\text{-}H)]^+$ -1349.43915362 Hartrees

Rh	0.00000	-1.05488	0.00007
P	2.24797	-0.74306	0.00011
P	-2.24797	-0.74306	0.00011
C	1.16414	1.62883	-0.00026

C	-1.16414	1.62883	-0.00026
C	1.20366	3.01425	-0.00043
C	-1.20366	3.01425	-0.00043
C	0.00000	3.70544	-0.00052
H	2.16556	3.51084	-0.00049
H	-2.16556	3.51084	-0.00049
H	0.00000	4.79054	-0.00065
O	-2.31708	0.94871	-0.00018
O	2.31708	0.94871	-0.00018
C	-3.29542	-1.12844	-1.43182
H	-3.46039	-2.20996	-1.47119
H	-4.26208	-0.62294	-1.35058
H	-2.79481	-0.82020	-2.35217
C	-3.29514	-1.12797	1.43238
H	-4.26187	-0.62261	1.35111
H	-3.45998	-2.20950	1.47222
H	-2.79440	-0.81931	2.35252
C	3.29542	-1.12844	-1.43182
H	4.26208	-0.62294	-1.35058
H	3.46039	-2.20997	-1.47119
H	2.79481	-0.82020	-2.35217
C	3.29514	-1.12797	1.43238
H	3.45998	-2.20950	1.47222
H	4.26187	-0.62261	1.35111
H	2.79440	-0.81931	2.35252
N	0.00000	0.92941	-0.00018

$[Rh(I-H)(H)(Me)]^+$ -1389.91282938 Hartrees

Rh	0.00000	-0.93134	-0.06362
P	2.24325	-0.56847	0.03885
P	-2.24325	-0.56848	0.03885
C	1.16388	1.84588	-0.04068
C	-1.16388	1.84587	-0.04068
C	1.21243	3.23226	-0.02883
C	-1.21246	3.23226	-0.02883
C	-0.00002	3.91480	-0.02864
H	2.16805	3.74056	-0.01341
H	-2.16807	3.74055	-0.01342
H	-0.00002	5.00020	-0.01844
O	-2.30494	1.13119	-0.02169
O	2.30494	1.13119	-0.02169
C	-3.35332	-0.98636	-1.33472
H	-3.51836	-2.06837	-1.33508
H	-4.31304	-0.47343	-1.22590
H	-2.89760	-0.70513	-2.28705
C	-3.20600	-0.90809	1.53497
H	-4.18882	-0.43185	1.48420
H	-3.33179	-1.99138	1.62932
H	-2.66471	-0.54606	2.41169
C	3.35332	-0.98634	-1.33472
H	4.31304	-0.47342	-1.22590
H	3.51836	-2.06835	-1.33509
H	2.89759	-0.70512	-2.28705
C	3.20600	-0.90809	1.53497
H	3.33179	-1.99136	1.62931
H	4.18882	-0.43183	1.48420
H	2.66471	-0.54605	2.41169
N	-0.00000	1.17305	-0.06771
C	0.00002	-2.97872	-0.15600
H	-0.88172	-3.45534	0.28140
H	0.00001	-3.19298	-1.23846
H	0.88177	-3.45533	0.28139

H	0.00000	-1.11204	1.42388

[Rh(I-H)(HMe)]$^+$ -1389.92979882 Hartrees

Rh	0.00000	-0.87857	0.00391
P	2.23847	-0.54437	0.02010
P	-2.23846	-0.54439	0.02010
C	1.16140	1.83224	-0.01653
C	-1.16142	1.83224	-0.01653
C	1.20439	3.21783	-0.02966
C	-1.20443	3.21782	-0.02966
C	-0.00002	3.90845	-0.03675
H	2.16560	3.71555	-0.03298
H	-2.16564	3.71554	-0.03299
H	-0.00003	4.99355	-0.04673
O	-2.31326	1.14704	-0.00682
O	2.31325	1.14705	-0.00681
C	-3.30729	-0.94758	-1.39222
H	-3.47370	-2.02924	-1.41633
H	-4.27222	-0.44013	-1.30446
H	-2.81966	-0.65057	-2.32320
C	-3.27222	-0.90600	1.46908
H	-4.24062	-0.40390	1.38878
H	-3.43411	-1.98688	1.53061
H	-2.76261	-0.57967	2.37817
C	3.30729	-0.94754	-1.39222
H	4.27223	-0.44008	-1.30446
H	3.47370	-2.02920	-1.41634
H	2.81966	-0.65053	-2.32320
C	3.27223	-0.90597	1.46908
H	3.43411	-1.98684	1.53060
H	4.24062	-0.40386	1.38878
H	2.76262	-0.57965	2.37817
N	-0.00000	1.13348	-0.01190
C	0.00003	-3.24262	-0.12034
H	-0.89773	-3.85629	-0.06267
H	0.00000	-2.71007	-1.09273
H	0.89786	-3.85622	-0.06268
H	0.00000	-2.59486	0.81127

