SUPPLEMENTARY INFORMATION

Computation Provides Chemical Insight into the Diverse ^{1}H NMR Chemical Shifts of $[Ru(NHC)_4(L)H]^{0/+}$ Species (NHC = *N*-heterocyclic carbene; L = vacant, H_2, N_2, CO, MeCN, O_2, P_4, SO_2, H^-, F^- and Cl^-) and their $[Ru(R_2PCH_2CH_2PR_2)_2(L)H]^+$ Congeners

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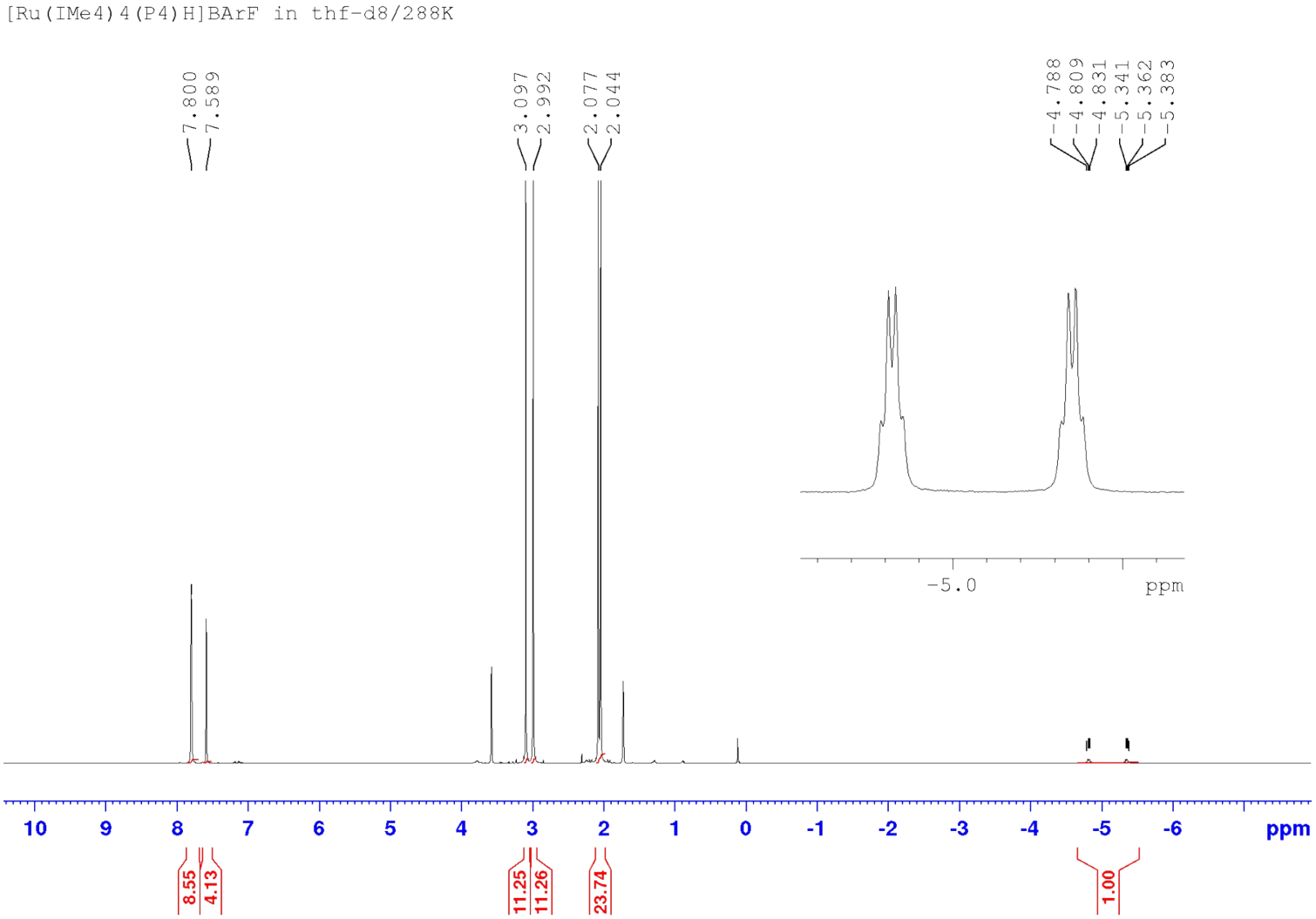

Figure S1. ^{1}H NMR spectrum (500 MHz, THF-d_8, 288 K) of $[Ru(IMe_4)_4(P_4)H]BAr_4^F$ (**1**). Inset shows expansion of Ru-H resonance.

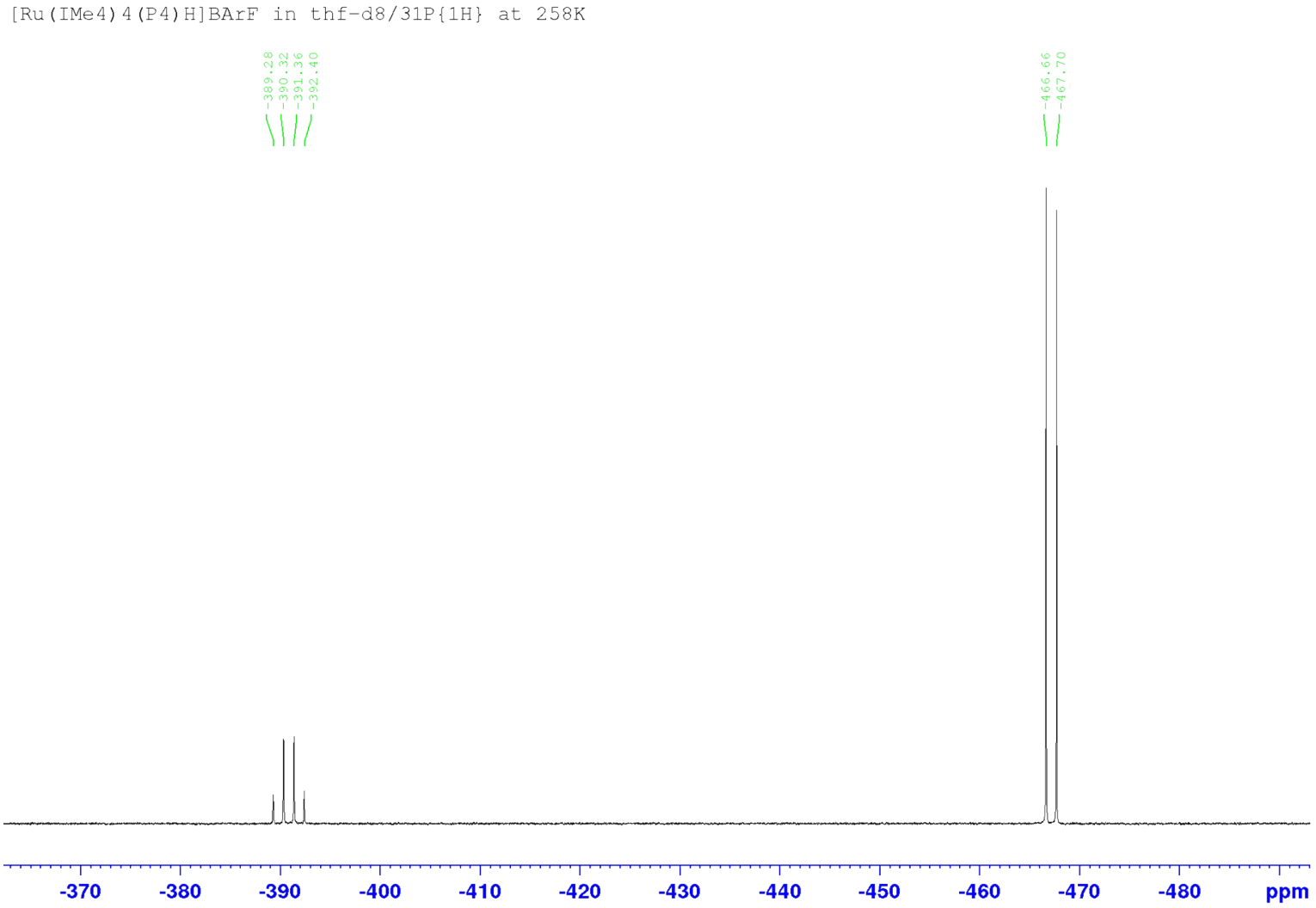

Figure S2. $^{31}P\{^{1}H\}$ NMR spectrum (202 MHz, THF-d_8, 258 K) of $[Ru(IMe_4)_4(P_4)H]BAr_4^F$ (**1**).

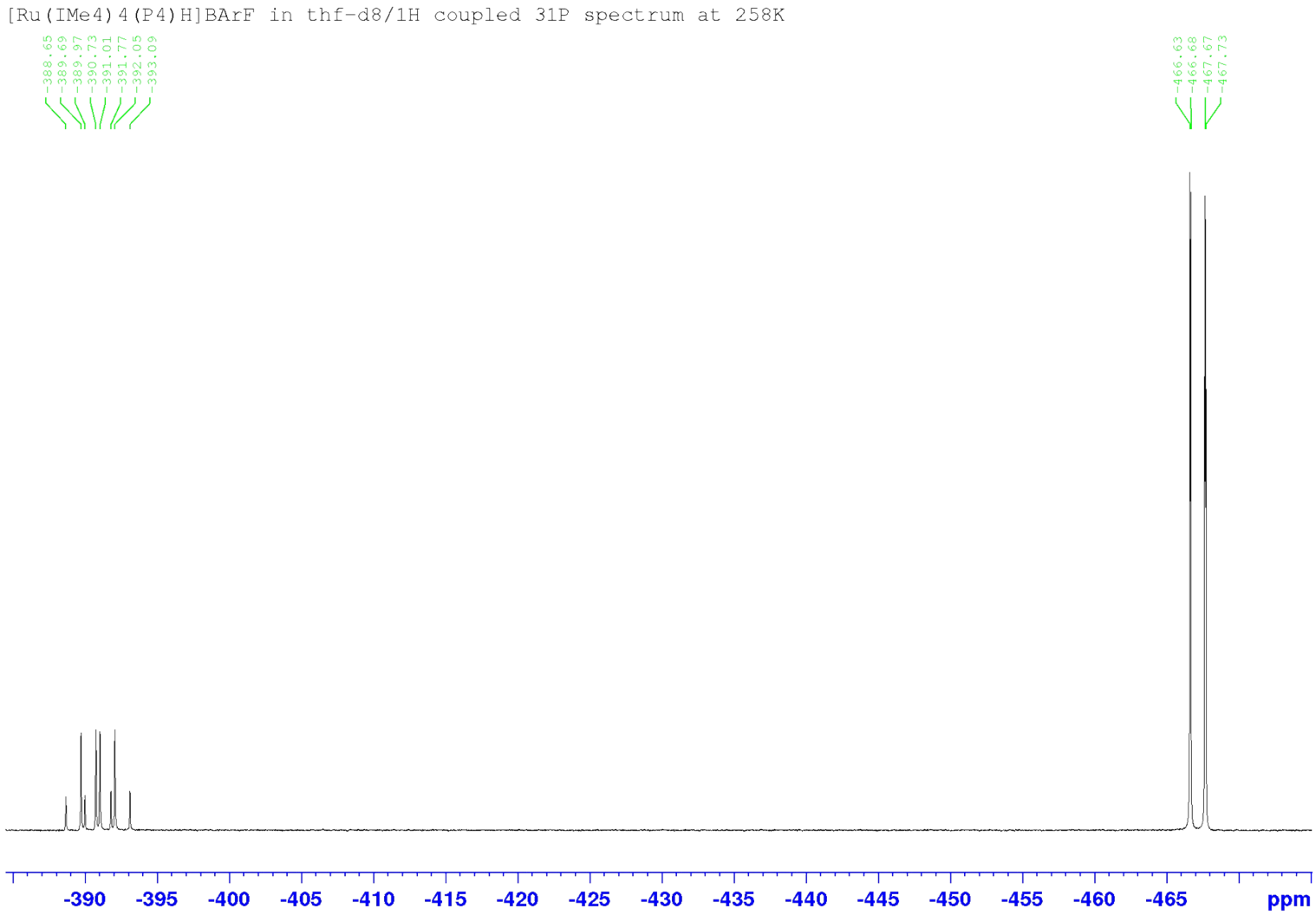

Figure S3. ^{31}P NMR spectrum (202 MHz, THF-d_8, 258 K) of [Ru(IMe$_4$)$_4$(P$_4$)H]BAr$_4^F$ (**1**).

