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Supporting Information

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Effect of the metal atom nature on hydrogen bonding and proton transfer to [Cp*MH₃(dppe)]: tungsten vs. molybdenum

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Figure 4. The optimized structures of the $[\text{CpW}(\text{dhpe})\text{H}_3]\cdot\text{TFE}$ adducts. (in color)

Figure 5. The optimized structures of the $[\text{CpW}(\text{dhpe})\text{H}_3]\cdot\text{HFIP}$ adducts. (in color)

Figure 10. Left: UV-visible spectra (toluene solution, 200 K, 0.12 cm cell) of: (a) *p*-nitrophenol ($3\cdot 10^{-4}$ M); (b) $[\text{Cp}^*\text{W}(\text{dppe})\text{H}_3]$ ($3\cdot 10^{-4}$ M); (c-h) *p*-nitrophenol in the presence of increasing amount of $[\text{Cp}^*\text{W}(\text{dppe})\text{H}_3]$: $3.7\cdot 10^{-5}$ M (c), $7.5\cdot 10^{-5}$ (d), $1.5\cdot 10^{-4}$ (e), $3\cdot 10^{-4}$ (f), $4.5\cdot 10^{-4}$ (g), $6\cdot 10^{-4}$ (h). Right: intensity changes at 380 nm. (in color)

Figure 1S. IR spectrum of $\text{Cp}^*\text{WH}_3(\text{dppe})$ and band decomposition.

Figure 2S. T_1 values for all investigated compounds (500 MHz).

Figure 3S. IR spectra of $[\text{Cp}^*\text{WH}_4(\text{dppe})]^+\text{BF}_4^-$ and of dppe .

Table 1S. Frequency parameters of the $[\text{CpW}(\text{dhpe})\text{H}_3]\cdot\text{HA}$ adducts (HA = TFE, HFIP).

Description of computational results for the $[\text{CpW}(\text{dhpe})\text{H}_3]\cdot 2\text{HFIP}$ adducts.

Table 2S. Main energetic and structural parameters of the $[\text{CpW}(\text{dhpe})\text{H}_3]\cdot 2\text{HFIP}$ adducts.

Description of computational results for the protonation product, $[\text{Cp}^*\text{WH}_4(\text{dppe})]^+$.

Description of the proton transfer pathway for the $[\text{Cp}^*\text{W}(\text{dhpe})\text{H}_3]+2(\text{HFIP})$ adduct **C2''**. **Figure 4S**

Figure 5S. Optimized structures of hydrogen bonded complexes and ion pairs resulting from proton transfer between $\text{Cp}^*\text{WH}_3(\text{dppe})$ and HFIP or $(\text{HFIP})_2$

Description of the dihydrogen elimination from $[\text{CpW}(\text{dhpe})\text{H}_4]^+$.

Potential energies (hartree) and Cartesian coordinates (Ångstrom) of all located minima.

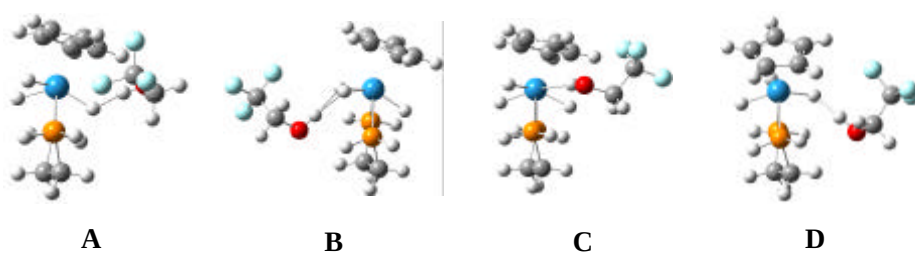


Figure 4.

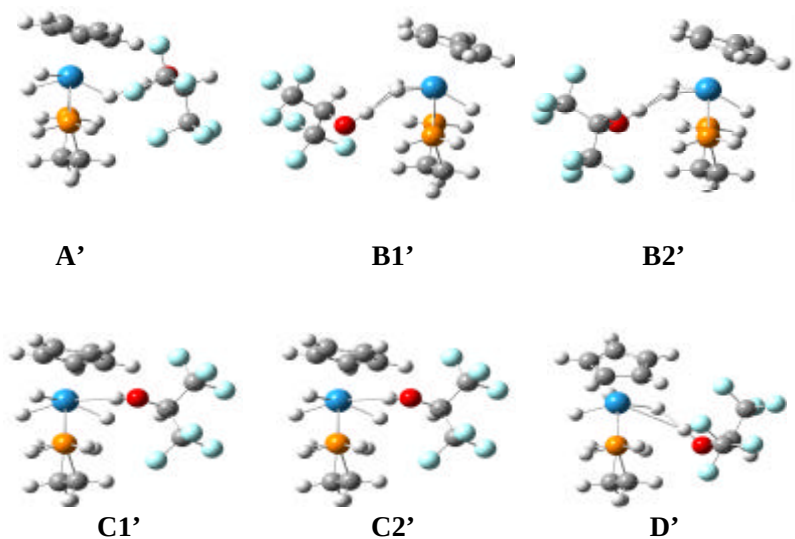


Figure 5.