[Rh(I-CF_3)]$^+$ -1686.15488106 Hartrees

Rh	-1.95791	0.00006	0.00715
P	-1.64851	2.24959	0.00305
P	-1.64871	-2.24950	0.00305
C	0.72329	1.16447	-0.02073
C	0.72318	-1.16458	-0.02071
C	2.10831	1.20496	-0.03733
C	2.10821	-1.20520	-0.03730
C	2.79548	-0.00016	-0.04254
H	2.61321	2.16224	-0.05328
H	2.61305	-2.16251	-0.05321
O	0.04615	-2.31604	-0.01581
O	0.04635	2.31598	-0.01584
C	-2.01359	-3.29659	1.43980
H	-3.09421	-3.46395	1.49256
H	-1.50722	-4.26224	1.35183
H	-1.69505	-2.79576	2.35654
C	-2.04548	-3.29531	-1.42614
H	-1.53707	-4.26095	-1.35049
H	-3.12697	-3.46290	-1.45479
H	-1.74771	-2.79350	-2.34929
C	-2.01329	3.29669	1.43982

H	-1.50687	4.26231	1.35184
H	-3.09390	3.46410	1.49262
H	-1.69475	2.79583	2.35655
C	-2.04522	3.29545	-1.42612
H	-3.12670	3.46314	-1.45473
H	-1.53673	4.26103	-1.35048
H	-1.74752	2.79361	-2.34929
N	0.02450	-0.00003	-0.01143
C	4.30698	-0.00011	0.00310
F	4.80285	-1.08508	-0.59572
F	4.72257	0.00184	1.27274
F	4.80277	1.08310	-0.59898

$[Rh(I\text{-}CF_3)(H)(Me)]^+$ -1726.62850806 Hartrees

Rh	1.82489	0.00000	-0.05947
P	1.46307	2.24479	0.03817
P	1.46308	-2.24479	0.03818
C	-0.95102	1.16407	-0.05985
C	-0.95102	-1.16407	-0.05986
C	-2.33743	1.21376	-0.06067
C	-2.33742	-1.21376	-0.06068
C	-3.01624	-0.00000	-0.06403
H	-2.85387	2.16491	-0.05941
H	-2.85386	-2.16491	-0.05942
O	-0.23972	-2.30346	-0.03676
O	-0.23973	2.30347	-0.03675
C	1.88741	-3.35180	-1.33521
H	2.96915	-3.51886	-1.32836
H	1.37222	-4.31091	-1.23176
H	1.61373	-2.89369	-2.28861
C	1.78448	-3.21098	1.53542
H	1.30467	-4.19171	1.47804
H	2.86640	-3.34181	1.63886
H	1.41733	-2.67015	2.41032
C	1.88739	3.35181	-1.33521
H	1.37218	4.31091	-1.23176
H	2.96913	3.51890	-1.32835
H	1.61373	2.89370	-2.28862
C	1.78448	3.21098	1.53542
H	2.86640	3.34184	1.63884
H	1.30465	4.19170	1.47804
H	1.41735	2.67015	2.41032
N	-0.27938	0.00001	-0.08088
C	3.87221	-0.00001	-0.12681
H	4.34310	-0.88182	0.31626
H	4.09789	-0.00020	-1.20696
H	4.34309	0.88196	0.31595
H	1.98190	0.00000	1.43083
C	-4.52829	-0.00001	0.00004
F	-4.92817	-0.00003	1.27496
F	-5.03222	-1.08378	-0.59418
F	-5.03223	1.08378	-0.59415

$[Rh(I\text{-}CF_3)(HMe)]^+$ -1726.64589479 Hartrees

Rh	1.76952	0.00002	0.00468
P	1.43790	2.24025	0.01781
P	1.43793	-2.24022	0.01781
C	-0.93851	1.16170	-0.02463
C	-0.93850	-1.16170	-0.02459
C	-2.32374	1.20581	-0.04344
C	-2.32372	-1.20583	-0.04341