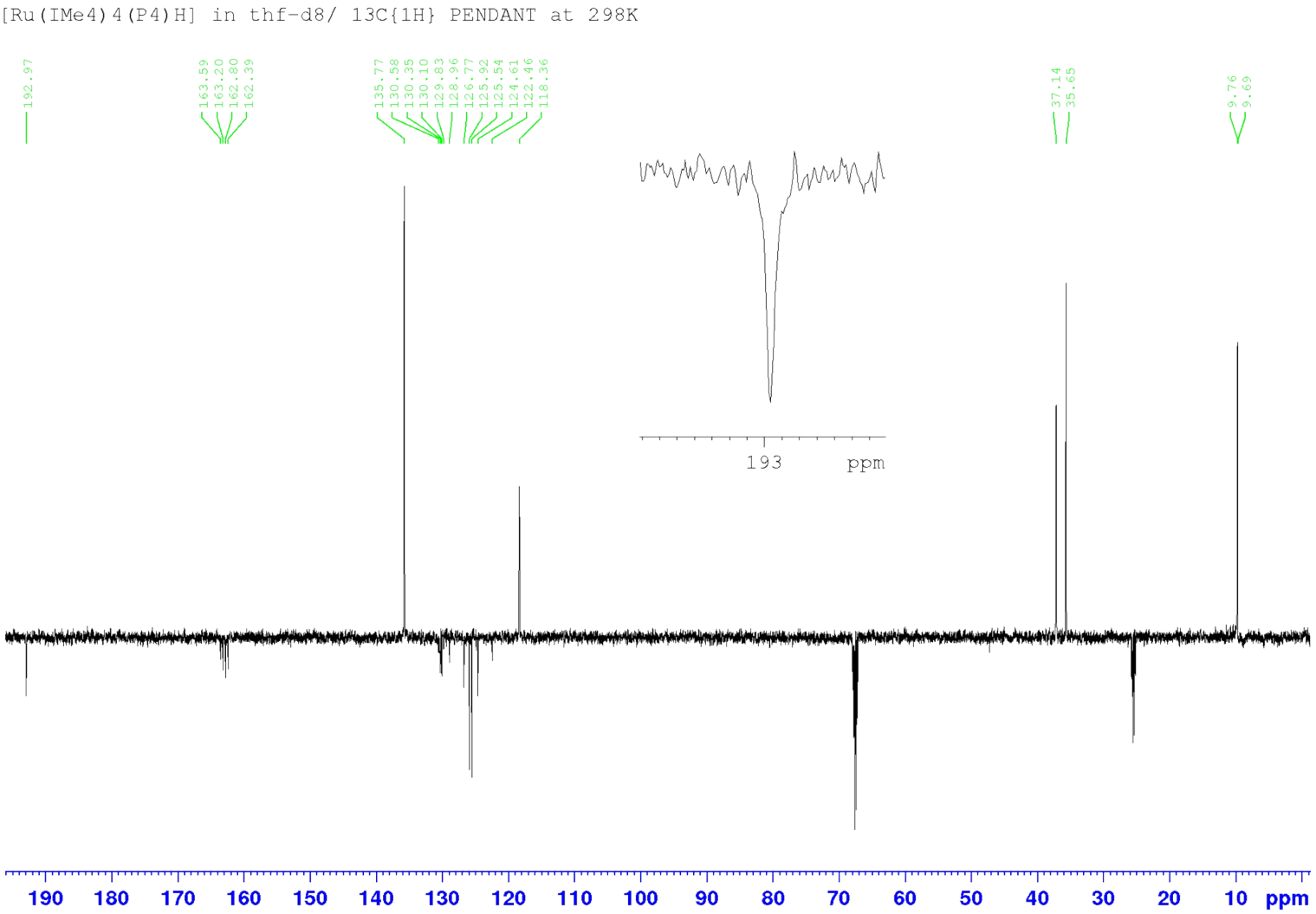

Figure S4. $^{13}C\{^{1}H\}$ PENDANT NMR spectrum (126 MHz, THF-d_8, 298 K) of $[Ru(IMe_4)_4(P_4)H]BAr_4^F$ (**1**). Inset shows Ru-C_{NHC} resonance.

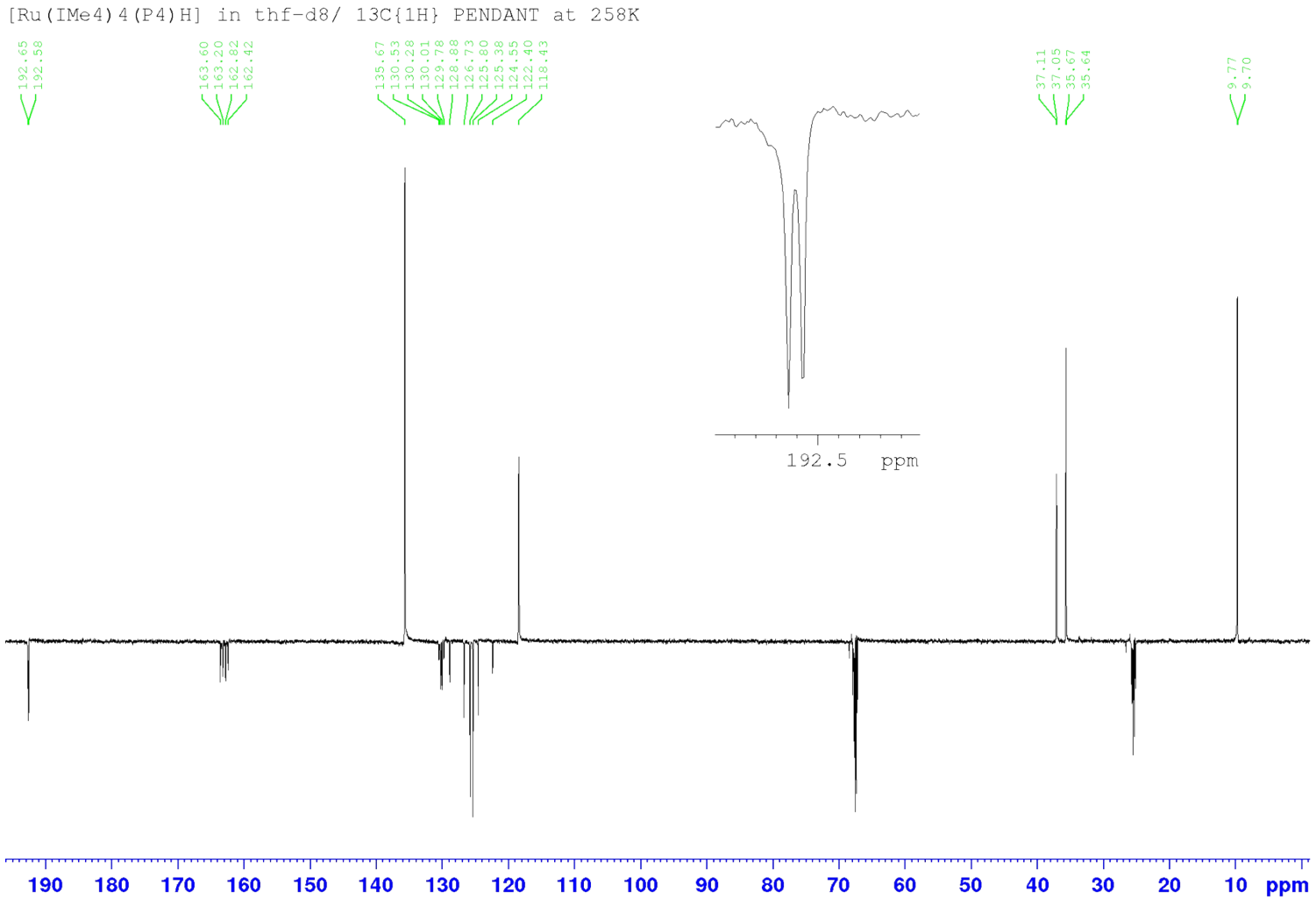

Figure S5. $^{13}C\{^{1}H\}$ PENDANT NMR spectrum (126 MHz, THF-d_8, 258 K) of $[Ru(IMe_4)_4(P_4)H]BAr_4^F$ (**1**). Inset shows doublet splitting of Ru-C_{NHC} resonance at this temperature.

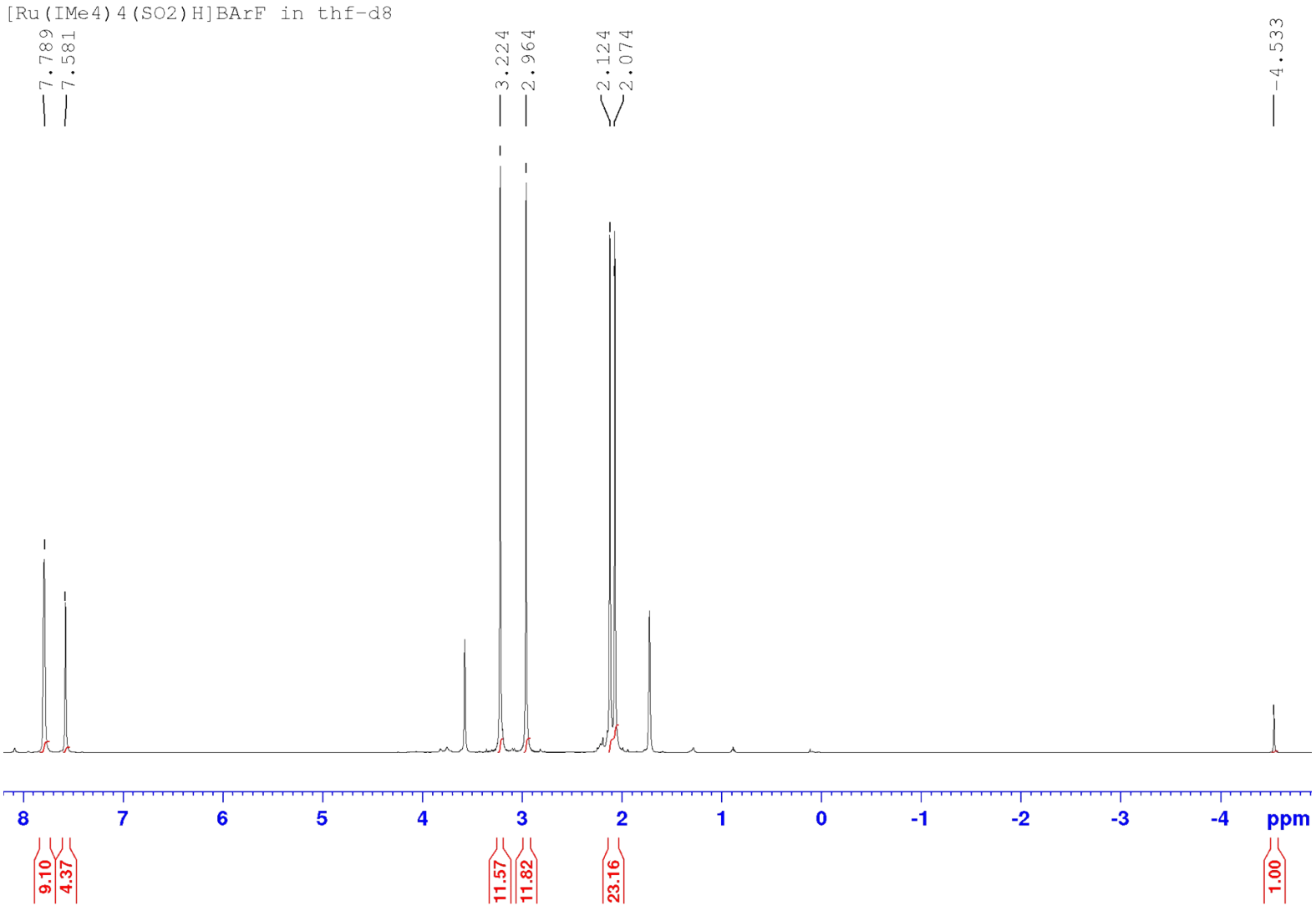

Figure S6. ^{1}H NMR spectrum (500 MHz, THF-d_8, 298 K) of $[Ru(IMe_4)_4(SO_2)H]BAr_4^F$ (**2**).

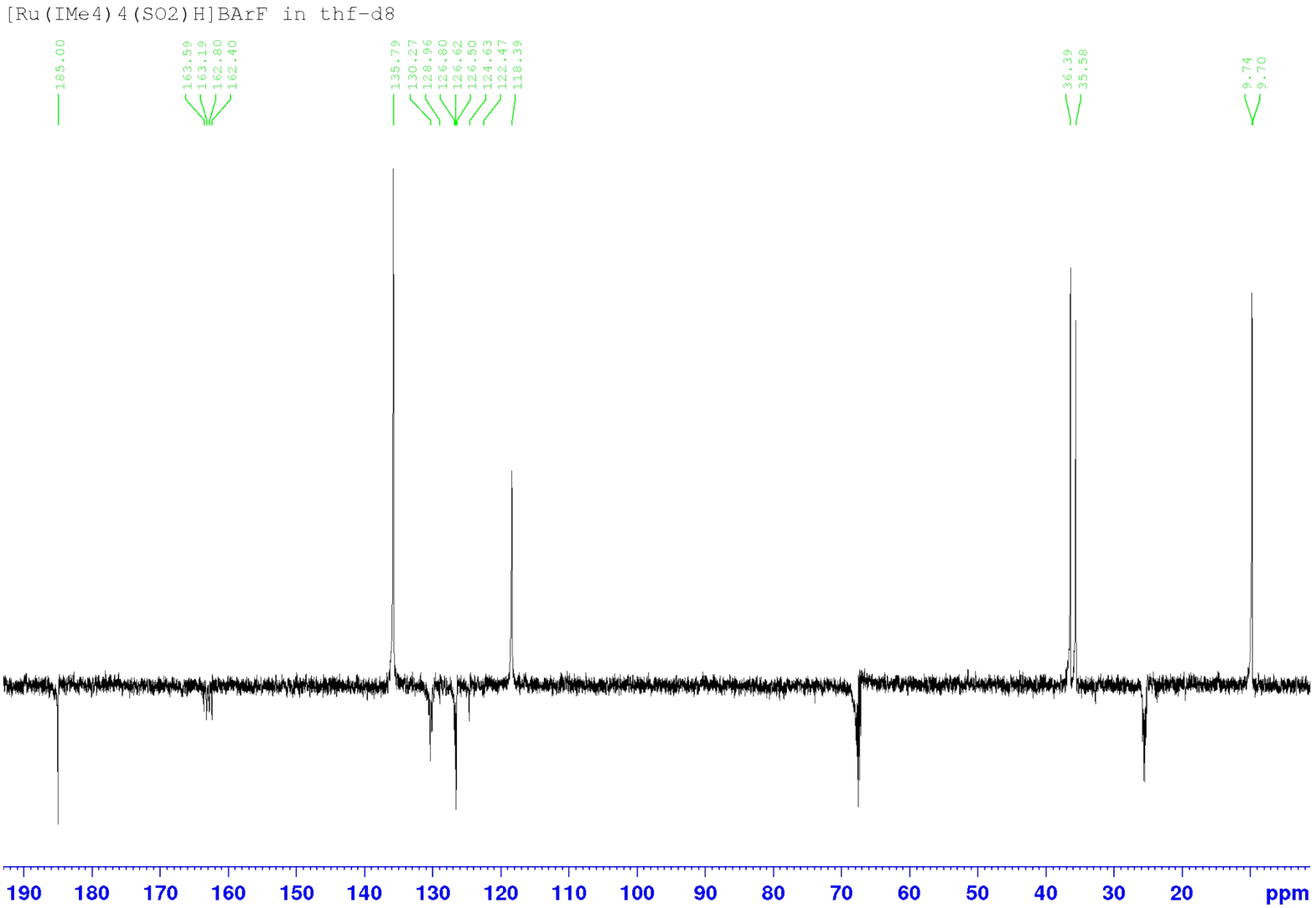

Figure S7. $^{13}C\{^{1}H\}$ PENDANT NMR spectrum (126 MHz, THF-d_8, 298 K) of $[Ru(IMe_4)_4(SO_2)H]BAr_4^F$ (**2**).