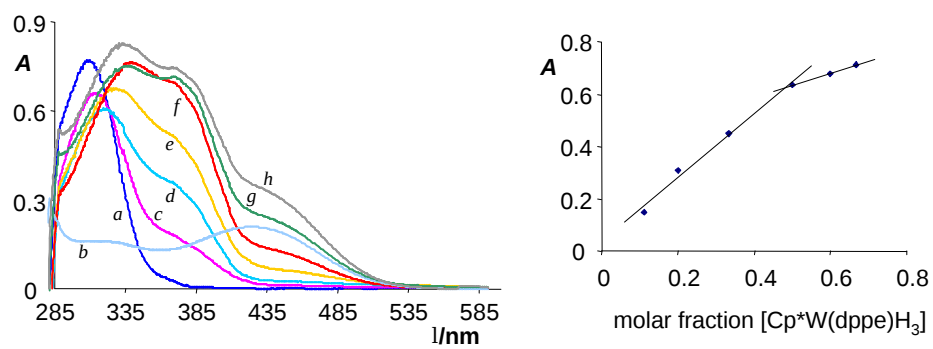


Figure 10.

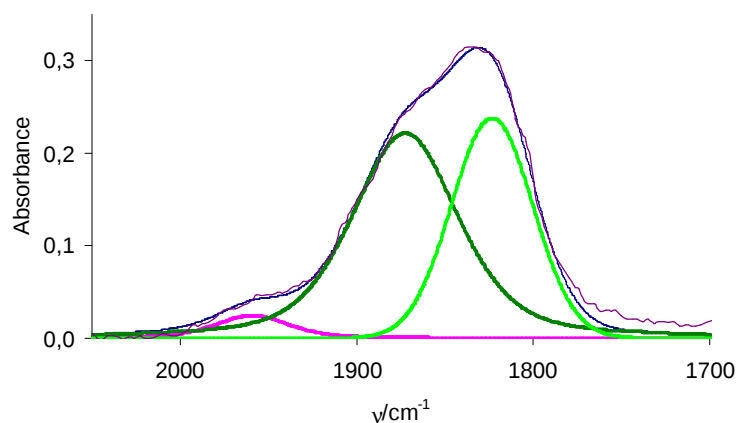


Figure 1S. IR spectrum in the ν_{MH} region of $\text{Cp}^*\text{WH}_3(\text{dppe})$ (0.025 g, 200K, CH_2Cl_2 , 0.12 cm) and band decomposition.

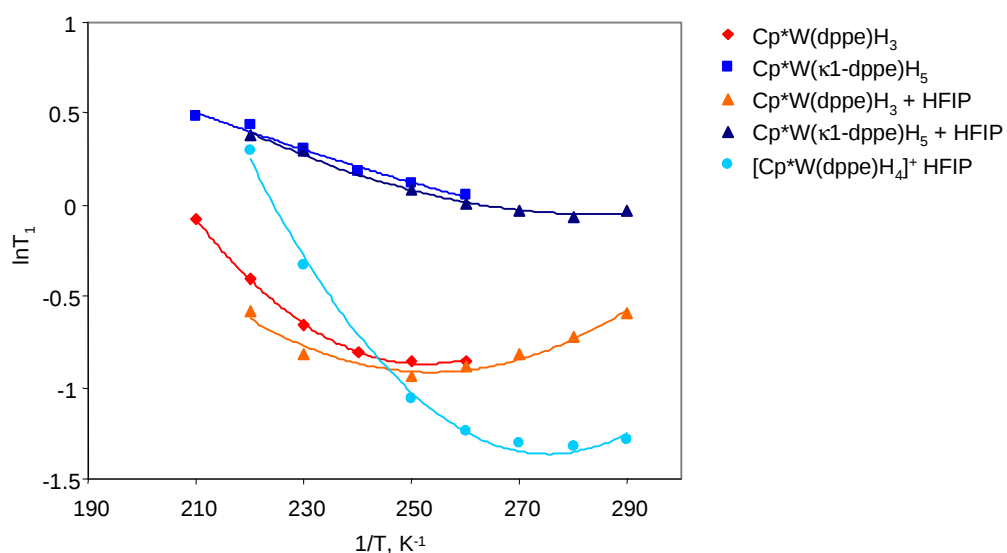


Figure 2S. T_1 values for all investigated compounds (500 MHz). Solvent = toluene- d_8 . Note: the trihydride sample used for this study contained also minor amount of pentahydride $\text{Cp}^*\text{WH}_5(\text{dppe})$, whose presence did not interfere with the interaction with HFIP as evident from the constant intensities of the corresponding ^1H ($\delta_{\text{WH}} -2.44$ ppm, 210K) and ^{31}P (δ 27 ppm) signals.