C	-3.01040	-0.00001	-0.05038
H	-2.82973	2.16239	-0.05840
H	-2.82970	-2.16241	-0.05833
O	-0.25645	-2.31213	-0.01561
O	-0.25647	2.31214	-0.01569
C	1.84259	-3.30644	-1.39518
H	2.92400	-3.47519	-1.41558
H	1.33298	-4.27054	-1.31057
H	1.55005	-2.81672	-2.32648
C	1.78976	-3.27484	1.46776
H	1.28615	-4.24217	1.38416
H	2.87004	-3.43916	1.53383
H	1.46053	-2.76545	2.37595
C	1.84261	3.30651	-1.39513
H	1.33297	4.27059	-1.31053
H	2.92402	3.47529	-1.41547
H	1.55013	2.81681	-2.32646
C	1.78965	3.27484	1.46780
H	2.86992	3.43916	1.53394
H	1.28604	4.24217	1.38419
H	1.46038	2.76543	2.37596
N	-0.24046	0.00000	-0.01619
C	4.13161	-0.00008	-0.09766
H	4.74516	-0.89801	-0.04223
H	3.59849	-0.00013	-1.07112
H	4.74527	0.89778	-0.04237
H	3.48439	0.00002	0.83299
C	-4.52152	-0.00002	-0.00611
F	-4.93978	-0.00004	1.26318
F	-5.01786	1.08400	-0.60684
F	-5.01785	-1.08404	-0.60687

$[Rh(I\text{-}NMe_3)]^{2+}$ -1522.79051253 Hartrees

Rh	1.98943	0.00012	0.00200
P	1.69482	-2.25745	0.00044
P	1.69440	2.25762	0.00045
C	-0.68626	-1.16241	-0.01159
C	-0.68648	1.16216	-0.01164
C	-2.07999	-1.20459	-0.02394
C	-2.08020	1.20405	-0.02402
C	-2.76833	-0.00034	-0.03862
H	-2.54118	-2.18168	-0.02965
H	-2.54166	2.18104	-0.02967
O	-0.02630	2.30782	-0.00603
O	-0.02587	-2.30795	-0.00598
C	2.05382	3.29890	1.43810
H	3.13504	3.46966	1.48058
H	1.54848	4.26560	1.35508
H	1.74937	2.79574	2.35835
C	2.06493	3.29737	-1.43552
H	1.55956	4.26443	-1.35721
H	3.14654	3.46737	-1.47037
H	1.76681	2.79341	-2.35742
C	2.05447	-3.29868	1.43806
H	1.54930	-4.26546	1.35505
H	3.13572	-3.46924	1.48051
H	1.74996	-2.79559	2.35833
C	2.06548	-3.29711	-1.43556
H	3.14712	-3.46693	-1.47045
H	1.56028	-4.26427	-1.35724
H	1.76724	-2.79320	-2.35744
N	0.01258	-0.00007	-0.00741

N	-4.26171	-0.00021	-0.00135
C	-4.83726	1.21055	-0.68620
H	-4.44817	1.26500	-1.70315
H	-5.92148	1.10028	-0.70324
H	-4.58609	2.10922	-0.12641
C	-4.83780	-1.21282	-0.68242
H	-4.44904	-1.27046	-1.69933
H	-4.58682	-2.10988	-0.11997
H	-5.92199	-1.10224	-0.69948
C	-4.69871	0.00205	1.44258
H	-4.30664	-0.89048	1.93036
H	-4.30639	0.89592	1.92766
H	-5.78961	0.00225	1.47346