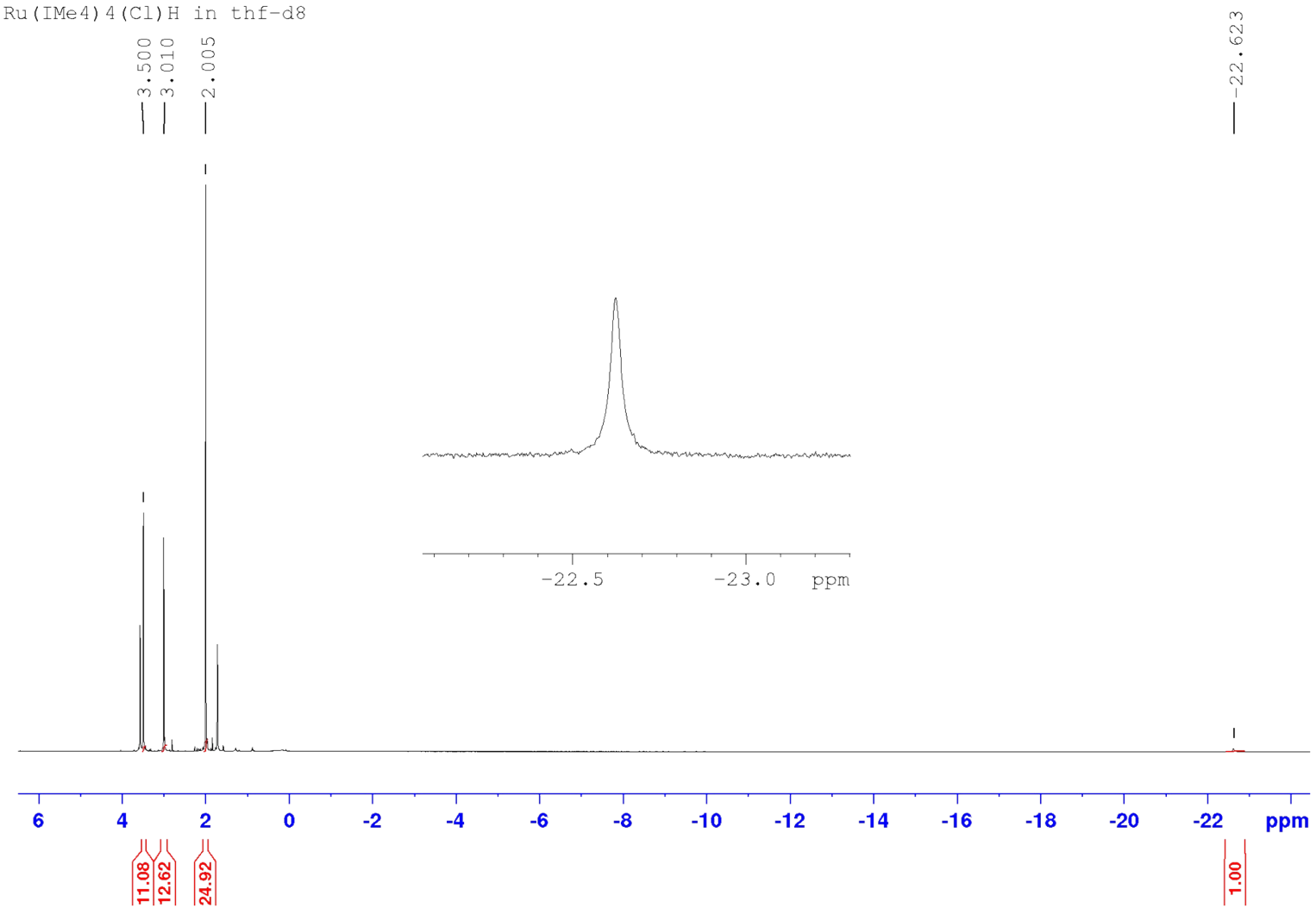

Figure S8. ^{1}H NMR spectrum (500 MHz, THF-d_8, 298 K) of [Ru(IMe$_4$)$_4$(Cl)H] (**3**). Inset shows expansion of Ru-H resonance.

Compound	**1**	**2**	**3**
Empirical formula	$C_{70}H_{83}N_8RuP_4BF_{24}O$	$C_{60}H_{61}N_8F_{24}SO_2RuB$	$C_{28}H_{49}ClN_8Ru$
Formula weight	1744.20	1526.10	634.27
Temperature/K	150.15	150.15	150(2)
Crystal system	monoclinic	monoclinic	tetragonal
Space group	$P2_1/a$	$C2$	$P4nc$
a/Å	20.6730(1)	25.9750(2)	11.7656(1)
b/Å	19.6270(1)	19.3490(2)	11.7656(1)
c/Å	20.6800(1)	18.3470(2)	11.17831(17)
α/°	90	90	90
β/°	110.534(1)	134.064(1)	90
γ/°	90	90	90
U/Å^3	7857.77(8)	6625.89(14)	1547.41(3)
Z	4	4	2
ρ_{calc}g/cm^3	1.474	1.530	1.361
μ/mm^{-1}	0.385	0.384	5.128
F(000)	3568.0	3096.0	668.0
Crystal size/mm^3	0.45 × 0.4 × 0.4	0.15 × 0.2 × 0.3	0.1433 × 0.1313 × 0.0679
2θ range for data collection/°	7.124 to 57.396	7.044 to 55.04	10.634 to 143.41
Index ranges	-27 ≤ h ≤ 27 -26 ≤ k ≤ 26 -27 ≤ l ≤ 27	-33 ≤ h ≤ 33 -24 ≤ k ≤ 25 -23 ≤ l ≤ 23	-11 ≤ h ≤ 14 -14 ≤ k ≤ 9 -11 ≤ l ≤ 13
Reflections collected	146852	63241	7545
Independent reflections, R_{int}	20231, 0.0501	15127, 0.0632	1456, 0.0319
Data/restraints/parameters	20231/81/1022	15127/3/904	1456/2/94
Goodness-of-fit on F^2	1.027	1.036	1.077
Final $R1$, $wR2$ indexes [I>=2σ (I)]	0.0619, 0.1656	0.0383, 0.0804	0.0293, 0.0785
Final $R1$, $wR2$ indexes [all data]	0.0760, 0.1829	0.0591, 0.0888	0.0296, 0.0792
Largest diff. peak/hole / e Å^{-3}	2.00, -1.52	0.55, -0.56	0.64, -0.77
Flack parameter	-	0.039(8)	0.003(7)

Table S1. Crystallographic details for **1**, **2** and **3**.

L	δ_{1c}^{iso}	$\delta_{2c-ZORA}^{iso}$	δ_{2c-X2C}^{iso}	Experiment
vacant	-25.0	-41.7	-41.1	-40.7
F^-	-15.8	-22.7	-23.1	-23.2
Cl^-	-15.4	-22.5	-22.3	-22.6
P_4	-3.5	-8.2	-7.6	-5.1
H^-	-4.3	-8.0	-8.1	-7.5
SO_2	-2.9	-7.6	-7.1	-4.5
MeCN	-7.6	-13.3	-12.9	-14.5
H_2	-3.6	-8.1	-7.5	-9.3
N_2	-5.7	-9.9	-9.6	-10.2
CO	-1.4	-4.2	-3.8	-4.0
O_2	3.4	0.7	1.4	4.8

Table S2. Computed ^{1}H chemical shifts (ppm) for $[Ru(IMe_4)_4(L)H]^{0/+}$ species with (i) the ZORA approximation using the B1PW91 hybrid density functional (δ_{iso}^{ZORA}); (ii) using the B1PW91 but without any correction for spin-orbit coupling effects (δ_{iso}^{1C}) and; (iii) with a X2C Hamiltonian with the B3PW91 hybrid density functional (δ_{iso}^{X2C}). Experimental data are provided for comparison – see main text for references.

Species	σ_{iso}	σ_{iso}^{d}	$\sigma_{//}^{d}$	$\sigma_{\perp}^{d}$	σ_{iso}^{p}	$\sigma_{//}^{p}$	$\sigma_{\perp}^{p}$	σ_{iso}^{so}	$\sigma_{//}^{so}$	$\sigma_{\perp}^{so}$
$[Ru(dippe)_2H]^+$	**64.0**	**24.7**	42.2	11.9; 20,1	**27.3**	-3.7	40.0; 45.7	**12.0**	-1.0	17.0; 20.2
$[Ru(dmpe)_2H]^+$	**73.5**	**25.8**	42.1	16.0; 19.3	**31.8**	1.7	44.3; 49.4	**15.9**	-1.1	22.4; 26.5
$[Ru(dmpe)(dmpe')H]^+$	**73.5**	**25.8**	42.1	16.0; 19.3	**31.9**	1.7	44.5; 49.6	**15.9**	-1.1	22.4; 26.5
$[Ru(dmpe)(dmpe')H]^+$ (3.50 Å)	**72.7**	**25.8**	42.4	16.5; 18.5	**31.4**	1.6	43.8; 48.8	**15.5**	-1.1	21.0; 26.7
$[Ru(dmpe)(dmpe')H]^+$ (3.25 Å)	**70.8**	**25.8**	42.6	16.3; 18.5	**30.3**	1.2	42.1; 47.6	**14.7**	-1.1	19.8; 25.5
$[Ru(dmpe)(dmpe')H]^+$ (3.00 Å)	**66.5**	**25.8**	42.6	15.5; 19.3	**28.1**	0.8	38.7; 44.7	**12.6**	-0.7	16.8; 22.2
$[Ru(dmpe)(dmpe')H]^+$ (2.75 Å)	**60.7**	**25.7**	42.5	15.0; 19.6	**25.2**	0.6	34.4; 40.6	**9.8**	-0.6	12.8; 17.6
$[Ru(dmpe)(dmpe')H]^+$ (2.50 Å)	**54.8**	**25.5**	42.2	14.8; 19.5	**22.3**	0.8	29.9; 36.2	**7.0**	-0.5	8.8; 13.0
$[Ru(dmpe)_2(\eta^2\text{-}O_2)H]^+$	**38.7**	**24.5**	39.7	11.1; 22.6	**12.2**	-13.3	20.7; 29.3	**2.0**	-0.5	-2.0; 8.2

Table S3. Calculated values (ZORA, B1PW91) for σ_{iso}, σ_{iso}^{d}, σ_{iso}^{p} and σ_{iso}^{so} for selected $[Ru(R_2PCH_2CH_2PR_2)_2(L)H]^+$ species, along with $\sigma_{||}$ and $\sigma_{\perp}$ contributions for σ_{iso}^{d}, σ_{iso}^{p} and σ_{iso}^{so}. The $[Ru(dmpe)(dmpe')H]^+$ species were computed with different values of the Ru□C$^{\beta}$ distance, as indicated. Two components are provided for the perpendicular terms due to the lower symmetry of these systems.

Species	$\sigma_{\parallel}^{p}$		$\sigma_{\perp}^{p}$		$\sigma_{\parallel}^{so}$	$\sigma_{\perp}^{so}$
	d_{π}	d_{xy}	d_{π}	d_{xy}	σ_{Ru-H}^{*}	σ_{Ru-H}^{*}
$[Ru(dippe)_2H]^+$	-1.7	-15.3	34.9; 41.7	0.3; 0.7	-0.7	6.9;7.6
$[Ru(dmpe)_2H]^+$	-2.3	-9.8	39.5; 46.0	0.4; 1.0	-0.9	7.8; 10.0
$[Ru(dmpe)(dmpe')H]^+$	-2.3	-9.9	39.7; 46.4	0.4; 1.0	-0.9	7.8; 10.2
$[Ru(dmpe)(dmpe')H]^+$ (3.50 Å)	-2.4	-9.7	39.0; 45.6	0.3; 1.0	-0.9	7.8; 10.4
$[Ru(dmpe)(dmpe')H]^+$ (3.25 Å)	-2.5	-9.8	37.3; 44.2	0.3; 1.0	-0.9	7.6; 10.2
$[Ru(dmpe)(dmpe')H]^+$ (3.00 Å)	-2.5	-9.9	33.1; 40.9	0.5; 1.2	-0.8	6.9; 9.2
$[Ru(dmpe)(dmpe')H]^+$ (2.75 Å)	-2.6	-9.8	28.0; 36.1	0.5; 1.4	-0.6	5.6; 7.6
$[Ru(dmpe)(dmpe')H]^+$ (2.50 Å)	-2.7	-9.3	22.1; 30.5	0.5; 1.8	-0.4	4.0; 5.7
$[Ru(dmpe)_2(\eta^2\text{-}O_2)H]^+$	-14.0	-11.1	0.2; 21.9	0.6; 2.4	-0.4	1.5; 3.8

Table S4. NCS analysis of the contributions (ppm) to σ_{iso}^{p} and σ_{iso}^{so} for selected $[Ru(R_2PCH_2CH_2PR_2)_2(L)H]^+$ species. The $[Ru(dmpe)(dmpe')H]^+$ species were computed with different values of the Ru□C$^{\beta}$ distance, as indicated. Two components are provided for the perpendicular terms due to the lower symmetry of these systems.

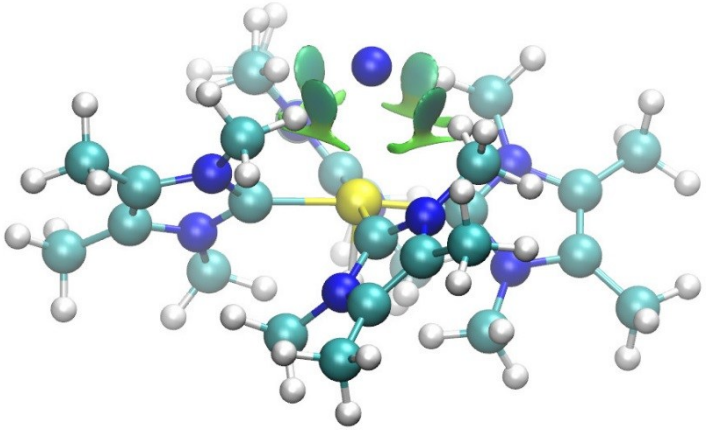

Figure S9. (a) Computed NCI Plot for [Ru(IMe$_4$)$_4$(Cl)H], **3**. Truncated isosurfaces highlighting Cl□H-C stabilizing interactions are plotted with a reduced density gradient isovalue of s = 0.5 a.u.