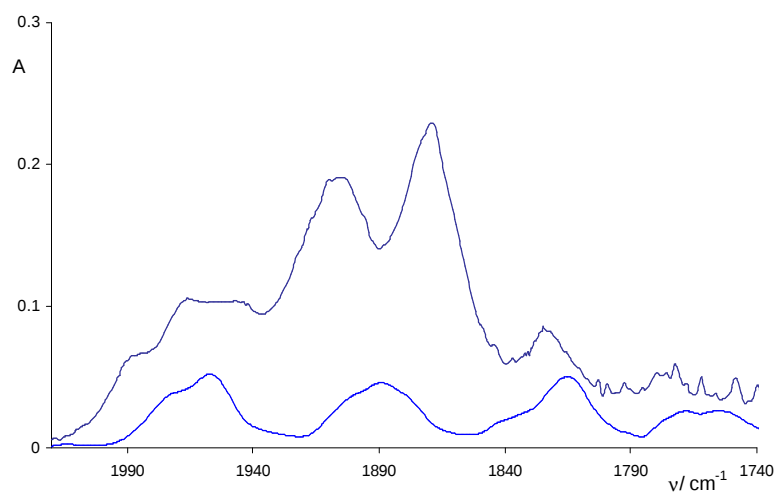


Figure 3S. IR spectra in the $\nu_{\text{W-H}}$ stretching region of $[\text{Cp}^*\text{WH}_4(\text{dppe})]^+\text{BF}_4^-$ (0.022M) and of dppe (0.011M) at 200K in CH_2Cl_2 , 0.22 cm.

Table 1S. Frequency parameters of the [CpW(dhpe)H₃](HA) adducts (HA = TFE, HFIP).

	ν_{W-H1} (cm ⁻¹) ^a	ν_{W-H2} (cm ⁻¹) ^a	ν_{W-H3} (cm ⁻¹) ^a	ν_{OH} (cm ⁻¹) ^a
TFE				3844 (0.38)
HFIP				3818 (0.66)
(HFIP)₂				3771 (2.50) ^b 3718 (4.02) ^c
[CpW(dhpe)H₃]·TFE adducts				
A	1966 (0.21)	1838 (0.38)	1809 (1.33)	3609 (5.26)
B	1930 (0.66)	1895 (0.44)	1809 (0.67)	3533 (7.70)
C	1953 (0.21)	1831 (0.41) ^d	1804 (1.01) ^e	3500 (8.12)
D	1811 (1.01)	1846 (0.96)	1901 (0.95)	3421 (8.37)
[CpW(dhpe)H₃]·HFIP adducts				
A'	1958 (0.21)	1839 (0.37)	1811 (1.75)	3472 (8.4)
B1'	1934 (0.64)	1886 (0.61)	1816 (0.78)	3433 (11.8)
B2'	1901 (0.45) ^f	1940 (0.99) ^g	1810 (0.71)	3432 (11.6)
C1'	1954 (0.20)	1820 (1.07) ^h	1849 (0.47) ⁱ	3331 (12.3)
C2'	1882 (0.75)	1848 (0.48)	1826 (1.37)	3184 (14.8)
D'	1813 (1.25)	1853 (0.96)	1901 (1.24)	3224 (12.6)
[CpW(dhpe)H₃]·2HFIP adducts				
A1''	1954 (0.21)	1826 (0.37)	1795 (2.94)	3581 (7.01) ^b 3238 (14.74) ^j
A2''	1898 (1.91)	1850 (1.17)	1822 (1.54)	3515 (7.50) ^b 2978 (20.23) ^j
B1''	1930 (0.64)	1879 (0.62)	1820 (0.82)	3619 (6.73) ^b 3157 (19.64) ^j
B2''	1956 (0.53)	1873 (0.76)	1818 (0.92)	3622 (6.85) ^b 3164 (19.39) ^j
C1''	1953 (0.24)	1830 (0.44)	1800 (1.05)	3661 (5.30) ^b 2994 (19.16) ^j
C2''	1919 (0.32)	1882 (0.35)	1818 (0.81)	3611 (8.07) ^b 2925 (28.13) ^j
D1''	1888 (0.78)	1840 (2.40)	1830.9 (0.55)	3567 (7.37) ^b 2917 (22.97) ^j

^aCalculated intensity in parentheses (A, 10⁴ L mol⁻¹cm⁻²). ^bFor the OH...O bonded HFIP molecule.

^cThis OH group interacts with one of the F atoms of the second HFIP molecule (r(H...F) = 2.048 Å). ^dSymmetric H2/H3 mode. ^eAsymmetric H3/H2 mode. ^fAsymmetric H1/H2 mode. ^gSymmetric H2/H1 mode. ^hAsymmetric H2/H3 mode. ⁱSymmetric H3/H2 mode. ^jFor the OH interacting with the WH₃ fragment.

Description of computational results for the $[\text{CpW}(\text{dhpe})\text{H}_3]\cdot 2\text{HFIP}$ adducts.

Seven species have been located, their main structural and energetic parameters being collected in Table 2S. The species located follow the same pattern as the simple adducts with HFIP and TFE, the species displaying a bifurcated interaction with two W-H bonds (**B1''** and **B2''**) being slightly more stabilized than those displaying a direct interaction with the metal centre (**C1''** and **C2''**), while the monodentated hydrogen bonded species that use the W-H3 binding site (**A1''** and **A2''**) are the least stabilized. Species **C2''** and **D''**, having energies intermediate between **A''** and **B''/C''**, feature significant difference from the original $[\text{CpW}(\text{dhpe})\text{H}_3]$ geometry with dhpe ligand tilted toward the Cp ring. The proton interacts with both W and H3 in **D''**, whereas the interaction in **C2''** can be regarded as a “pure” H-bond to the tungsten atom.