$[Rh(I\text{-}NMe_3)(H)(Me)]^{2+}$ -1563.26378004 Hartrees

Rh	1.86079	0.00006	-0.06075
P	1.51278	2.25152	0.03333
P	1.51305	-2.25144	0.03333
C	-0.91547	1.16250	-0.05329
C	-0.91533	-1.16271	-0.05328
C	-2.31124	1.21297	-0.04529
C	-2.31110	-1.21334	-0.04529
C	-2.99063	-0.00022	-0.05686
H	-2.78410	2.18432	-0.03172
H	-2.78380	-2.18476	-0.03171
O	-0.22066	-2.29433	-0.02633
O	-0.22093	2.29421	-0.02633
C	1.90250	-3.34792	-1.35498
H	2.98349	-3.52451	-1.35764
H	1.38466	-4.30585	-1.25306
H	1.62957	-2.88079	-2.30422
C	1.82214	-3.22931	1.52198
H	1.33379	-4.20565	1.46097
H	2.90399	-3.37588	1.61217
H	1.47636	-2.69076	2.40686
C	1.90210	3.34804	-1.35497
H	1.38415	4.30591	-1.25306
H	2.98307	3.52478	-1.35763
H	1.62924	2.88088	-2.30422
C	1.82175	3.22943	1.52198
H	2.90358	3.37614	1.61217
H	1.33327	4.20571	1.46097
H	1.47603	2.69083	2.40686
N	-0.24768	-0.00006	-0.08599
C	3.90470	0.00017	-0.10002
H	4.36791	-0.88210	0.34794
H	4.13284	0.00016	-1.17960
H	4.36782	0.88252	0.34790
H	2.00075	0.00007	1.43260
N	-4.48577	-0.00013	-0.00218
C	-5.07079	1.21090	-0.67839
H	-4.69074	1.26975	-1.69849
H	-6.15477	1.09744	-0.68627
H	-4.81830	2.10905	-0.11848
C	-5.07127	-1.21094	-0.67836
H	-4.69121	-1.27001	-1.69845
H	-4.81925	-2.10920	-0.11842
H	-6.15520	-1.09701	-0.68630
C	-4.90646	-0.00001	1.44634
H	-4.50908	-0.89337	1.92828
H	-4.50881	0.89327	1.92821
H	-5.99697	0.00016	1.48928

$[Rh(I\text{-}NMe_3)(HMe)]^{2+}$ -1563.28556752 Hartrees

Rh	1.79876	-0.00717	0.00150
P	1.46490	-2.25236	0.01124
P	1.50368	2.24276	0.01124
C	-0.91258	-1.14580	-0.00076
C	-0.89040	1.17470	-0.00063
C	-2.30427	-1.17600	-0.00363
C	-2.28631	1.23504	-0.00353
C	-2.98149	0.03744	-0.00525
H	-2.78269	-2.14662	-0.00379
H	-2.73947	2.21554	-0.00372
O	-0.21679	2.31382	0.00308
O	-0.25557	-2.29511	0.00283
C	1.86566	3.27933	1.45299
H	2.94742	3.44422	1.49984
H	1.36560	4.24879	1.37202
H	1.55549	2.77468	2.37049
C	1.87753	3.29458	-1.41659
H	1.37516	4.26239	-1.33037
H	2.95935	3.46186	-1.45179
H	1.57631	2.79935	-2.34220
C	1.81068	-3.29371	1.45353
H	1.29490	-4.25496	1.37326
H	2.88960	-3.47620	1.50038
H	1.50885	-2.78352	2.37075
C	1.82304	-3.31027	-1.41605
H	2.90215	-3.49426	-1.45089
H	1.30577	-4.27019	-1.32963
H	1.52974	-2.81083	-2.34193
N	-0.20355	0.00999	-0.00046
C	4.15389	-0.02812	-0.07973
H	4.77758	0.86386	-0.04632
H	3.53826	-0.02499	0.86683
H	4.76072	-0.93181	-0.05150
H	3.59601	-0.01992	-1.04426
N	-4.47398	0.01524	-0.00777
C	-4.96807	-0.69863	1.22465
H	-4.59089	-0.17666	2.10446
H	-6.05879	-0.68461	1.21402
H	-4.61334	-1.72765	1.21898
C	-5.07501	1.39023	-0.01009
H	-4.76774	1.92426	0.88897
H	-4.76396	1.92277	-0.90874
H	-6.15893	1.27662	-0.01218
C	-4.96424	-0.70109	-1.24031
H	-4.58427	-0.18090	-2.11997
H	-4.60975	-1.73016	-1.23149
H	-6.05498	-0.68695	-1.23307

$[Rh(II)]^{+}$ -2539.13219464 Hartrees

Rh	0.00000	-0.59977	-0.00019
P	-2.21399	-0.25118	-0.00008
P	2.21399	-0.25118	-0.00008
C	-1.15990	2.09625	-0.00023
C	1.15990	2.09625	-0.00023
C	-1.20489	3.47734	-0.00024
C	1.20489	3.47734	-0.00024
C	0.00000	4.16906	-0.00025
H	-2.16758	3.97316	-0.00025
H	2.16758	3.97316	-0.00024