Cartesian Coordinates (Å) and computed energies (in Hartrees) for all optimised structures.

$[Ru(IMe_4)_4(H)]^+$

N	-0.58613	2.97955	0.90691
C	0.00000	2.09199	0.01559
N	0.59828	2.95433	-0.89706
C	0.38820	4.30824	-0.58785
C	-0.36261	4.32325	0.56237
Ru	0.00000	0.00000	0.00763
C	0.00000	-2.09199	0.01559
N	0.58613	-2.97955	0.90691
C	0.36261	-4.32325	0.56237
C	-0.38820	-4.30824	-0.58785
N	-0.59828	-2.95433	-0.89706
C	1.34866	-2.58737	2.08702
C	-1.31192	-2.51403	-2.08822
C	1.31192	2.51403	-2.08822
C	-1.34866	2.58737	2.08702
C	-2.09199	0.00000	0.01559
N	-2.97955	-0.58613	0.90691
C	-4.32325	-0.36261	0.56237
C	-4.30824	0.38820	-0.58785
N	-2.95433	0.59828	-0.89706
C	-2.58737	-1.34866	2.08702
C	-2.51403	1.31192	-2.08822
C	2.09199	0.00000	0.01559
N	2.95433	-0.59828	-0.89706
C	4.30824	-0.38820	-0.58785
C	4.32325	0.36261	0.56237
N	2.97955	0.58613	0.90691
C	2.51403	-1.31192	-2.08822
C	2.58737	1.34866	2.08702
H	0.00000	0.00000	1.56333
C	-0.92826	-5.42604	-1.42183
C	0.88621	-5.46589	1.37262
C	-0.88621	5.46589	1.37262
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C	5.42604	-0.92826	-1.42183
C	-5.46589	-0.88621	1.37262
C	-5.42604	0.92826	-1.42183
H	2.78798	-0.76494	-3.00807
H	2.96158	-2.31871	-2.13191
H	1.42091	-1.41380	-2.02936
H	1.30932	-1.49257	2.15293
H	0.91186	-3.03193	2.99761
H	2.39928	-2.91396	2.00355
H	-0.76494	-2.78798	-3.00807
H	-2.31871	-2.96158	-2.13191
H	-1.41380	-1.42091	-2.02936
H	-2.91396	-2.39928	2.00355
H	-1.49257	-1.30932	2.15293
H	-3.03193	-0.91186	2.99761
H	-2.96158	2.31871	-2.13191
H	-1.42091	1.41380	-2.02936
H	-2.78798	0.76494	-3.00807
H	-0.91186	3.03193	2.99761
H	-2.39928	2.91396	2.00355
H	-1.30932	1.49257	2.15293
H	0.76494	2.78798	-3.00807
H	2.31871	2.96158	-2.13191
H	1.41380	1.42091	-2.02936
H	2.91396	2.39928	2.00355
H	1.49257	1.30932	2.15293
H	3.03193	0.91186	2.99761
H	0.60570	-6.42335	0.90798
H	1.98805	-5.44810	1.45466
H	0.48200	-5.46813	2.40141
H	-2.03281	-5.42035	-1.46489
H	-0.55980	-5.38651	-2.46317
H	-0.62218	-6.39651	-1.00252
H	6.39651	-0.62218	-1.00252
H	5.42035	-2.03281	-1.46489
H	5.38651	-0.55980	-2.46317
H	5.44810	1.98805	1.45466
H	5.46813	0.48200	2.40141
H	6.42335	0.60570	0.90798
H	-6.42335	-0.60570	0.90798
H	-5.44810	-1.98805	1.45466
H	-5.46813	-0.48200	2.40141
H	-5.42035	2.03281	-1.46489
H	-5.38651	0.55980	-2.46317
H	-6.39651	0.62218	-1.00252
H	-1.98805	5.44810	1.45466
H	-0.48200	5.46813	2.40141
H	-0.60570	6.42335	0.90798
H	0.62218	6.39651	-1.00252
H	2.03281	5.42035	-1.46489
H	0.55980	5.38651	-2.46317

SCF = -1629.42945755
H(0 K)= -1628.704372
H(298 K)= -1628.656037
G(298 K)= -1628.786250
Lowest Frequency = 15.7567cm-1

$[Ru(IMe_4)_4(H)(H_2)]^+$

N	-1.94339	-2.36860	0.95809
C	-1.63919	-1.31665	0.10123
N	-2.70524	-1.34884	-0.78717
C	-3.63303	-2.35901	-0.48455
C	-3.15201	-3.00671	0.62643
Ru	0.00000	0.00000	0.15188
H	0.26409	-0.34968	1.85118
H	-0.26411	0.34967	1.85117
C	-2.87499	-0.45153	-1.92600
C	-4.86856	-2.59789	-1.29333
C	-3.71217	-4.16206	1.39455
C	-1.14129	-2.75350	2.11538
C	-1.31692	1.64250	-0.01485
N	-2.40894	1.97504	0.77626
C	-3.04036	3.15900	0.35648
C	-2.34361	3.59301	-0.74412
N	-1.31159	2.66306	-0.95223
C	-2.83868	1.23130	1.95648
C	-0.35275	2.79895	-2.04503
C	-2.55129	4.78705	-1.62076
C	-4.23333	3.74263	1.04523
C	1.63919	1.31664	0.10126
N	2.70524	1.34884	-0.78714
C	3.63303	2.35901	-0.48450
C	3.15201	3.00670	0.62649
N	1.94339	2.36858	0.95813
C	2.87499	0.45156	-1.92598
C	4.86857	2.59790	-1.29327
C	3.71218	4.16203	1.39462
C	1.14129	2.75348	2.11542
C	1.31692	-1.64251	-0.01487
N	2.40893	-1.97505	0.77625
C	3.04035	-3.15900	0.35645
C	2.34362	-3.59299	-0.74417
N	1.31159	-2.66304	-0.95228

C	2.83865	-1.23134	1.95650
C	4.23332	-3.74265	1.04519
C	2.55132	-4.78701	-1.62085
C	0.35276	-2.79890	-2.04508
H	0.00000	0.00001	-1.47131
H	-1.42977	-2.18180	3.01596
H	-1.28106	-3.82487	2.32090
H	-0.08366	-2.56268	1.89351
H	-0.16327	-1.83659	-2.15405
H	0.88093	-3.05001	-2.97901
H	-0.38562	-3.59012	-1.82907
H	2.36810	-1.62665	2.87538
H	3.93109	-1.30559	2.06387
H	2.55730	-0.17841	1.83128
H	3.63913	-0.31755	-1.71890
H	1.90964	-0.03747	-2.11036
H	3.18183	1.02611	-2.81488
H	1.28105	3.82484	2.32094
H	0.08366	2.56265	1.89355
H	1.42977	2.18178	3.01600
H	-0.88093	3.04996	-2.97899
H	0.38556	3.59025	-1.82906
H	0.16336	1.83668	-2.15395
H	-2.36817	1.62659	2.87539
H	-3.93113	1.30553	2.06383
H	-2.55732	0.17837	1.83125
H	-3.63914	0.31756	-1.71891
H	-1.90965	0.03750	-2.11036
H	-3.18181	-1.02607	-2.81491
H	3.37971	-5.40131	-1.23672
H	1.65460	-5.43062	-1.66550
H	2.80563	-4.50623	-2.65934
H	5.11447	-3.07643	0.99941
H	4.03763	-3.95760	2.11102
H	4.51891	-4.69142	0.56609
H	-4.68605	-4.45671	0.97483
H	-3.05809	-5.05259	1.35391
H	-3.87321	-3.91894	2.46014
H	-5.50357	-1.69627	-1.35861
H	-4.63908	-2.91251	-2.32801
H	-5.47412	-3.39554	-0.83692
H	5.47412	3.39555	-0.83686
H	5.50357	1.69628	-1.35856
H	4.63909	2.91251	-2.32795
H	3.05810	5.05256	1.35401
H	3.87322	3.91889	2.46021
H	4.68605	4.45669	0.97490
H	-1.65459	5.43068	-1.66536
H	-2.80555	4.50630	-2.65927
H	-3.37971	5.40133	-1.23666
H	-4.51893	4.69141	0.56613
H	-5.11448	3.07640	0.99944
H	-4.03764	3.95758	2.11105

SCF = -1630.62525271
H(0 K)= -1629.881927
H(298 K)= -1629.833655
G(298 K)= -1629.963460
Lowest Frequency = 23.2342cm-1

$[Ru(IMe_4)_4(H)(N_2)]^+$

N	0.92965	2.97554	0.74341
C	1.04845	1.83534	-0.03676
N	2.03482	2.19531	-0.94067
C	2.51878	3.49530	-0.72016
C	1.81795	3.99139	0.35151
Ru	0.00000	0.00000	0.10417
N	0.00000	0.00000	2.07095
N	0.00000	0.00000	3.21611
C	2.53634	1.35436	-2.02483
C	3.59186	4.11902	-1.55502
C	1.90103	5.31469	1.04401
C	0.00000	3.14833	1.85821
C	1.83534	-1.04845	-0.03676
N	2.97554	-0.92965	0.74341
C	3.99139	-1.81795	0.35151
C	3.49530	-2.51878	-0.72016
N	2.19531	-2.03482	-0.94067
C	3.14833	0.00000	1.85821
C	1.35436	-2.53634	-2.02483
C	4.11902	-3.59186	-1.55502
C	5.31469	-1.90103	1.04401
C	-1.04845	-1.83534	-0.03676
N	-2.03482	-2.19531	-0.94067
C	-2.51878	-3.49530	-0.72016
C	-1.81795	-3.99139	0.35151
N	-0.92965	-2.97554	0.74341
C	-2.53634	-1.35436	-2.02483
C	-3.59186	-4.11902	-1.55502
C	-1.90103	-5.31469	1.04401
C	0.00000	-3.14833	1.85821
C	-1.83534	1.04845	-0.03676
N	-2.97554	0.92965	0.74341
C	-3.99139	1.81795	0.35151
C	-3.49530	2.51878	-0.72016
N	-2.19531	2.03482	-0.94067
C	-3.14833	0.00000	1.85821
C	-5.31469	1.90103	1.04401
C	-4.11902	3.59186	-1.55502
C	-1.35436	2.53634	-2.02483
H	0.00000	0.00000	-1.53105
H	0.51223	3.03814	2.82872
H	-0.45517	4.14984	1.80907
H	-0.78647	2.39026	1.77571
H	-0.55522	1.80402	-2.19585
H	-1.95739	2.65317	-2.93921
H	-0.90763	3.51168	-1.76588
H	-3.03814	0.51223	2.82872
H	-4.14984	-0.45517	1.80907
H	-2.39026	-0.78647	1.77571
H	-3.51168	-0.90763	-1.76588
H	-1.80402	-0.55522	-2.19585
H	-2.65317	-1.95739	-2.93921
H	0.45517	-4.14984	1.80907
H	0.78647	-2.39026	1.77571
H	-0.51223	-3.03814	2.82872
H	1.95739	-2.65317	-2.93921
H	0.90763	-3.51168	-1.76588
H	0.55522	-1.80402	-2.19585
H	3.03814	-0.51223	2.82872
H	4.14984	0.45517	1.80907
H	2.39026	0.78647	1.77571
H	3.51168	0.90763	-1.76588
H	1.80402	0.55522	-2.19585
H	2.65317	1.95739	-2.93921
H	-5.11221	3.85146	-1.15836
H	-3.51418	4.51615	-1.56448
H	-4.25808	3.27954	-2.60628
H	-5.89621	0.96515	0.95540
H	-5.20673	2.11975	2.12137
H	-5.92312	2.70528	0.60340
H	2.70528	5.92312	0.60340
H	0.96515	5.89621	0.95540
H	2.11975	5.20673	2.12137
H	4.51615	3.51418	-1.56448

H	3.27954	4.25808	-2.60628
H	3.85146	5.11221	-1.15836
H	-3.85146	-5.11221	-1.15836
H	-4.51615	-3.51418	-1.56448
H	-3.27954	-4.25808	-2.60628
H	-0.96515	-5.89621	0.95540
H	-2.11975	-5.20673	2.12137
H	-2.70528	-5.92312	0.60340
H	3.51418	-4.51615	-1.56448
H	4.25808	-3.27954	-2.60628
H	5.11221	-3.85146	-1.15836
H	5.92312	-2.70528	0.60340
H	5.89621	-0.96515	0.95540
H	5.20673	-2.11975	2.12137

SCF = -1738.98706910
H(0 K)= -1738.249720
H(298 K)= -1738.200595
G(298 K)= -1738.329337
Lowest Frequency = 23.9677cm-1