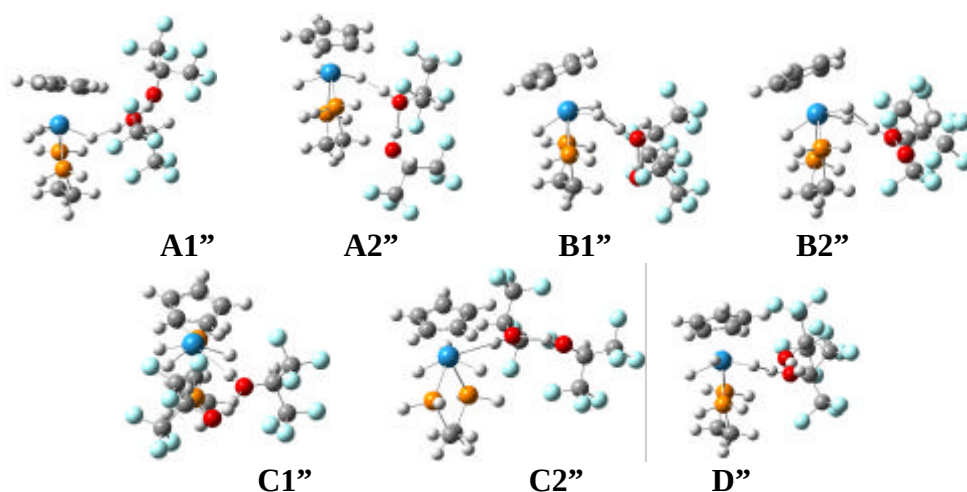
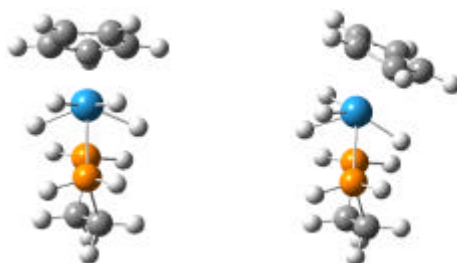


Table 2S. Main energetic and structural parameters of the [CpW(dhpe)H₃] $\cdot$ 2HFIP adducts. Energies are given relative to the separated [CpWH₃(dpe)] and (HFIP)₂ species.

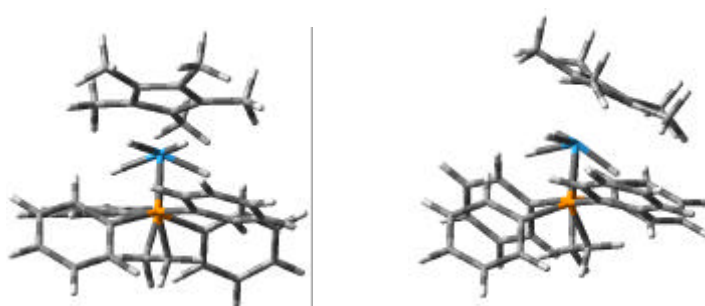
	A1''	A2''	B1''	B2''	C1''	C2''	D''
? E _{gas phase} (kcal.mol ⁻¹)	-12.9	-13.4	-16.6	-15.9	-15.7	-14.6	-14.7
? E _{BSE} (kcal.mol ⁻¹)	-6.5	-6.0	-10.4	-10.5	-7.0	-8.3	-8.0
? E _{DCM} (kcal.mol ⁻¹)	-3.6	-1.2	-3.6	-2.0	-4.4	-4.9	-2.7
Dist. O-H $\cdots$ HW (Å)	1.559	1.474	1.721 (H1) 1.816 (H2)	1.846 (H1) 1.651 (H2)	1.920	2.221	1.540
Dist. O-H $\cdots$ W(Å)	2.944	2.883	2.663	2.683	2.531	2.502	2.574
$\angle$ O-H $\cdots$ H(W)	155.6	150.7	146.7 (H1) 141.4 (H2)	141.3 (H1) 147.0 (H2)	138.3	142.3	149.8
$\angle$ O-H $\cdots$ W	152.5	163.7	170.3	171.0	178.2	175.3	168.5
r _{W-H1} (Å) ^a	1.694	1.735	1.706	1.722	1.697	1.740	1.726
r _{W-H2} (Å) ^a	1.735	1.724	1.722	1.704	1.737	1.707	1.727
r _{W-H3} (Å) ^a	1.747	1.732	1.734	1.735	1.742	1.722	1.742
Δq_W^b	0.013	0.040	-0.173	-0.143	-0.299	-0.405	-0.085
Δq_{H1}^b	0.005	0.010	-0.012	-0.063	0.011	0.081	-0.003
Δq_{H2}^b	0.007	-0.034	-0.081	-0.044	0.017	-0.009	-0.006
Δq_{H3}^b	-0.125	-0.094	0.023	0.017	-0.004	0.092	-0.097

Description of computational results for the protonation product, $[\text{Cp}^*\text{WH}_4(\text{dppe})]^+$.