H	0.00000	5.25405	-0.00026
O	2.32036	1.40625	-0.00022
O	-2.32036	1.40625	-0.00023
C	3.30641	-0.68312	1.47398
C	3.30688	-0.68334	-1.47373
C	-3.30640	-0.68312	1.47399
C	-3.30690	-0.68335	-1.47371
N	0.00000	1.39327	-0.00023
F	4.50117	-0.11953	1.40694
F	2.68578	-0.27254	2.57728
F	3.43368	-2.00827	1.50150
F	4.50130	-0.11901	-1.40680
F	3.43492	-2.00843	-1.50043
F	2.68622	-0.27378	-2.57739
F	-3.43497	-2.00844	-1.50038
F	-2.68623	-0.27383	-2.57738
F	-4.50130	-0.11898	-1.40680
F	-4.50117	-0.11955	1.40695
F	-3.43363	-2.00826	1.50155
F	-2.68577	-0.27248	2.57728

$[Rh(II)(H)(Me)]^+$ -2579.60637982 Hartrees

Rh	0.00000	-0.57268	-0.09984
P	2.20494	-0.16346	0.00871
P	-2.20494	-0.16347	0.00871
C	1.15782	2.22805	-0.11377
C	-1.15782	2.22805	-0.11377
C	1.21425	3.61019	-0.11261
C	-1.21425	3.61019	-0.11261
C	-0.00000	4.29293	-0.11952
H	2.17028	4.11827	-0.09802
H	-2.17028	4.11827	-0.09802
H	-0.00000	5.37825	-0.11737
O	-2.30525	1.49803	-0.08031
O	2.30525	1.49803	-0.08031
C	-3.34852	-0.64644	-1.40791
C	-3.23553	-0.50918	1.54601
C	3.34852	-0.64644	-1.40791
C	3.23553	-0.50918	1.54601
N	0.00000	1.55397	-0.13932
C	0.00002	-2.61717	-0.14025
H	-0.88677	-3.06740	0.30925
H	0.00003	-2.82905	-1.22240
H	0.88681	-3.06739	0.30926
H	-0.00000	-0.74148	1.39113
F	-2.59460	0.00480	2.59333
F	-3.32933	-1.82814	1.68409
F	-4.44572	0.02072	1.46621
F	-3.59975	-1.94780	-1.30558
F	-2.68482	-0.41167	-2.54361
F	-4.48166	0.03280	-1.41467
F	2.68482	-0.41167	-2.54361
F	3.59975	-1.94780	-1.30558
F	3.32933	-1.82814	1.68409
F	4.44572	0.02072	1.46621
F	2.59460	0.00480	2.59333
F	4.48166	0.03280	-1.41467

$[Rh(II)(HMe)]^+$ -2579.62946017 Hartrees

Rh	0.00000	-0.50689	-0.03535
P	2.19916	-0.13703	0.00243

P	-2.19915	-0.13702	0.00242
C	1.15718	2.21569	-0.09534
C	-1.15718	2.21569	-0.09536
C	1.20602	3.59652	-0.13118
C	-1.20602	3.59652	-0.13119
C	0.00000	4.28703	-0.15045
H	2.16771	4.09388	-0.14109
H	-2.16771	4.09388	-0.14113
H	0.00001	5.37169	-0.17803
O	-2.31596	1.51857	-0.07124
O	2.31597	1.51857	-0.07119
C	-3.34405	-0.63426	-1.40821
C	-3.24462	-0.50621	1.52637
C	3.34402	-0.63425	-1.40823
C	3.24467	-0.50623	1.52635
N	0.00000	1.51478	-0.08120
C	-0.00009	-2.86256	-0.21124
H	-0.90145	-3.46883	-0.13389
H	-0.00015	-2.36163	-1.19643
H	0.90115	-3.46903	-0.13410
H	0.00007	-2.21619	0.72735
F	-3.54003	-1.95068	-1.31514
F	-2.72768	-0.36216	-2.55700
F	-4.50772	-0.00689	-1.37616
F	-2.61621	-0.00252	2.58595
F	-3.32496	-1.83152	1.64837
F	-4.46208	0.00763	1.45262
F	3.32499	-1.83154	1.64834
F	4.46213	0.00759	1.45256
F	2.61629	-0.00254	2.58595
F	4.50768	-0.00686	-1.37622
F	3.54003	-1.95067	-1.31514
F	2.72761	-0.36218	-2.55700