[Ru(IMe$_4$)$_4$(H)(CO)]$^+$

N	0.00000	3.12302	0.74579
C	0.44778	2.06701	-0.03164
N	1.27301	2.69764	-0.94763
C	1.34722	4.08424	-0.73718
C	0.53999	4.35526	0.34027
Ru	0.00000	0.00000	0.13318
C	2.06701	-0.44778	-0.03164
N	2.69764	-1.27301	-0.94763
C	4.08424	-1.34722	-0.73718
C	4.35526	-0.53999	0.34027
N	3.12302	0.00000	0.74579
C	2.03806	-1.99535	-2.03305
C	4.99527	-2.17647	-1.58573
C	5.64985	-0.23253	1.02424
C	3.01180	0.91568	1.88057
C	1.99535	2.03806	-2.03305
C	2.17647	4.99527	-1.58573
C	0.23253	5.64985	1.02424
C	-0.91568	3.01180	1.88057
C	-0.44778	-2.06701	-0.03164
N	0.00000	-3.12302	0.74579
C	-0.53999	-4.35526	0.34027
C	-1.34722	-4.08424	-0.73718
N	-1.27301	-2.69764	-0.94763
C	0.91568	-3.01180	1.88057
C	-1.99535	-2.03806	-2.03305
C	-2.17647	-4.99527	-1.58573
C	-0.23253	-5.64985	1.02424
C	0.00000	0.00000	2.01925
O	0.00000	0.00000	3.20503
C	-2.06701	0.44778	-0.03164
N	-2.69764	1.27301	-0.94763
C	-4.08424	1.34722	-0.73718
C	-4.35526	0.53999	0.34027
N	-3.12302	0.00000	0.74579
C	-2.03806	1.99535	-2.03305
C	-4.99527	2.17647	-1.58573
C	-5.64985	0.23253	1.02424
C	-3.01180	-0.91568	1.88057
H	0.00000	0.00000	-1.55201
H	-2.94516	-0.36677	2.83475
H	-3.89408	-1.57270	1.90812
H	-2.11022	-1.52546	1.75412
H	-1.51260	-1.06870	-2.21555
H	-1.94603	-2.65926	-2.94104
H	-3.05434	-1.87689	-1.76789
H	0.36677	-2.94516	2.83475
H	1.57270	-3.89408	1.90812
H	1.52546	-2.11022	1.75412
H	1.87689	-3.05434	-1.76789
H	1.06870	-1.51260	-2.21555
H	2.65926	-1.94603	-2.94104
H	3.89408	1.57270	1.90812
H	2.11022	1.52546	1.75412
H	2.94516	0.36677	2.83475
H	1.94603	2.65926	-2.94104
H	3.05434	1.87689	-1.76789
H	1.51260	1.06870	-2.21555
H	-0.36677	2.94516	2.83475
H	-1.57270	3.89408	1.90812
H	-1.52546	2.11022	1.75412
H	-1.87689	3.05434	-1.76789
H	-1.06870	1.51260	-2.21555
H	-2.65926	1.94603	-2.94104
H	-2.13439	-6.02213	-1.19214
H	-3.23833	-4.69177	-1.60677
H	-1.82414	-5.03195	-2.63288
H	0.83413	-5.92799	0.94122
H	-0.48299	-5.62224	2.09964
H	-0.81675	-6.46473	0.57055
H	-6.46473	0.81675	0.57055
H	-5.92799	-0.83413	0.94122
H	-5.62224	0.48299	2.09964
H	-4.69177	3.23833	-1.60677
H	-5.03195	1.82414	-2.63288
H	-6.02213	2.13439	-1.19214
H	6.02213	-2.13439	-1.19214
H	4.69177	-3.23833	-1.60677
H	5.03195	-1.82414	-2.63288
H	5.92799	0.83413	0.94122
H	5.62224	-0.48299	2.09964
H	6.46473	-0.81675	0.57055
H	3.23833	4.69177	-1.60677
H	1.82414	5.03195	-2.63288
H	2.13439	6.02213	-1.19214
H	0.81675	6.46473	0.57055
H	-0.83413	5.92799	0.94122
H	0.48299	5.62224	2.09964

SCF = -1742.81006877
H(0 K)= -1742.072942
H(298 K)= -1742.023908
G(298 K)= -1742.152938
Lowest Frequency = 25.6202cm-1

[Ru(IMe$_4$)$_4$(H)(MeCN)]$^+$

N	2.83264	-0.96181	-1.03422
C	2.09461	-0.19670	-0.13992
N	3.09313	0.41242	0.61131
C	4.38495	0.03395	0.20729
C	4.21840	-0.84050	-0.83767
Ru	0.00038	0.00031	-0.00862
C	0.19764	2.09442	-0.14032
N	0.96396	2.83205	-1.03394
C	0.84247	4.21789	-0.83814
C	-0.03337	4.38499	0.20555
N	-0.41262	3.09334	0.60949
C	1.79388	2.26750	-2.09500
C	1.57297	5.22763	-1.66558
C	-0.54529	5.62671	0.86395
C	-1.38149	2.87434	1.67777
C	2.87383	1.38146	1.67954

C	5.62629	0.54502	0.86705
C	5.22856	-1.56988	-1.66559
C	2.26855	-1.79036	-2.09659
C	-0.19631	-2.09377	-0.14186
N	0.41294	-3.09286	0.60859
C	0.03456	-4.38440	0.20351
C	-0.84009	-4.21706	-0.84115
N	-0.96161	-2.83116	-1.03652
C	1.38322	-2.87471	1.67591
C	-1.79052	-2.26630	-2.09821
C	-1.56962	-5.22659	-1.66969
C	0.54576	-5.62622	0.86226
N	-0.00277	-0.00177	2.05045
C	-0.00727	-0.00436	3.23450
C	-2.09360	0.19721	-0.14213
N	-3.09302	-0.41287	0.60725
C	-4.38442	-0.03380	0.20229
C	-4.21666	0.84180	-0.84147
N	-2.83071	0.96336	-1.03634
C	-2.87512	-1.38259	1.67497
C	-5.62657	-0.54555	0.86003
C	-5.22585	1.57214	-1.66971
C	-2.26551	1.79307	-2.09722
H	0.00115	0.00106	-1.63775
H	0.98172	-3.20737	2.64889
H	2.30974	-3.43693	1.47043
H	1.60902	-1.80357	1.71439
H	1.24476	-1.44109	-2.28355
H	2.87425	-1.68496	-3.01061
H	2.24350	-2.85549	-1.80741
H	3.20213	0.97781	2.65308
H	3.43895	2.30689	1.47733
H	1.80309	1.60955	1.71499
H	2.85862	2.24249	-1.80438
H	1.44480	1.24366	-2.28200
H	1.68971	2.87283	-3.00940
H	-2.30444	3.44454	1.47873
H	-1.61453	1.80456	1.70972
H	-0.97561	3.19748	2.65227
H	-2.86991	1.68819	-3.01217
H	-2.24132	2.85796	-1.80706
H	-1.24134	1.44437	-2.28306
H	-3.20229	-0.97835	2.64886
H	-3.44273	-2.30656	1.47320
H	-1.80496	-1.61358	1.70976
H	-2.85564	-2.24213	-1.80896
H	-1.44176	-1.24213	-2.28403
H	-1.68482	-2.87092	-3.01292
H	6.24337	-1.36986	-1.28923
H	5.07567	-2.66375	-1.64107
H	5.20627	-1.26007	-2.72660
H	5.73215	1.64129	0.77281
H	5.65421	0.30626	1.94582
H	6.51659	0.09050	0.40647
H	0.09189	-6.51621	0.40043
H	1.64212	-5.73151	0.76857
H	0.30629	-5.65542	1.94084
H	-2.66352	-5.07393	-1.64455
H	-1.26027	-5.20325	-2.73080
H	-1.36926	-6.24172	-1.29435
H	1.37269	6.24262	-1.28982
H	2.66678	5.07454	-1.63971
H	1.26440	5.20500	-2.72694
H	-1.64129	5.73321	0.76720
H	-0.30891	5.65475	1.94323
H	-0.08924	6.51667	0.40420
H	-5.07294	2.66597	-1.64371
H	-5.20231	1.26357	-2.73105
H	-6.24111	1.37172	-1.29477
H	-6.51626	-0.09026	0.39901
H	-5.73258	-1.64167	0.76423
H	-5.65571	-0.30809	1.93905
C	-0.01638	-0.00740	4.69506
H	0.07678	1.01818	5.09374
H	-0.95595	-0.43842	5.08357
H	0.82183	-0.60461	5.09521

SCF = -1762.20690616
H(0 K)= -1761.433487
H(298 K)= -1761.381591
G(298 K)= -1761.519751
Lowest Frequency = 19.0961cm-1

$[Ru(IMe_4)_4(H)(O_2)]^+$

N	0.13277	3.15834	-0.41426
C	-0.37640	2.03347	0.20396
N	-1.20349	2.55819	1.17877
C	-1.22563	3.96145	1.15404
C	-0.37874	4.34085	0.14148
Ru	-0.00001	0.00001	-0.27258
C	-2.10902	-0.32892	-0.22008
N	-2.85050	-1.08056	0.68227
C	-4.22400	-1.06912	0.38633
C	-4.36669	-0.28506	-0.73235
N	-3.07787	0.14885	-1.07801
C	-2.33017	-1.81035	1.83435
C	-5.24109	-1.81032	1.19529
C	-5.58509	0.09055	-1.51374
C	-2.84317	1.02877	-2.22567
C	-1.99910	1.79196	2.13435
C	-2.05644	4.78566	2.08578
C	-0.01170	5.69897	-0.36563
C	1.12790	3.20035	-1.48961
C	0.37638	-2.03342	0.20409
N	-0.13257	-3.15832	-0.41424
C	0.37886	-4.34080	0.14164
C	1.22553	-3.96134	1.15436
N	1.20333	-2.55808	1.17905
C	-1.12742	-3.20038	-1.48986
C	1.99874	-1.79179	2.13475
C	2.05619	-4.78549	2.08628
C	0.01200	-5.69895	-0.36553
O	0.09569	0.68893	-2.25539
O	-0.09584	-0.68907	-2.25533
C	2.10900	0.32892	-0.22022
N	2.85056	1.08040	0.68221
C	4.22404	1.06899	0.38615
C	4.36664	0.28507	-0.73264
N	3.07779	-0.14879	-1.07825
C	2.33034	1.80998	1.83446
C	5.24120	1.81007	1.19514
C	5.58497	-0.09046	-1.51416
C	2.84301	-1.02858	-2.22600
H	0.00002	0.00007	1.33727
H	3.24969	-0.56533	-3.13952
H	3.34839	-1.99668	-2.06644
H	1.75589	-1.16746	-2.34377
H	1.50814	-0.82512	2.30009
H	2.05595	-2.34372	3.08479
H	3.01975	-1.61812	1.75577
H	-0.72525	-3.76163	-2.34828
H	-2.04176	-3.70360	-1.13274
H	-1.35462	-2.17665	-1.81018
H	-2.35269	-2.90017	1.66074
H	-1.29333	-1.49903	2.00560

H	-2.93641	-1.58663	2.72746
H	-3.34857	1.99684	-2.06598
H	-1.75606	1.16769	-2.34349
H	-3.24989	0.56561	-3.13923
H	-2.05646	2.34392	3.08437
H	-3.02004	1.61832	1.75520
H	-1.50856	0.82528	2.29981
H	0.72597	3.76156	-2.34816
H	2.04214	3.70358	-1.13226
H	1.35519	2.17661	-1.80983
H	2.35277	2.89983	1.66101
H	1.29354	1.49857	2.00581
H	2.93671	1.58617	2.72746
H	1.95513	-5.85210	1.83547
H	3.12934	-4.53199	2.02324
H	1.74888	-4.66806	3.14156
H	-1.07271	-5.89421	-0.29150
H	0.29795	-5.83633	-1.42373
H	0.52744	-6.47513	0.21973
H	6.48327	0.35169	-1.05727
H	5.73484	-1.18432	-1.55057
H	5.53312	0.26628	-2.55847
H	5.03336	2.89450	1.23667
H	5.29816	1.44764	2.23801
H	6.24042	1.68454	0.75145
H	-6.24034	-1.68474	0.75170
H	-5.03323	-2.89475	1.23664
H	-5.29797	-1.44805	2.23822
H	-5.73497	1.18441	-1.55001
H	-5.53331	-0.26606	-2.55809
H	-6.48334	-0.35166	-1.05683
H	-3.12959	4.53221	2.02253
H	-1.74934	4.66824	3.14113
H	-1.95528	5.85227	1.83497
H	-0.52723	6.47520	0.21950
H	1.07299	5.89418	-0.29137
H	-0.29741	5.83635	-1.42390

SCF = -1779.79965243
H(0 K)= -1779.063482
H(298 K)= -1779.014946
G(298 K)= -1779.143470
Lowest Frequency = 25.1104cm-1

$[Ru(IMe_4)_4(H)(P_4)]^+$

N	1.86883	-2.57219	0.29859
C	1.63675	-1.39497	-0.39906
N	2.73633	-1.34177	-1.24902
C	3.61587	-2.42196	-1.06435
C	3.06556	-3.20343	-0.07948
Ru	0.03201	-0.00795	-0.29161
P	-0.24816	-0.02756	2.07261
P	-0.89454	-1.30181	3.83176
P	0.67517	0.31829	4.11765
P	-1.49123	0.88451	3.73117
C	2.97506	-0.33473	-2.28087
C	4.88113	-2.59261	-1.84439
C	3.55244	-4.47175	0.54697
C	0.98348	-3.15517	1.30141
C	-1.50178	1.43097	-0.56720
N	-1.72744	2.63835	0.08370
C	-2.83652	3.33165	-0.43009
C	-3.33795	2.55737	-1.44609
N	-2.51552	1.42068	-1.51809
C	-0.87471	3.24666	1.10186
C	-2.71520	0.39918	-2.54394
C	-4.51412	2.77663	-2.34425
C	-3.30022	4.64391	0.11828
C	-1.35223	-1.59133	-0.59665
N	-1.23729	-2.64719	-1.49426
C	-2.33822	-3.51886	-1.45020
C	-3.19760	-3.00686	-0.51110
N	-2.58990	-1.84077	-0.01595
C	-0.14588	-2.84701	-2.44563
C	-2.44969	-4.74443	-2.30094
C	-4.52079	-3.50534	-0.02275
C	-3.28268	-0.98157	0.93995
C	1.46595	1.55269	-0.38271
N	2.61912	1.76187	0.36170
C	3.33262	2.90008	-0.04914
C	2.62585	3.43976	-1.09466
N	1.50825	2.60956	-1.28522
C	3.13825	0.88315	1.40556
C	4.59654	3.34959	0.61276
C	2.89562	4.65630	-1.92277
C	0.55863	2.84817	-2.37033
H	0.34023	-1.87993	-2.62109
H	-0.55395	-3.23223	-3.39282
H	0.60176	-3.56275	-2.06313
H	-3.35646	-5.30779	-2.03353
H	-1.58796	-5.42276	-2.16949
H	-2.51995	-4.50634	-3.37823
H	-4.77092	-4.45918	-0.51127
H	-5.34386	-2.80044	-0.24013
H	-4.52039	-3.68155	1.06778
H	-3.35383	-1.46220	1.93011
H	-4.30240	-0.76676	0.57915
H	-2.72989	-0.03937	1.02885
H	-1.77272	-0.14535	-2.67529
H	-2.99824	0.88265	-3.49194
H	-3.50801	-0.31370	-2.25928
H	-5.04275	3.69784	-2.05620
H	-5.24140	1.94711	-2.28838
H	-4.22126	2.88610	-3.40455
H	-4.18848	4.99224	-0.42996
H	-2.53036	5.43176	0.03160
H	-3.57695	4.57291	1.18564
H	-0.05752	2.55486	1.33285
H	-1.45047	3.45907	2.01705
H	-0.44755	4.19203	0.72418
H	0.05129	1.90310	-2.59891
H	1.10135	3.20144	-3.26078
H	-0.19588	3.60431	-2.09215
H	3.78469	5.18194	-1.54279
H	2.05410	5.37146	-1.89998
H	3.08976	4.41126	-2.98311
H	4.97332	4.26476	0.13162
H	5.39697	2.59063	0.54846
H	4.44662	3.57647	1.68374
H	2.43772	0.05183	1.53554
H	3.24188	1.42784	2.35806
H	4.12590	0.48641	1.11401
H	2.01557	0.13131	-2.53644
H	3.40043	-0.81897	-3.17357
H	3.67371	0.44610	-1.93365
H	5.44208	-3.46154	-1.46826
H	5.54265	-1.71173	-1.76427
H	4.69430	-2.76647	-2.92009
H	4.53827	-4.74198	0.13927
H	2.87501	-5.32402	0.35598
H	3.66098	-4.37860	1.64228
H	0.00373	-2.67054	1.22462
H	1.38272	-3.01176	2.32031
H	0.87179	-4.23579	1.11737
H	0.12382	0.00816	-1.89746