The product of the proton transfer to $[\text{Cp}^*\text{W}(\text{dppe})\text{H}_3]$ is a cationic tungsten tetrahydride complex, $[\text{Cp}^*\text{W}(\text{dppe})\text{H}_4]^+$. Two different isomers of this complex have been located. For the model system $[\text{CpWH}_4(\text{dpe})]^+$, the difference between the most stable isomer (left) and the less stable (right) is $10.9 \text{ kcal.mol}^{-1}$.



The most stable isomer is more symmetric and has the four hydrogen atoms located almost in a plane, two of them at each side of the P-W-P plane, as described in the main text. The other isomer is asymmetric and contains three of the four hydrides on one side of the P-W-P plane. The metal hydride distances for this isomer are 1.682, 1.724 and 1.684 Å for the three hydrides on the same side of the P-W-P plane, the longest distance corresponding to the central hydride ligand. The W-H distance for the hydride on the other side of the P-W-P plane is 1.706 Å.



The results on the model system are close to those obtained when considering the real ligands of the system. We can observe the geometry of the most stable isomer on the left, and the other one on the right. The energy difference is slightly decreased from the model system to the real one, from 10.9 to $9.0 \text{ kcal mol}^{-1}$. The metal hydride distances for the most stable isomer are shown in the main text. For the less stable isomer, the three hydrides on the same side of the P-W-P plane have distances of 1.675, 1.716 and 1.681 Å, the longest one corresponding to the central hydride, whereas the W-H distance to the hydride on the other side of the plane is 1.707 Å.

Description of the proton transfer pathway for the $[\text{Cp}^*\text{W}(\text{dhpe})\text{H}_3]+2(\text{HFIP})$ adduct **C2''**.

Species **C2''** is homologous of species **C2'**, used in the system with only one HFIP molecule. The variation of the relative energy in gas phase and dichloromethane along the coordinate O-H is presented in Figure 5S.

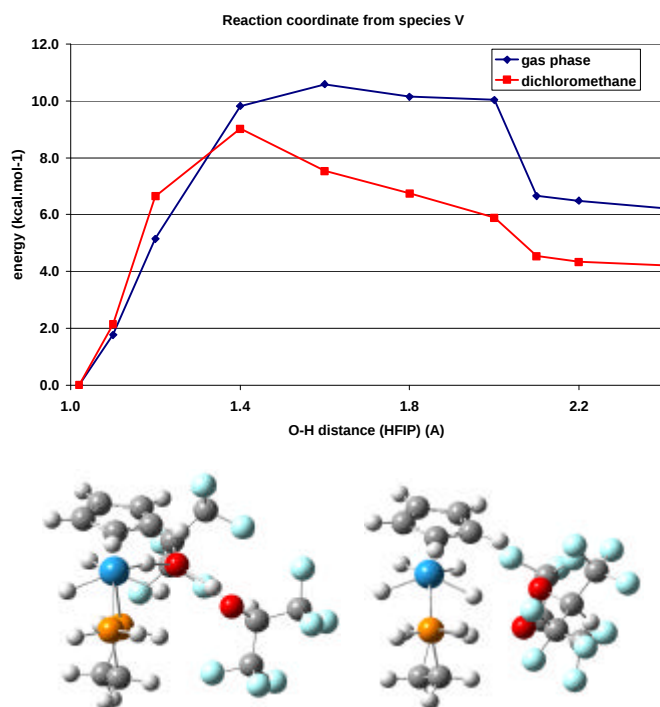
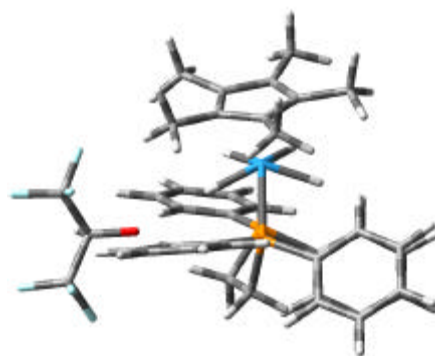


Figure 4S. Proton transfer reaction coordinate for species **C2''** in the gas phase and in dichloromethane. The geometries of the maximum of the coordinate (left) and the product of the proton transfer (right) are also shown.

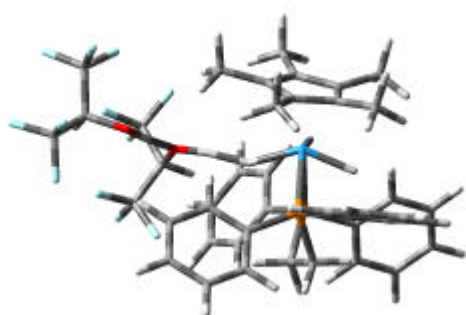
The coordinate has a maximum at 10.6 kcal mol⁻¹ in gas phase for an O-H distance of 1.6 Å. When the effect of the solvent is taken into account, this maximum slightly decreases to 9.0 kcal.mol⁻¹ and moves to 1.4 Å. The W-H distance is 1.791 Å and the distances between the transferring proton and the closest hydrides are 1.858 Å and 1.928 Å. The product of the protonation is the most stable tetrahydride. The M-H distances in this case are 1.727, 1.695, 1.687 and 1.704 Å, the shorter (M)H-O distance is 2.290 Å and the shortest (P)H-O distance is 1.863 Å. The product of this pathway differs from that of the other pathway described in the main text only for the conformation and position of the conjugate anion. The difference in energy between both minima is 3.6 kcal mol⁻¹ in gas phase.