$[Rh(III)]^+$ -1365.44698694 Hartrees

Rh	0.00000	-1.05298	0.00001
P	-2.25432	-0.73488	0.00009
P	2.25432	-0.73488	-0.00006
C	-1.15564	1.62363	-0.00011
C	1.15564	1.62363	0.00003
C	-1.14068	3.01702	-0.00011
C	1.14067	3.01702	-0.00001
H	-2.07785	3.56398	-0.00013
H	2.07784	3.56398	0.00000
O	2.31451	0.96434	0.00010
O	-2.31451	0.96434	-0.00017
C	3.30032	-1.11232	1.43366
H	3.46925	-2.19325	1.47497
H	4.26518	-0.60351	1.35165
H	2.79817	-0.80413	2.35322
C	3.30014	-1.11208	-1.43398
H	4.26475	-0.60274	-1.35229
H	3.46965	-2.19293	-1.47508
H	2.79762	-0.80437	-2.35349
C	-3.30006	-1.11203	1.43408
H	-4.26493	-0.60322	1.35216
H	-3.46899	-2.19294	1.47563
H	-2.79773	-0.80368	2.35348
C	-3.30039	-1.11238	-1.43357
H	-3.46981	-2.19325	-1.47449
H	-4.26503	-0.60312	-1.35176
H	-2.79808	-0.80474	-2.35322

N	-0.00000	0.91842	-0.00003
N	-0.00000	3.69300	-0.00006

[Rh(III)(H)(Me)]$^+$ -1405.91958817 Hartrees

Rh	-0.00000	-0.93077	-0.06267
P	2.24874	-0.56203	0.03553
P	-2.24874	-0.56202	0.03554
C	1.15658	1.84185	-0.04081
C	-1.15658	1.84186	-0.04081
C	1.14943	3.23703	-0.02229
C	-1.14942	3.23704	-0.02230
H	2.07861	3.79705	-0.00617
H	-2.07859	3.79706	-0.00619
O	-2.30245	1.14632	-0.02317
O	2.30246	1.14631	-0.02316
C	-3.35328	-0.96912	-1.34472
H	-3.52536	-2.05013	-1.34770
H	-4.31022	-0.45035	-1.23892
H	-2.89159	-0.68906	-2.29453
C	-3.21814	-0.89299	1.52826
H	-4.19687	-0.40881	1.47344
H	-3.35335	-1.97535	1.62134
H	-2.67754	-0.53604	2.40750
C	3.35328	-0.96912	-1.34472
H	4.31022	-0.45035	-1.23892
H	3.52537	-2.05013	-1.34770
H	2.89159	-0.68907	-2.29453
C	3.21814	-0.89301	1.52825
H	3.35335	-1.97537	1.62132
H	4.19686	-0.40882	1.47344
H	2.67754	-0.53607	2.40750
N	0.00000	1.16560	-0.07127
C	-0.00001	-2.97751	-0.12795
H	-0.88215	-3.44797	0.31470
H	-0.00010	-3.20232	-1.20841
H	0.88219	-3.44797	0.31457
H	-0.00000	-1.08234	1.42843
N	0.00001	3.90214	-0.01899

[Rh(III)(HMe)]$^+$ -1405.93812513 Hartrees

Rh	0.00000	-0.87637	0.00254
P	2.24467	-0.53686	0.01272
P	-2.24467	-0.53687	0.01272
C	1.15304	1.82661	-0.01042
C	-1.15304	1.82661	-0.01043
C	1.14135	3.21995	-0.01904
C	-1.14136	3.21995	-0.01905
H	2.07763	3.76825	-0.02182
H	-2.07764	3.76825	-0.02183
O	-2.31080	1.16189	-0.00429
O	2.31080	1.16189	-0.00428
C	-3.30594	-0.92458	-1.40825
H	-3.47925	-2.00506	-1.43883
H	-4.26808	-0.41146	-1.32263
H	-2.81132	-0.62576	-2.33496
C	-3.28430	-0.89824	1.45632
H	-4.24875	-0.38880	1.37470
H	-3.45445	-1.97828	1.51089
H	-2.77629	-0.58044	2.36935
C	3.30593	-0.92456	-1.40826
H	4.26807	-0.41145	-1.32265