SCF = -1655.79685926
H(0 K)= -1655.061431
H(298 K)= -1655.008531
G(298 K)= -1655.149039
Lowest Frequency = 4.3028cm-1

$[Ru(IMe_4)_4(H)(SO_2)]^+$

N	-3.11403	-0.46873	0.66086
C	-1.96866	-0.80514	-0.04152
N	-2.42610	-1.79518	-0.90018
C	-3.78753	-2.08315	-0.71080
C	-4.22307	-1.24297	0.28365
Ru	0.00000	0.00001	0.09429
C	0.83663	-1.93407	-0.21924
N	1.76256	-2.30345	-1.18202
C	2.09547	-3.66548	-1.10710
C	1.35779	-4.18679	-0.07275
N	0.59683	-3.12525	0.44300
C	2.35292	-1.42923	-2.19444
C	3.08091	-4.31937	-2.02317
C	1.30513	-5.57289	0.48710
C	-0.32760	-3.32531	1.55978
C	-1.65002	-2.44635	-1.95336
C	-4.52158	-3.12744	-1.49111
C	-5.56869	-1.10665	0.92292
C	-3.24135	0.58227	1.67126
S	-0.00002	0.00000	2.34732
O	-1.03523	-0.72419	3.19313
O	1.03519	0.72417	3.19316
C	-0.83663	1.93410	-0.21923
N	-1.76251	2.30349	-1.18204
C	-2.09545	3.66551	-1.10710
C	-1.35785	4.18680	-0.07269
N	-0.59688	3.12525	0.44307
C	-2.35279	1.42929	-2.19453
C	-3.08085	4.31942	-2.02320
C	-1.30524	5.57287	0.48721
C	0.32748	3.32529	1.55990
C	1.96866	0.80516	-0.04148
N	2.42614	1.79517	-0.90015
C	3.78757	2.08314	-0.71073
C	4.22308	1.24295	0.28372
N	3.11403	0.46869	0.66090
C	1.65009	2.44634	-1.95335
C	4.52163	3.12742	-1.49102
C	5.56868	1.10660	0.92300
C	3.24131	-0.58234	1.67126
H	0.79509	1.80659	-2.20247
H	2.28301	2.57817	-2.84462
H	1.27853	3.43479	-1.63374
H	5.54927	3.22872	-1.11065
H	4.04172	4.11926	-1.41411
H	4.59550	2.87952	-2.56591
H	6.02776	0.11879	0.73569
H	5.52005	1.24474	2.01746
H	6.25671	1.86665	0.52305
H	2.38914	-1.26442	1.57801
H	3.24848	-0.15635	2.68584
H	4.17110	-1.14485	1.49278
H	1.69446	-0.56333	-2.33090
H	2.44325	-1.97850	-3.14415
H	3.35293	-1.07946	-1.88655
H	3.23179	-5.36841	-1.72728
H	4.06707	-3.82290	-1.99668
H	2.74090	-4.32264	-3.07493
H	2.02526	-6.22043	-0.03532
H	0.30726	-6.03424	0.37535
H	1.55766	-5.59454	1.56200
H	-0.98124	-2.45331	1.65991
H	0.22348	-3.46181	2.50527
H	-0.93745	-4.22380	1.37497
H	0.00001	0.00002	-1.52418
H	-0.79502	-1.80659	-2.20247
H	-2.28292	-2.57819	-2.84464
H	-1.27846	-3.43479	-1.63373
H	-5.54922	-3.22875	-1.11076
H	-4.04166	-4.11927	-1.41418
H	-4.59542	-2.87954	-2.56600
H	-6.02777	-0.11884	0.73561
H	-5.52007	-1.24481	2.01737
H	-6.25670	-1.86670	0.52294
H	-2.38919	1.26438	1.57805
H	-3.24852	0.15624	2.68583
H	-4.17115	1.14478	1.49278
H	-1.69430	0.56341	-2.33099
H	-2.44308	1.97859	-3.14423
H	-3.35281	1.07947	-1.88671
H	-3.23176	5.36843	-1.72729
H	-4.06701	3.82293	-1.99678
H	-2.74078	4.32271	-3.07495
H	-2.02535	6.22042	-0.03524
H	-0.30737	6.03424	0.37554
H	-1.55784	5.59449	1.56210
H	0.98112	2.45329	1.66004
H	-0.22365	3.46177	2.50536
H	0.93733	4.22380	1.37515

SCF = -1790.10659935
H(0 K)= -1789.367809
H(298 K)= -1789.317663
G(298 K)= -1789.449427
Lowest Frequency = 26.0887cm-1

$[Ru(IMe_4)_4(H)_2]$

C	-0.41989	4.30191	0.54356
N	-0.65689	2.95526	0.85974
C	0.00000	2.07063	0.00000
N	0.65689	2.95526	-0.85974
C	0.41989	4.30191	-0.54356
C	1.48694	2.52904	-1.97782
C	-1.48694	2.52904	1.97782
Ru	0.00000	0.00000	0.00000
C	2.07063	0.00000	0.00000
N	2.95526	-0.65689	-0.85974
C	4.30191	-0.41989	-0.54356
C	4.30191	0.41989	0.54356
N	2.95526	0.65689	0.85974
C	2.52904	-1.48694	-1.97782
C	2.52904	1.48694	1.97782
C	5.43928	-1.01570	-1.31123
C	5.43928	1.01570	1.31123
C	1.01570	5.43928	-1.31123
C	-1.01570	5.43928	1.31123
H	0.00000	0.00000	-1.70871
C	-2.07063	0.00000	0.00000
N	-2.95526	0.65689	-0.85974
C	-4.30191	0.41989	-0.54356
C	-4.30191	-0.41989	0.54356
N	-2.95526	-0.65689	0.85974
C	-2.52904	1.48694	-1.97782
C	-2.52904	-1.48694	1.97782
C	-5.43928	1.01570	-1.31123
C	-5.43928	-1.01570	1.31123

C	0.00000	-2.07063	0.00000
N	-0.65689	-2.95526	-0.85974
C	-0.41989	-4.30191	-0.54356
C	0.41989	-4.30191	0.54356
N	0.65689	-2.95526	0.85974
C	-1.48694	-2.52904	-1.97782
C	1.48694	-2.52904	1.97782
C	-1.01570	-5.43928	-1.31123
C	1.01570	-5.43928	1.31123
H	-2.55516	2.56157	-1.72073
H	-3.18264	1.31272	-2.84949
H	-1.49045	1.19320	-2.20644
H	-5.40220	2.12098	-1.32262
H	-6.40024	0.72230	-0.85925
H	-5.45775	0.68353	-2.36664
H	-5.45775	-0.68353	2.36664
H	-5.40220	-2.12098	1.32262
H	-6.40024	-0.72230	0.85925
H	-2.55516	-2.56157	1.72073
H	-3.18264	-1.31272	2.84949
H	-1.49045	-1.19320	2.20644
H	0.00000	0.00000	1.70871
H	-2.56157	-2.55516	-1.72073
H	-1.31272	-3.18264	-2.84949
H	-1.19320	-1.49045	-2.20644
H	-2.12098	-5.40220	-1.32262
H	-0.72230	-6.40024	-0.85925
H	-0.68353	-5.45775	-2.36664
H	0.68353	-5.45775	2.36664
H	2.12098	-5.40220	1.32262
H	0.72230	-6.40024	0.85925
H	2.56157	-2.55516	1.72073
H	1.31272	-3.18264	2.84949
H	1.19320	-1.49045	2.20644
H	2.55516	-2.56157	-1.72073
H	3.18264	-1.31272	-2.84949
H	1.49045	-1.19320	-2.20644
H	5.40220	-2.12098	-1.32262
H	6.40024	-0.72230	-0.85925
H	5.45775	-0.68353	-2.36664
H	5.45775	0.68353	2.36664
H	5.40220	2.12098	1.32262
H	6.40024	0.72230	0.85925
H	2.55516	2.56157	1.72073
H	3.18264	1.31272	2.84949
H	1.49045	1.19320	2.20644
H	2.56157	2.55516	-1.72073
H	1.31272	3.18264	-2.84949
H	1.19320	1.49045	-2.20644
H	2.12098	5.40220	-1.32262
H	0.72230	6.40024	-0.85925
H	0.68353	5.45775	-2.36664
H	-0.68353	5.45775	2.36664
H	-2.12098	5.40220	1.32262
H	-0.72230	6.40024	0.85925
H	-2.56157	2.55516	1.72073
H	-1.31272	3.18264	2.84949
H	-1.19320	1.49045	2.20644

SCF = -1630.15154685
H(0 K)= -1629.420687
H(298 K)= -1629.373882
G(298 K)= -1629.496733
Lowest Frequency = 23.0478cm-1

[Ru(IMe$_4$)$_4$(H)(F)]

C	-3.11970	2.98516	-0.63483
N	-1.90666	2.34309	-0.92999
C	-1.61236	1.31199	-0.03787
N	-2.70484	1.35644	0.82081
C	-3.62948	2.35241	0.47338
C	-2.87233	0.45217	1.95813
C	-1.05432	2.72330	-2.04731
Ru	0.00001	0.00000	-0.01315
C	-1.31200	-1.61235	-0.03787
N	-1.35644	-2.70484	0.82081
C	-2.35245	-3.62945	0.47340
C	-2.98523	-3.11964	-0.63477
N	-2.34314	-1.90662	-0.92994
C	-0.45213	-2.87238	1.95809
C	-2.72338	-1.05424	-2.04723
C	-2.59992	-4.89010	1.23952
C	-4.13029	-3.65220	-1.43636
C	-4.89012	2.59987	1.23950
C	-3.65230	4.13017	-1.43645
F	0.00007	0.00002	2.26699
C	1.31201	1.61236	-0.03792
N	1.35647	2.70485	0.82075
C	2.35245	3.62948	0.47330
C	2.98519	3.11967	-0.63489
N	2.34311	1.90664	-0.93003
C	0.45220	2.87239	1.95806
C	2.72331	1.05428	-2.04735
C	2.59993	4.89013	1.23941
C	4.13021	3.65224	-1.43653
C	1.61237	-1.31201	-0.03796
N	2.70487	-1.35648	0.82069
C	3.62950	-2.35245	0.47321
C	3.11967	-2.98518	-0.63499
N	1.90664	-2.34309	-0.93010
C	2.87240	-0.45224	1.95804
C	1.05426	-2.72327	-2.04741
C	4.89016	-2.59994	1.23929
C	3.65223	-4.13017	-1.43665
H	-0.39619	3.53088	1.69616
H	1.00221	3.32443	2.80044
H	0.09455	1.86512	2.24275
H	1.70226	5.53391	1.28481
H	3.40336	5.47497	0.76379
H	2.90849	4.69351	2.28346
H	3.85328	3.85213	-2.48911
H	4.98815	2.95431	-1.45651
H	4.48793	4.60129	-1.00651
H	3.65768	0.50261	-1.83729
H	2.86626	1.65866	-2.95992
H	1.90118	0.33735	-2.19181
H	-0.00003	0.00001	-1.62896
H	3.53078	0.39623	1.69611
H	3.32457	-1.00224	2.80035
H	1.86512	-0.09471	2.24281
H	5.53394	-1.70227	1.28471
H	5.47501	-3.40336	0.76363
H	4.69356	-2.90856	2.28333
H	3.85209	-3.85323	-2.48924
H	2.95431	-4.98813	-1.45663
H	4.60130	-4.48789	-1.00667
H	0.50267	-3.65771	-1.83739
H	1.65862	-2.86612	-2.96001
H	0.33728	-1.90118	-2.19179
H	0.39629	-3.53080	1.69611
H	-1.00209	-3.32452	2.80045
H	-0.09453	-1.86513	2.24283
H	-1.70226	-5.53390	1.28487
H	-3.40339	-5.47492	0.76393
H	-2.90844	-4.69348	2.28358

H	-3.85340	-3.85212	-2.48894
H	-4.98821	-2.95425	-1.45633
H	-4.48802	-4.60123	-1.00631
H	-3.65768	-0.50248	-1.83707
H	-2.86651	-1.65863	-2.95977
H	-1.90121	-0.33739	-2.19180
H	-3.53071	-0.39630	1.69620
H	-3.32448	1.00214	2.80048
H	-1.86506	0.09462	2.24287
H	-5.53389	1.70220	1.28492
H	-5.47498	3.40330	0.76388
H	-4.69349	2.90845	2.28354
H	-3.85221	3.85324	-2.48903
H	-2.95438	4.98812	-1.45645
H	-4.60134	4.48787	-1.00642
H	-0.50264	3.65766	-1.83723
H	-1.65872	2.86630	-2.95986
H	-0.33741	1.90117	-2.19181

SCF = -1729.44989076
H(0 K)= -1728.722418
H(298 K)= -1728.674383
G(298 K)= -1728.801819
Lowest Frequency = 22.9525cm-1

[Ru(IMe$_4$)$_4$(H)(Cl)]