$[\text{Cp}^*\text{WH}_3(\text{dppe})]\cdot\text{HOCH}(\text{CF}_3)_2$



$[\text{Cp}^*\text{WH}_4(\text{dppe})]^+[\text{OCH}(\text{CF}_3)_2]^-$



$[\text{Cp}^*\text{WH}_3(\text{dppe})]\cdot[(\text{CF}_3)_2\text{CHOH}]_2$



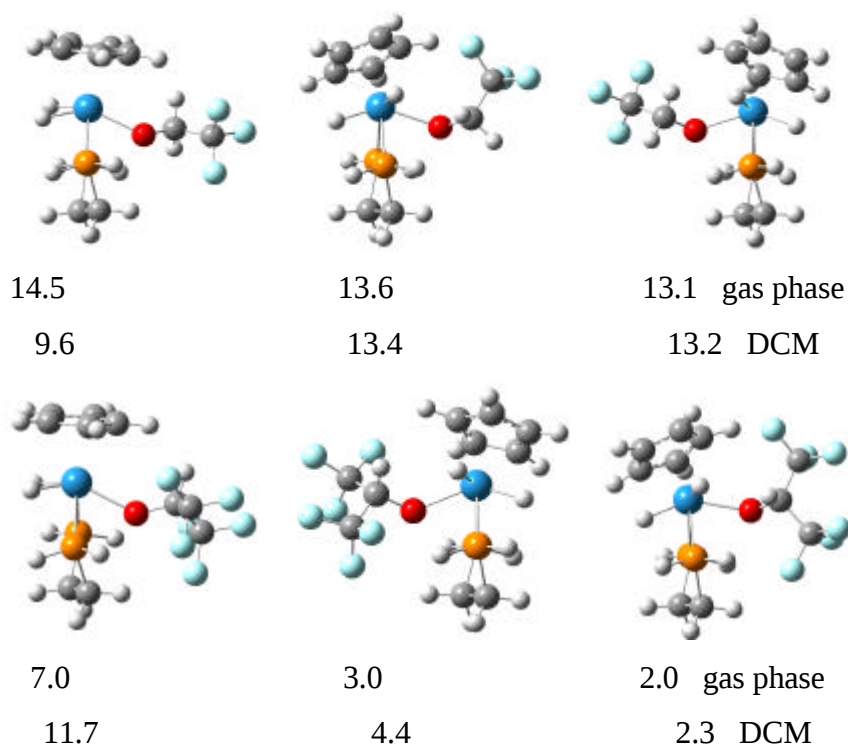
$[\text{Cp}^*\text{WH}_4(\text{dppe})]^+[(\text{CF}_3)_2\text{CHOH OCH}(\text{CF}_3)_2]^-$

Figure 5S. Optimized structures of hydrogen bonded complexes and ion pairs resulting from proton transfer between Cp*WH₃(dppe) and HFIP or (HFIP)₂

Description of the dihydrogen elimination from $[\text{CpW}(\text{dhpe})\text{H}_4]^+$.

The elimination of H_2 from the $[\text{CpW}(\text{dhpe})\text{H}_4]^+(\text{OR}_\text{F})^-$ salt ($\text{R}_\text{F}\text{O}^-$ = conjugate base of TFE or HFIP) would lead to the formation of $\text{CpW}(\text{dhpe})\text{H}_2(\text{OR}_\text{F})$. Three different isomers of this system have been located when considering TFE as proton donor and three more when considering HFIP. When considering $(\text{TFE})_2$ as the proton donor, therefore the elimination occurs from the $[\text{CpW}(\text{dhpe})\text{H}_4]^+(\text{CF}_3\text{CH}_2\text{OHOCH}_2\text{CF}_3)^-$ salt, the three optimized isomers were found at 14.5, 13.6 and 13.1 kcal mol^{-1} above the reactants in the gas phase, or at 9.6, 13.4 and 13.2 kcal mol^{-1} in dichloromethane. These energies are much higher than those of the corresponding Mo system, which leads a $\text{CpMo}(\text{dhpe})\text{H}_2(\text{OCH}_2\text{CF}_3)$ only +7.3 kcal mol^{-1} higher than the reagents in the gas phase or +0.2 kcal mol^{-1} higher in CH_2CH_2 solution. When considering $(\text{HFIP})_2$, the isomers were located at 7.0, 3.0 and 2.0 kcal mol^{-1} in the gas phase and at 11.7, 4.4 and 2.3 kcal mol^{-1} in dichloromethane. The smaller value obtained in this case is related to the difference in proton transfer thermodynamics and not to the thermodynamics of the H_2 evolution step.

The $[\text{CpW}(\text{dpe})\text{H}_2(\text{OR}_\text{F})]$ complexes could further evolve, leading to the elimination of a second H_2 molecule and form either $[\text{CpW}(\text{dpe})(\text{OR}_\text{F})]$ or $[\text{CpW}(\text{dpe})(\text{OR}_\text{F})(\text{HOR}_\text{F})]$ by the addition of an additional molecule of proton donor. The formation of these species was previously studied for the molybdenum complex but it has not been studied for the tungsten complex, since this process is not experimentally observed.