H	3.47923	-2.00504	-1.43885
H	2.81130	-0.62574	-2.33496
C	3.28431	-0.89825	1.45631
H	3.45447	-1.97828	1.51087
H	4.24876	-0.38881	1.37468
H	2.77631	-0.58046	2.36935
N	-0.00000	1.12186	-0.00717
C	0.00001	-3.23682	-0.07542
H	-0.89833	-3.85110	-0.03995
H	0.00013	-2.67995	-1.03951
H	0.89820	-3.85131	-0.03978
H	-0.00005	-2.60948	0.86375
N	-0.00001	3.89573	-0.02361

$[Rh(III-H)]^{2+}$ -1365.70233748 Hartrees

Rh	0.00000	-1.05870	0.00002
P	-2.27608	-0.78561	0.00014
P	2.27608	-0.78561	-0.00011
C	-1.17043	1.59074	0.00003
C	1.17043	1.59074	-0.00010
C	-1.18021	2.98520	-0.00001
C	1.18021	2.98520	-0.00014
H	-2.09617	3.56191	0.00002
H	2.09618	3.56191	-0.00021
O	2.31187	0.95042	-0.00014
O	-2.31187	0.95043	0.00011
C	3.30369	-1.14229	1.44327
H	3.47831	-2.22364	1.48178
H	4.27004	-0.63477	1.36475
H	2.79636	-0.84230	2.36290
C	3.30352	-1.14235	-1.44358
H	4.26977	-0.63459	-1.36532
H	3.47840	-2.22366	-1.48190
H	2.79598	-0.84266	-2.36319
C	-3.30350	-1.14230	1.44365
H	-4.26986	-0.63476	1.36528
H	-3.47814	-2.22364	1.48216
H	-2.79603	-0.84234	2.36321
C	-3.30372	-1.14234	-1.44320
H	-3.47856	-2.22366	-1.48153
H	-4.26998	-0.63461	-1.36478
H	-2.79632	-0.84260	-2.36288
N	0.00000	0.89237	-0.00002
N	0.00000	3.61511	-0.00009
H	0.00000	4.63419	-0.00012

$[Rh(III-H)(H)(Me)]^{2+}$ -1406.17434596 Hartrees

Rh	-0.00000	-0.94669	-0.06136
P	2.26507	-0.62312	0.02968
P	-2.26507	-0.62312	0.02968
C	1.17205	1.81016	-0.03643
C	-1.17205	1.81016	-0.03643
C	1.18945	3.21054	-0.00873
C	-1.18944	3.21055	-0.00873
H	2.09543	3.80262	0.01048
H	-2.09542	3.80263	0.01049
O	-2.29552	1.13584	-0.01669
O	2.29552	1.13583	-0.01670
C	-3.34741	-0.98264	-1.37391
H	-3.53403	-2.06255	-1.38718
H	-4.30258	-0.45893	-1.27293

H	-2.87092	-0.70593	-2.31750
C	-3.24893	-0.92105	1.51307
H	-4.22098	-0.42433	1.44674
H	-3.40776	-2.00239	1.59692
H	-2.71301	-0.58541	2.40360
C	3.34741	-0.98265	-1.37391
H	4.30258	-0.45895	-1.27292
H	3.53402	-2.06257	-1.38718
H	2.87092	-0.70594	-2.31750
C	3.24894	-0.92105	1.51307
H	3.40775	-2.00239	1.59693
H	4.22099	-0.42433	1.44674
H	2.71301	-0.58540	2.40360
N	0.00000	1.15319	-0.08041
C	-0.00002	-2.98806	-0.06992
H	-0.88327	-3.44468	0.38116
H	-0.00000	-3.21543	-1.15012
H	0.88322	-3.44469	0.38118
H	0.00000	-1.07743	1.43451
N	0.00001	3.82623	-0.00402
H	0.00001	4.84588	0.01355