Ru	0.00000	0.00000	0.02822
Cl	0.00000	0.00000	2.75055
N	3.01202	0.73295	0.69222
N	2.91635	-0.71101	-0.91543
C	2.08465	0.00000	-0.04549
C	4.33705	0.48774	0.29981
C	4.27784	-0.43390	-0.71594
C	2.67349	1.72262	1.71241
H	2.73146	2.74730	1.30078
H	3.37540	1.63782	2.55784
H	1.65802	1.50897	2.07643
C	5.51508	1.14351	0.94815
H	5.46814	2.24616	0.88469
H	6.44792	0.82333	0.45742
H	5.59973	0.88537	2.02034
C	5.37048	-1.08283	-1.50535
H	5.31759	-0.83951	-2.58353
H	5.34934	-2.18535	-1.42200
H	6.35370	-0.74402	-1.14232
C	2.44743	-1.62247	-1.95111
H	2.52610	-2.67827	-1.63378
H	3.04078	-1.48364	-2.87054
H	1.39220	-1.38369	-2.14325
H	0.00000	0.00000	-1.57886
N	0.73295	-3.01202	0.69222
N	-0.71101	-2.91635	-0.91543
C	0.00000	-2.08465	-0.04549
C	0.48774	-4.33705	0.29981
C	-0.43390	-4.27784	-0.71594
C	1.72262	-2.67349	1.71241
H	2.74730	-2.73146	1.30078
H	1.63782	-3.37540	2.55784
H	1.50897	-1.65802	2.07643
C	1.14351	-5.51508	0.94815
H	2.24616	-5.46814	0.88469
H	0.82333	-6.44792	0.45742
H	0.88537	-5.59973	2.02034
C	-1.08283	-5.37048	-1.50535
H	-0.83951	-5.31759	-2.58353
H	-2.18535	-5.34934	-1.42200
H	-0.74402	-6.35370	-1.14232
C	-1.62247	-2.44743	-1.95111
H	-2.67827	-2.52610	-1.63378
H	-1.48364	-3.04078	-2.87054
H	-1.38369	-1.39220	-2.14325
N	-3.01202	-0.73295	0.69222
N	-2.91635	0.71101	-0.91543
C	-2.08465	0.00000	-0.04549
C	-4.33705	-0.48774	0.29981
C	-4.27784	0.43390	-0.71594
C	-2.67349	-1.72262	1.71241
H	-2.73146	-2.74730	1.30078
H	-3.37540	-1.63782	2.55784
H	-1.65802	-1.50897	2.07643
C	-5.51508	-1.14351	0.94815
H	-5.46814	-2.24616	0.88469
H	-6.44792	-0.82333	0.45742
H	-5.59973	-0.88537	2.02034
C	-5.37048	1.08283	-1.50535
H	-5.31759	0.83951	-2.58353
H	-5.34934	2.18535	-1.42200
H	-6.35370	0.74402	-1.14232
C	-2.44743	1.62247	-1.95111
H	-2.52610	2.67827	-1.63378
H	-3.04078	1.48364	-2.87054
H	-1.39220	1.38369	-2.14325
N	-0.73295	3.01202	0.69222
N	0.71101	2.91635	-0.91543
C	0.00000	2.08465	-0.04549
C	-0.48774	4.33705	0.29981
C	0.43390	4.27784	-0.71594
C	-1.72262	2.67349	1.71241
H	-2.74730	2.73146	1.30078
H	-1.63782	3.37540	2.55784
H	-1.50897	1.65802	2.07643
C	-1.14351	5.51508	0.94815
H	-2.24616	5.46814	0.88469
H	-0.82333	6.44792	0.45742
H	-0.88537	5.59973	2.02034
C	1.08283	5.37048	-1.50535
H	0.83951	5.31759	-2.58353
H	2.18535	5.34934	-1.42200
H	0.74402	6.35370	-1.14232
C	1.62247	2.44743	-1.95111
H	2.67827	2.52610	-1.63378
H	1.48364	3.04078	-2.87054
H	1.38369	1.39220	-2.14325

(b) Ru-phosphine complexes

$[Ru(dmpe)_2(H)]^+$

```
C   0.00000  3.43755 -0.40612
C  -1.38535  3.18933  0.20095
P  -1.89454  1.38526 -0.07073
Ru  0.00000  0.00000  0.07797
P  -1.17268 -2.03310  0.07519
C   0.00000 -3.43755 -0.40612
C   1.38535 -3.18933  0.20095
P   1.89454 -1.38526 -0.07073
P   1.17268  2.03310  0.07519
C   3.34731 -1.22531  1.09682
C   2.74696 -1.46020 -1.73161
C  -1.82000 -2.60048  1.74071
C  -2.63754 -2.36831 -1.03141
C  -2.74696  1.46020 -1.73161
C  -3.34731  1.22531  1.09682
C   2.63754  2.36831 -1.03141
C   1.82000  2.60048  1.74071
H   0.00000  0.00000 -1.47939
H  -0.04849  3.44021 -1.50983
H  -2.14992  3.86323 -0.22337
H  -1.37110  3.35434  1.29355
H   0.42369  4.40679 -0.09010
H   1.37110 -3.35434  1.29355
H   2.14992 -3.86323 -0.22337
H   0.04849 -3.44021 -1.50983
H  -0.42369 -4.40679 -0.09010
H   2.94309  3.42541 -0.96515
H   3.48725  1.73536 -0.73091
H   2.36803  2.13062 -2.07212
H   2.24619  3.61514  1.67259
H   1.00407  2.60051  2.48073
H   2.59979  1.90457  2.08770
H  -4.06773  2.04591  0.94445
H  -3.86017  0.26637  0.92163
H  -2.98964  1.24662  2.13846
H  -3.55972  2.20482 -1.72297
H  -2.01044  1.72502 -2.50556
H  -3.16169  0.47110 -1.97763
H   3.55972 -2.20482 -1.72297
H   2.01044 -1.72502 -2.50556
H   3.16169 -0.47110 -1.97763
H  -2.94309 -3.42541 -0.96515
H  -3.48725 -1.73536 -0.73091
H  -2.36803 -2.13062 -2.07212
H  -2.24619 -3.61514  1.67259
H  -1.00407 -2.60051  2.48073
H  -2.59979 -1.90457  2.08770
H   4.06773 -2.04591  0.94445
H   3.86017 -0.26637  0.92163
H   2.98964 -1.24662  2.13846
```

```
SCF  =          -598.434308122
H(0 K)=         -598.015549
H(298 K)=       -597.987021
G(298 K)=       -598.070968
Lowest Frequency = 34.2878cm-1
```

$[Ru(dippe)_2(H)]^+$

```
C  -2.72549  4.03527 -0.97989
C  -2.53605  2.50703 -1.02188
C  -3.87512  1.78555 -1.27157
P  -1.56916  1.70766  0.44457
Ru -0.02019 -0.03154 -0.04234
P   1.48476 -1.86893  0.41173
C   2.93105 -2.54834 -0.66230
C   2.49928 -2.86006 -2.10489
C  -0.55849  3.13079  1.16653
C   0.66052  3.40698  0.28778
P   1.52340  1.78945 -0.21543
C   3.11796  1.80596  0.83714
C   4.18026  2.85819  0.47557
C  -2.86344  1.44459  1.83081
C  -3.69076  2.69607  2.18707
C   1.94764  2.21949 -2.04495
C   2.80873  1.14936 -2.73256
C   2.50356  3.62898 -2.33733
C  -2.20860  0.86943  3.10078
C   2.72700  1.91179  2.32519
P  -1.57282 -1.77880 -0.47898
C  -0.72474 -3.47129 -0.43755
C   0.43665 -3.45401  0.55913
C  -1.94117 -1.46350 -2.32815
C  -2.21349 -2.66696 -3.24513
C  -3.25071 -2.10645  0.36495
C  -4.21948 -3.01064 -0.41693
C  -0.75307 -0.62719 -2.85341
C  -3.01528 -2.64113  1.79077
C   2.32751 -1.85116  2.14527
C   3.17743 -3.10320  2.44746
C   1.32419 -1.62468  3.29108
C   4.18182 -1.65588 -0.63062
H   0.03017 -0.00106  1.51133
H   1.94703  4.43765 -1.83870
H   2.36767  2.92571  2.57409
H  -0.50373  0.22579 -2.16290
H  -0.98845 -0.15203 -3.82351
H  -3.96898 -2.67099  2.34580
H   1.87163 -1.48995  4.24049
H   4.56629 -1.49967  0.39076
H  -1.18259  4.03195  1.28742
H   0.34407  3.89885 -0.64795
H   1.08474 -4.33893  0.43468
H  -0.24930  2.79757  2.17186
H   1.37772  4.08719  0.77885
H  -1.45890 -4.25892 -0.19467
H  -0.36290 -3.67706 -1.45819
H   0.04915 -3.47237  1.59223
H  -1.86866  2.27501 -1.87427
H  -4.28396  2.07504 -2.25541
H  -3.76845  0.68795 -1.26636
H  -4.63123  2.05042 -0.51416
H  -3.22438  4.36705 -1.90821
H  -3.35759  4.35920 -0.13782
H  -1.77029  4.58112 -0.91493
H  -3.54584  0.67955  1.41631
H  -2.98976  0.57805  3.82455
H  -1.58916 -0.01457  2.88478
H  -1.56975  1.61878  3.59997
H  -4.26462  3.09404  1.33708
H  -4.41638  2.44003  2.97952
H  -3.05620  3.50696  2.58280
H   0.92939  2.16586 -2.48265
H   3.56184  3.72241 -2.05173
H   2.44302  3.81651 -3.42430
H   3.84485  1.15911 -2.35179
H   2.39814  0.13778 -2.59088
H   2.86316  1.34546 -3.81816
H   3.54243  0.80112  0.65901
H   1.94012  1.19162  2.60277
H   3.60881  1.71867  2.96115
```

H	3.77783	3.88530	0.50847
H	5.00726	2.81168	1.20679
H	4.61633	2.69083	-0.52119
H	-2.83956	-0.81835	-2.30870
H	0.14334	-1.24879	-2.99773
H	-2.45761	-2.31083	-4.26235
H	-1.32719	-3.31748	-3.33939
H	-3.05399	-3.28780	-2.90156
H	-3.69759	-1.09703	0.43821
H	-2.62149	-3.67244	1.77193
H	-2.31098	-2.01517	2.36208
H	-4.51187	-2.57776	-1.38661
H	-3.79428	-4.01323	-0.59847
H	-5.14442	-3.15494	0.16953
H	2.99535	-0.97098	2.09860
H	0.69510	-0.73496	3.13131
H	0.65529	-2.49267	3.42692
H	3.60400	-3.01670	3.46240
H	2.56870	-4.02371	2.43382
H	4.02163	-3.23937	1.75463
H	3.17868	-3.50892	-0.17391
H	4.99250	-2.12557	-1.21597
H	3.98718	-0.66897	-1.07829
H	3.34353	-3.30518	-2.66108
H	1.66654	-3.58090	-2.14904
H	2.19576	-1.94974	-2.64878

SCF = -1227.37535131
H(0 K)= -1226.512724
H(298 K)= -1226.462617
G(298 K)= -1226.591018
Lowest Frequency = 18.7889cm-1

$[Ru(dmpe)_2(H)(O_2)]^+$

C	2.14337	-2.27033	1.87543
P	1.24955	-2.02023	0.26976
C	2.50056	-2.54206	-1.01285
Ru	0.00000	0.00000	0.09642
P	1.74527	1.41315	-0.64158
C	3.13254	1.59092	0.58308
P	-1.24955	2.02023	0.26976
C	-2.14337	2.27033	1.87543
C	0.00000	3.43299	0.23321
C	1.06954	3.16145	-0.83260
C	-2.50056	2.54206	-1.01285
P	-1.74527	-1.41315	-0.64158
C	-2.61238	-1.11369	-2.25474
C	-1.06954	-3.16145	-0.83260
C	0.00000	-3.43299	0.23321
C	-3.13254	-1.59092	0.58308
C	2.61238	1.11369	-2.25474
H	0.00000	0.00000	-1.52390
H	0.64166	3.22424	-1.84941
H	-0.51723	4.39171	0.05539
H	0.44671	3.47200	1.24187
H	1.90369	3.88281	-0.77868
H	-0.44671	-3.47200	1.24187
H	0.51723	-4.39171	0.05539
H	-0.64166	-3.22424	-1.84941
H	-1.90369	-3.88281	-0.77868
H	3.35572	1.90593	-2.43996
H	3.12120	0.13882	-2.23133
H	1.87131	1.10421	-3.06853
H	3.82557	2.38844	0.26902
H	2.71258	1.81761	1.57437
H	3.68000	0.63843	0.65255
H	-2.38289	3.33503	2.02725
H	-3.07482	1.68399	1.87550
H	-1.49192	1.89604	2.67858
H	-2.86148	3.56385	-0.81102
H	-2.05236	2.50396	-2.01790
H	-3.36244	1.85663	-0.98577
H	2.86148	-3.56385	-0.81102
H	2.05236	-2.50396	-2.01790
H	3.36244	-1.85663	-0.98577
H	-3.35572	-1.90593	-2.43996
H	-3.12120	-0.13882	-2.23133
H	-1.87131	-1.10421	-3.06853
H	-3.82557	-2.38844	0.26902
H	-2.71258	-1.81761	1.57437
H	-3.68000	-0.63843	0.65255
H	2.38289	-3.33503	2.02725
H	3.07482	-1.68399	1.87550
H	1.49192	-1.89604	2.67858
O	-0.55181	-0.43613	2.05959
O	0.55181	0.43613	2.05959

SCF = -748.804497601
H(0 K)= -748.379073
H(298 K)= -748.348406
G(298 K)= -748.436130
Lowest Frequency = 37.4049cm-1