Potential energies (hartree) and Cartesian coordinates (Ångstrom) of all located minima.

H₂				8	-1.004906	-1.289864	0.730802
-1.17853933613 h				1	0.043108	-1.292143	0.026413
1	.000000	.000000	.371398	8	0.936296	-1.200326	-0.696038
1	.000000	.000000	-.371398	6	1.366920	0.110005	-0.604285
CF₃CH₂OH				1	0.698467	0.745748	0.001303
-452.661169511 h				6	2.739828	0.216161	0.030845
1	-2.789851	0.269459	0.000681	9	2.798555	-0.263937	1.335623
8	-1.950736	-0.207082	-0.000114	9	3.174143	1.559617	0.093041
6	-0.903028	0.755602	-0.000152	9	3.733540	-0.462243	-0.679968
1	-0.912523	1.396598	0.890762	1	-1.771004	-1.224036	-1.210147
6	0.407989	0.007821	-0.000003	1	1.473375	0.607484	-1.589849
9	1.458273	0.925872	-0.000200	(CF₃)₂CHOH			
9	0.559262	-0.795767	-1.117862	-789.612307522 h			
9	0.559237	-0.795261	1.118235	6	0.003828	0.541690	-0.502343
1	-0.912461	1.396464	-0.891164	1	0.000133	0.482735	-1.598500
CF₃CH₂O⁻				6	1.290136	-0.128720	-0.033850
-452.056207649 h				6	-1.267507	-0.161071	-0.026333
8	-2.072238	-0.189759	-0.000018	9	1.297865	-1.467758	-0.400059
6	-1.080760	0.673877	-0.000517	9	2.378023	0.476918	-0.636156
1	-0.984065	1.392537	0.890073	9	1.461370	-0.056692	1.331392
6	0.329306	0.024159	-0.000114	9	-1.313914	-0.354287	1.336317
9	1.393551	0.974819	-0.001971	9	-1.445007	-1.384365	-0.645692
9	0.583756	-0.792406	-1.113108	9	-2.353005	0.646341	-0.377432
9	0.584344	-0.788466	1.115703	8	0.042299	1.865909	-0.016454
1	-0.984170	1.391802	-0.891755	1	-0.725253	2.337182	-0.370040
(CF₃CH₂OH)₂				(CF₃)₂CHO⁻			
-905.345796184 h				-789.040531096 h			
6	1.566448	-0.135149	-1.032107	6	-0.000001	0.702696	-0.497179
1	2.095360	-0.282869	-1.979515	1	-0.000008	0.506032	-1.620204
6	2.564600	-0.261145	0.093611	6	1.271189	-0.090640	-0.040679
8	0.904720	1.133398	-0.984068	6	-1.271166	-0.090663	-0.040671
1	-0.372864	1.339347	0.372294	9	-1.426824	-0.166250	1.343286
8	-1.178264	1.493257	0.899208	9	-1.356963	-1.425705	-0.504177
6	-2.287887	1.200906	0.076865	9	-2.423484	0.529539	-0.526857
1	-2.186616	1.587759	-0.945290	9	2.423577	0.530395	-0.525569
6	-2.542513	-0.287885	-0.030310	9	1.426054	-0.167551	1.343320
1	1.576431	1.829056	-1.043415	9	1.357677	-1.425188	-0.505448
9	-3.644802	-0.539558	-0.843552	8	-0.000057	1.936057	-0.066202
9	-2.778200	-0.889965	1.191081	((CF₃)₂CHOH)₂			
9	-1.455248	-0.959743	-0.609546	-1579.23893084 h			
9	3.496216	0.781430	0.026525	6	2.450256	-0.170200	0.669980
9	3.260943	-1.455915	0.007795	1	2.985762	-0.513640	1.562279
9	1.971302	-0.196608	1.341189	6	2.808505	1.297230	0.462288
1	0.795204	-0.895867	-0.924320	6	2.862882	-1.084390	-0.482390
1	-3.174966	1.652198	0.529351	8	1.043567	-0.209050	0.836968
(CF₃CH₂OHOCH₂CF₃)⁻				1	-0.209267	0.291604	-0.572453
-904.788836050 h				8	-1.099576	0.224527	-0.957892
6	-2.052223	-1.142665	-0.138060	6	-2.028317	0.242365	0.097077
1	-2.882848	-1.868255	0.018342	1	-1.656548	0.751338	0.993767
6	-2.721719	0.219451	-0.020754	6	-2.358326	-1.192137	0.515958
9	-3.803988	0.349632	-0.922513	6	-3.246829	1.030215	-0.377512
9	-3.257284	0.476560	1.242098	1	0.750220	-1.121795	0.994380
9	-1.868195	1.288705	-0.305020	9	-3.199120	-1.240218	1.613001
				9	-2.913587	-1.943688	-0.491157
				9	-1.167209	-1.836797	0.902049

9	-4.232573	1.055477	0.601367
9	-3.802641	0.506943	-1.525886
9	-2.880144	2.338384	-0.632695
9	2.342920	-2.351905	-0.220469
9	4.233061	-1.201972	-0.584757
9	2.362752	-0.667707	-1.698341
9	2.551716	2.007185	1.620272
9	4.150833	1.438455	0.161893
9	2.070534	1.865863	-0.558943