$[Rh(III-H)(HMe)]^{2+}$ -1406.19952013 Hartrees

Rh	-0.00001	-0.88168	-0.00043
P	-2.26646	-0.58960	-0.00001
P	2.26643	-0.58975	-0.00001
C	-1.16766	1.78936	-0.00016
C	1.16780	1.78928	-0.00015
C	-1.18037	3.18249	0.00009
C	1.18060	3.18242	0.00010
H	-2.09597	3.75939	0.00017
H	2.09624	3.75925	0.00019
O	2.30884	1.14390	-0.00035
O	-2.30874	1.14405	-0.00038
C	3.30081	-0.94141	1.44132
H	3.48290	-2.02120	1.48114
H	4.26363	-0.42787	1.36096
H	2.79363	-0.64325	2.36159
C	3.30242	-0.94180	-1.44007
H	4.26499	-0.42792	-1.35887
H	3.48488	-2.02154	-1.47920
H	2.79617	-0.64417	-2.36101
C	-3.30085	-0.94117	1.44134
H	-4.26364	-0.42756	1.36096
H	-3.48302	-2.02094	1.48117
H	-2.79366	-0.64303	2.36160
C	-3.30247	-0.94159	-1.44005
H	-3.48500	-2.02132	-1.47919
H	-4.26501	-0.42765	-1.35885
H	-2.79621	-0.64399	-2.36100
N	0.00005	1.08944	-0.00025
C	-0.00028	-3.22427	0.00018
H	0.89767	-3.84039	-0.00009
H	-0.00011	-2.64169	0.96006
H	-0.89854	-3.83993	-0.00011
H	-0.00014	-2.64110	-0.95949
N	0.00014	3.81410	0.00019
H	0.00017	4.83254	0.00036

$[Ir(I-H)(HMe)]^{2+}$, transition state for ox. add. -1383.73877358 Hartrees

Ir	-0.00000	-0.76812	0.00039

P	2.24313	-0.42169	0.07409
P	-2.24313	-0.42168	0.07409
C	1.16859	1.97225	-0.05474
C	-1.16859	1.97226	-0.05471
C	1.20919	3.35688	-0.10170
C	-1.20917	3.35688	-0.10168
C	0.00001	4.04138	-0.12842
H	2.16687	3.86110	-0.11154
H	-2.16686	3.86111	-0.11151
H	0.00001	5.12617	-0.16450
O	-2.31231	1.27811	-0.01155
O	2.31231	1.27809	-0.01160
C	-3.36363	-0.85717	-1.28519
H	-3.51930	-1.94064	-1.28031
H	-4.32844	-0.35537	-1.17086
H	-2.91313	-0.57631	-2.23956
C	-3.20436	-0.73160	1.57983
H	-4.17624	-0.23272	1.53143
H	-3.35811	-1.81053	1.68240
H	-2.64636	-0.37765	2.44904
C	3.36366	-0.85721	-1.28515
H	4.32846	-0.35540	-1.17081
H	3.51933	-1.94067	-1.28024
H	2.91318	-0.57637	-2.23954
C	3.20433	-0.73157	1.57986
H	3.35809	-1.81050	1.68246
H	4.17621	-0.23268	1.53147
H	2.64630	-0.37762	2.44905
N	0.00000	1.28414	-0.04326
C	-0.00002	-2.88008	-0.49165
H	-0.88419	-3.47461	-0.25164
H	0.00018	-2.67731	-1.57155
H	0.88395	-3.47479	-0.25136
H	0.00003	-2.12978	0.81397

$[Ir(III)(HMe)]^{2+}$, transition state for ox. add. -1399.74532075 Hartrees

Ir	0.00000	-0.76861	-0.00225
P	2.24781	-0.41537	0.07229
P	-2.24782	-0.41534	0.07230
C	1.16085	1.96965	-0.05473
C	-1.16082	1.96967	-0.05472
C	1.14671	3.36315	-0.09850
C	-1.14667	3.36316	-0.09850
H	2.07836	3.91894	-0.11015
H	-2.07831	3.91897	-0.11018
O	-2.30890	1.29379	-0.01232
O	2.30892	1.29377	-0.01231
C	-3.36588	-0.83944	-1.29145
H	-3.52866	-1.92194	-1.28842
H	-4.32749	-0.33124	-1.17852
H	-2.91125	-0.56032	-2.24442
C	-3.21087	-0.71695	1.57723
H	-4.17877	-0.21054	1.52750
H	-3.37320	-1.79481	1.67878
H	-2.65121	-0.36765	2.44728
C	3.36591	-0.83945	-1.29144
H	4.32749	-0.33119	-1.17852
H	3.52875	-1.92195	-1.28837
H	2.91127	-0.56039	-2.24442
C	3.21083	-0.71701	1.57724
H	3.37316	-1.79487	1.67877
H	4.17874	-0.21060	1.52755

H	2.65115	-0.36773	2.44729
N	0.00001	1.27861	-0.04474
C	-0.00007	-2.87917	-0.46247
H	-0.88426	-3.46767	-0.20887
H	-0.00005	-2.69986	-1.54726
H	0.88406	-3.46776	-0.20887
H	0.00006	-2.09207	0.86195
N	0.00003	4.03052	-0.12318