[Ru(dmpe)(dmpe′)(H)]$^+$

C	3.08776	-1.63063	-0.42203
C	3.52997	-0.37302	0.33382
P	2.24929	1.00118	0.09311
Ru	0.09262	0.06694	-0.00196
P	-1.05832	2.11130	0.03776
C	-2.79592	1.86444	-0.66567
C	-3.35848	0.51759	-0.19860
P	-2.04724	-0.83728	-0.39558
P	1.25949	-1.97145	-0.07699
C	-2.75528	-2.23727	0.64562
C	-2.38728	-1.45109	-2.12797
C	-1.40757	2.82096	1.73766
C	-0.48978	3.62763	-0.88970
C	2.86897	1.84476	-1.45449
C	2.74926	2.22016	1.42108
C	0.88638	-3.31653	-1.31588
C	1.33692	-2.95023	1.52050
H	0.21951	0.18156	-1.55037
H	3.18033	-1.48768	-1.51363
H	4.52428	-0.02113	0.00787
H	3.58890	-0.56781	1.41999
H	3.69295	-2.51290	-0.14958
H	-3.62336	0.55770	0.87292
H	-4.27073	0.23600	-0.75277
H	-2.69268	1.88900	-1.76531
H	-3.44428	2.70902	-0.37328
H	1.64925	-4.11105	-1.27089
H	-0.09866	-3.75996	-1.10087
H	0.86885	-2.88397	-2.32815
H	2.02345	-3.80751	1.42214
H	1.68232	-2.30354	2.34260
H	0.33169	-3.32232	1.77233
H	3.82961	2.43496	1.37262
H	2.19405	3.16226	1.28888
H	2.50653	1.80657	2.41275
H	3.91612	2.16723	-1.33359
H	2.79253	1.14656	-2.30205
H	2.24112	2.72097	-1.67460
H	-3.43777	-1.76803	-2.23370
H	-2.17129	-0.64542	-2.84625
H	-1.72595	-2.30026	-2.35590
H	-1.25159	4.42282	-0.83988
H	0.44625	4.00753	-0.45092
H	-0.30776	3.36265	-1.94271
H	-2.06135	3.70611	1.66729
H	-1.89458	2.06089	2.36875
H	-0.45961	3.11099	2.21726
H	-3.80074	-2.40369	0.32763
H	-2.18949	-3.14435	0.36529
C	-2.66986	-1.99338	2.15986
H	-1.63037	-1.81074	2.48397
H	-3.27618	-1.12649	2.47227
H	-3.04560	-2.86799	2.71639

SCF = -637.745512091
H(0 K)= -637.298792
H(298 K)= -637.268913
G(298 K)= -637.356508
Lowest Frequency = 33.7071cm-1

[Ru(dmpe)(dmpe′)(H)]$^+$ (Ru-C = 3.5 A)

C	3.33533	-0.96459	-0.46642
C	3.50023	0.33132	0.33452
P	1.96376	1.41277	0.10706
Ru	0.04579	0.04858	-0.03534
P	-1.49179	1.82130	-0.07287
C	-3.12300	1.20038	-0.79763
C	-3.42618	-0.20140	-0.25800
P	-1.86369	-1.27966	-0.31905
P	1.62192	-1.69908	-0.14498
C	-2.11585	-2.45584	1.11878
C	-2.16199	-2.31853	-1.83977
C	-2.02496	2.52487	1.58120
C	-1.21553	3.38133	-1.05941
C	2.41815	2.39826	-1.41450
C	2.18304	2.68130	1.46413
C	1.54730	-3.04814	-1.43296
C	1.92782	-2.70106	1.41118
H	0.16240	0.18720	-1.58426
H	3.39687	-0.76841	-1.55195
H	4.40313	0.89190	0.03573
H	3.58679	0.11775	1.41532
H	4.11283	-1.70818	-0.21847
H	-3.74040	-0.15081	0.79976
H	-4.24003	-0.69359	-0.81758
H	-2.98727	1.18156	-1.89385
H	-3.93349	1.91600	-0.57320
H	2.48864	-3.62167	-1.44811
H	0.72013	-3.73784	-1.20324
H	1.37420	-2.60019	-2.42337
H	2.76984	-3.39816	1.26695
H	2.15581	-2.02893	2.25353
H	1.02451	-3.27771	1.66423
H	3.19729	3.11299	1.44073
H	1.44938	3.49287	1.33566
H	2.01320	2.20761	2.44396
H	3.37743	2.92176	-1.26983
H	2.49492	1.71761	-2.27624
H	1.63073	3.13542	-1.62973
H	-3.12513	-2.84935	-1.76695
H	-2.17163	-1.66301	-2.72464
H	-1.35068	-3.05084	-1.96198
H	-2.13165	3.99421	-1.07727
H	-0.40500	3.97411	-0.60709
H	-0.93307	3.11691	-2.09002
H	-2.83425	3.26284	1.45351
H	-2.37475	1.71431	2.23965
H	-1.16516	3.01320	2.06608
H	-3.16320	-2.80338	1.16412
H	-1.48479	-3.34195	0.92711
C	-1.68817	-1.74990	2.41596
H	-0.65123	-1.36975	2.33916
H	-2.34494	-0.89542	2.65223
H	-1.72658	-2.43486	3.28012

SCF = -637.742961992

[Ru(dmpe)(dmpe′)(H)]$^+$ (Ru-C = 3.25 A)

C	3.40187	-0.72387	-0.42656
C	3.43679	0.54699	0.42824
P	1.84140	1.52475	0.15267
Ru	0.03265	0.02958	-0.05089
P	-1.61858	1.69569	-0.17776
C	-3.19372	0.92624	-0.88344
C	-3.42246	-0.45299	-0.25520
P	-1.79475	-1.43491	-0.21677
P	1.73426	-1.59501	-0.21446
C	-1.88190	-2.36254	1.41194
C	-2.07310	-2.73210	-1.52802
C	-2.23495	2.49039	1.40454
C	-1.41245	3.19374	-1.27143
C	2.29297	2.55715	-1.33899
C	1.91606	2.78850	1.52856
C	1.77759	-2.81928	-1.62220
C	2.07940	-2.70935	1.25401
H	0.16295	0.18835	-1.59868
H	3.49678	-0.47883	-1.49969
H	4.31245	1.17863	0.19758
H	3.48170	0.29848	1.50417
H	4.22024	-1.41978	-0.17220
H	-3.76198	-0.35331	0.79129
H	-4.19298	-1.02994	-0.79432
H	-3.03441	0.84156	-1.97329
H	-4.05131	1.60277	-0.72119
H	2.75671	-3.32386	-1.66645
H	0.99497	-3.58043	-1.48181
H	1.59078	-2.29089	-2.56937
H	2.96016	-3.34485	1.06427
H	2.26108	-2.09863	2.15243
H	1.20770	-3.35456	1.44499
H	2.89734	3.29067	1.55013
H	1.13232	3.54744	1.37626
H	1.74057	2.29299	2.49649
H	3.21130	3.13691	-1.14985
H	2.44662	1.89430	-2.20438
H	1.47146	3.24761	-1.57965
H	-3.01488	-3.27477	-1.34573
H	-2.11719	-2.24451	-2.51446
H	-1.23839	-3.44872	-1.53206
H	-2.36765	3.73557	-1.36761
H	-0.66483	3.87534	-0.83623
H	-1.06956	2.87493	-2.26755
H	-3.05850	3.19364	1.19722
H	-2.58950	1.71664	2.10322
H	-1.40828	3.03423	1.88769
H	-2.90461	-2.71530	1.63267
H	-1.24157	-3.25628	1.30970
C	-1.34125	-1.42711	2.50898
H	-0.35056	-1.00883	2.21866
H	-2.02415	-0.58397	2.70313
H	-1.19543	-1.95657	3.46614

SCF = -637.740983546

[Ru(dmpe)(dmpe′)(H)]$^+$ (Ru-C = 3.0 A)

C	3.42732	-0.57534	-0.41174
C	3.38446	0.66164	0.49167
P	1.75941	1.58730	0.20459
Ru	0.02485	0.01919	-0.05292
P	-1.71217	1.58792	-0.28597
C	-3.22995	0.68360	-0.96244
C	-3.40787	-0.66059	-0.24648
P	-1.72975	-1.54204	-0.09101
P	1.78979	-1.51902	-0.29228
C	-1.68453	-2.16879	1.67915
C	-1.95127	-3.06877	-1.13964
C	-2.41933	2.48582	1.20120
C	-1.55231	2.99726	-1.49850
C	2.20776	2.68572	-1.24019
C	1.75008	2.80719	1.62078
C	1.86450	-2.58825	-1.81925
C	2.16097	-2.76676	1.05680
H	0.17228	0.19573	-1.60167
H	3.54571	-0.28310	-1.47059
H	4.24125	1.33501	0.31379
H	3.40479	0.37301	1.55838
H	4.26583	-1.24722	-0.15905
H	-3.79280	-0.51215	0.77824
H	-4.12428	-1.31446	-0.77187
H	-3.03867	0.53111	-2.03962
H	-4.12488	1.32357	-0.86719
H	2.83349	-3.10978	-1.88453
H	1.05692	-3.33537	-1.79548
H	1.72474	-1.95311	-2.70726
H	3.06705	-3.34728	0.81692
H	2.30790	-2.24655	2.01650
H	1.31269	-3.46104	1.16500
H	2.71403	3.33786	1.69014
H	0.94808	3.54631	1.46663
H	1.55916	2.27497	2.56591
H	3.10096	3.28963	-1.01065
H	2.40272	2.06001	-2.12473
H	1.36840	3.35655	-1.47550
H	-2.86686	-3.61121	-0.85290
H	-2.01731	-2.77616	-2.19927
H	-1.08496	-3.73619	-1.01295
H	-2.53459	3.46365	-1.67980
H	-0.87100	3.76203	-1.09403
H	-1.14267	2.61889	-2.44719
H	-3.26504	3.12819	0.90482
H	-2.76728	1.76176	1.95435
H	-1.63719	3.10945	1.66168
H	-2.67545	-2.47995	2.05358
H	-1.03472	-3.06089	1.68778
C	-1.06639	-1.04245	2.53206
H	-0.10899	-0.66777	2.07979
H	-1.75217	-0.19097	2.65680
H	-0.79041	-1.39280	3.54210

SCF = -637.739419406

[Ru(dmpe)(dmpe′)(H)]$^+$ (Ru-C = 2.75 A)

C	3.42268	-0.47645	-0.47487
C	3.36172	0.74545	0.44842
P	1.70307	1.62647	0.21423
Ru	0.01705	0.00636	-0.04067
P	-1.77439	1.51047	-0.33079
C	-3.25140	0.52665	-0.98839
C	-3.39451	-0.79832	-0.22844
P	-1.68630	-1.60644	-0.01463
P	1.81947	-1.47257	-0.33095
C	-1.54141	-2.01592	1.81182
C	-1.86476	-3.24393	-0.88918
C	-2.53829	2.44274	1.10740
C	-1.65052	2.87572	-1.59633
C	2.09149	2.77425	-1.20906
C	1.68278	2.81062	1.65983
C	1.87760	-2.51475	-1.87619
C	2.25957	-2.73205	0.98588
H	0.16287	0.18817	-1.59748
H	3.50555	-0.16512	-1.53166
H	4.19358	1.44725	0.26233
H	3.41540	0.44129	1.50966
H	4.28848	-1.12392	-0.25224
H	-3.80899	-0.63276	0.78188
H	-4.07206	-1.49672	-0.74784
H	-3.04015	0.34153	-2.05663
H	-4.16939	1.13747	-0.92765
H	2.84988	-3.02578	-1.96949
H	1.07645	-3.26888	-1.84901
H	1.71364	-1.86544	-2.74963
H	3.17862	-3.27868	0.71742
H	2.40982	-2.22578	1.95260
H	1.43698	-3.45626	1.09730
H	2.62581	3.37876	1.71899
H	0.84737	3.51912	1.54418
H	1.53758	2.24840	2.59567
H	2.97648	3.39182	-0.98416
H	2.27756	2.17803	-2.11558
H	1.23257	3.43305	-1.40449
H	-2.74754	-3.79137	-0.52067
H	-1.97114	-3.06867	-1.97134
H	-0.96578	-3.85632	-0.71836
H	-2.64809	3.29111	-1.81439
H	-1.01134	3.68502	-1.21029
H	-1.20491	2.47788	-2.52034
H	-3.38618	3.05923	0.76600
H	-2.89884	1.74016	1.87519
H	-1.78055	3.09579	1.56809
H	-2.50166	-2.25720	2.30068
H	-0.89472	-2.90622	1.89622
C	-0.85296	-0.78682	2.44458
H	0.11441	-0.51376	1.92339
H	-1.51778	0.08518	2.50464
H	-0.51398	-0.99854	3.47564

SCF = -637.736692383

[Ru(dmpe)(dmpe′)(H)]$^+$ (Ru-C = 2.5 A)

C	3.40831	-0.43236	-0.53316
C	3.35319	0.78645	0.39501
P	1.67680	1.64488	0.20846
Ru	0.01294	-0.00619	-0.00922
P	-1.80814	1.46377	-0.34819
C	-3.24272	0.43704	-1.03357
C	-3.38483	-0.88065	-0.25958
P	-1.66651	-1.63991	0.03233
P	1.82751	-1.45517	-0.34599
C	-1.47554	-1.86280	1.88402
C	-1.80503	-3.34787	-0.70223
C	-2.63792	2.38472	1.06213
C	-1.69168	2.82310	-1.61972
C	2.01149	2.80006	-1.22181
C	1.68171	2.82753	1.65543
C	1.85448	-2.49727	-1.89103
C	2.32317	-2.70627	0.95901
H	0.13424	0.16919	-1.58327
H	3.45510	-0.11729	-1.59101
H	4.17000	1.50037	0.18947
H	3.43911	0.48031	1.45364
H	4.29101	-1.06538	-0.33685
H	-3.84932	-0.71581	0.72869
H	-4.01802	-1.60393	-0.80033
H	-2.99222	0.23946	-2.09095
H	-4.17466	1.02908	-1.01213
H	2.82880	-2.99874	-2.01091
H	1.06170	-3.25913	-1.84109
H	1.65921	-1.84908	-2.75874
H	3.23657	-3.24764	0.66212
H	2.50346	-2.19485	1.91807
H	1.51050	-3.43607	1.10291
H	2.61103	3.42019	1.68054
H	0.82400	3.51368	1.57245
H	1.58642	2.26188	2.59567
H	2.90207	3.41912	-1.02479
H	2.16658	2.20828	-2.13692
H	1.14526	3.45832	-1.38346
H	-2.67678	-3.88158	-0.28985
H	-1.91299	-3.26717	-1.79543
H	-0.89321	-3.92337	-0.47897
H	-2.69563	3.20346	-1.86986
H	-1.09161	3.65592	-1.22128
H	-1.20599	2.43281	-2.52645
H	-3.48596	2.98159	0.68835
H	-3.01356	1.68042	1.82151
H	-1.91059	3.05655	1.54466
H	-2.41524	-2.00962	2.44568
H	-0.84756	-2.75564	2.04750
C	-0.71852	-0.58271	2.31083
H	0.29364	-0.43407	1.80044
H	-1.35325	0.31022	2.32256
H	-0.35317	-0.68628	3.35275

SCF = -637.729116772