$((CF_3)_2CHOHOCH(CF_3)_2)^-$

-1578.72613722 h

6	1.805859	-0.200410	0.077848
1	1.315884	0.232857	0.968282
6	3.104722	-0.831287	0.589353
6	2.083091	0.990506	-0.848517
9	3.930588	0.081032	1.264398
9	2.824236	-1.840974	1.498954
9	3.883221	-1.392137	-0.413717
9	2.802298	0.652890	-1.987692
9	2.791864	2.026292	-0.226639
9	0.884819	1.551655	-1.280254
8	1.050513	-1.136366	-0.575500
1	0.000007	-1.205710	0.000191
8	-1.050491	-1.136236	0.575845
6	-1.805828	-0.200423	-0.077731
1	-1.315767	0.232752	-0.968161
6	-3.104584	-0.831448	-0.589310
6	-2.083232	0.990600	0.848437
9	-2.823923	-1.841450	-1.498501
9	-3.930269	0.080667	-1.264851
9	-3.883324	-1.391937	0.413783
9	-0.885029	1.552030	1.280007
9	-2.792213	2.026158	0.226411
9	-2.802320	0.653072	1.987706

$[CpW(dhpe)H_3]$

-357.175886080 h

6	-2.066868	1.207171	0.454283
6	-2.354855	0.712153	-0.847838
6	-2.417532	-0.713120	-0.776299
6	-2.154525	-1.116892	0.566170
6	-1.933354	0.082183	1.322122
74	-0.183808	-0.087165	-0.244242
15	1.575810	1.546228	0.002090
6	3.300993	0.769291	-0.160855
6	3.284278	-0.677051	0.370355
15	1.711151	-1.565991	-0.212411
1	0.575271	-0.302905	1.302337
1	-0.154333	-1.086760	-1.614655
1	0.309588	0.677166	-1.710583
1	1.825049	-2.737556	0.606423
1	2.186353	-2.169531	-1.414601
1	1.729614	2.667846	-0.861995
1	1.745628	2.260140	1.233018
1	4.172738	-1.231308	0.048365
1	3.261518	-0.683232	1.467440
1	4.052995	1.380432	0.350438
1	3.531800	0.775449	-1.233967
1	-2.506117	1.309878	-1.735913

1	-2.636993	-1.373453	-1.603564
1	-2.190077	-2.125153	0.952783
1	-1.727924	0.127358	2.382799
1	-1.985421	2.248341	0.735044

$[CpW(dhpe)H_4]^+$

-357.591437813 h

6	-1.954305	1.493384	0.109858
6	-2.193401	0.766543	-1.095742
6	-2.570872	-0.561327	-0.736293
6	-2.559758	-0.654106	0.692482
6	-2.174244	0.616734	1.214767
74	-0.348276	-0.258563	-0.016783
15	1.281685	1.666747	0.037324
6	3.037926	1.098961	-0.266003
6	3.278499	-0.289830	0.360352
15	1.864702	-1.434287	-0.067842
1	-0.430406	-1.709370	0.845180
1	-0.421294	-1.594723	-1.052540
1	0.280328	0.028349	-1.593833
1	2.049020	-2.531873	0.803265
1	2.254521	-2.011778	-1.300030
1	1.114364	2.708266	-0.909256
1	1.364278	2.436517	1.225991
1	4.227967	-0.714011	0.018937
1	3.316151	-0.224281	1.454039
1	3.739475	1.839289	0.130126
1	3.170323	1.063111	-1.353704
1	-2.126979	1.157891	-2.101300
1	-2.850357	-1.349901	-1.420335
1	-2.832478	-1.523597	1.273298
1	-2.090404	0.875080	2.261147
1	-1.697455	2.542823	0.176297
1	0.326513	-0.167205	1.565879

$[CpW(dhpe)H_4]^+$

-357.574072518 h

6	2.185665	-1.100852	0.837928
6	2.601590	-0.743538	-0.490265
6	2.600276	0.670973	-0.582663
6	2.181579	1.197342	0.686368
6	1.988728	0.100774	1.573362
74	0.348294	-0.020223	-0.227173
15	-1.598106	-1.586067	0.076156
6	-3.234784	-0.669491	0.044418
6	-3.098801	0.760553	0.608310
15	-1.568097	1.592149	-0.075707
1	-0.360277	0.083228	1.320764
1	0.432755	1.253441	-1.325347
1	0.450267	-1.432333	-1.134552
1	-1.422467	2.730914	0.756377
1	-2.012323	2.212336	-1.268709
1	-1.805206	-2.617408	-0.869800
1	-1.649474	-2.344878	1.274226
1	-3.986148	1.356164	0.372176
1	-2.989999	0.743104	1.699049
1	-3.993034	-1.236782	0.592880
1	-3.542601	-0.638484	-1.007639
1	2.891763	-1.434398	-1.269707
1	2.886268	1.254629	-1.446721

1	2.113464	2.246223	0.941980
1	1.711464	0.168723	2.616632
1	2.120118	-2.107621	1.228163
1	-0.470777	-0.126194	-1.740488

[Cp*W(dppe)H₃]

-1477.72989395 h

74	-0.089169	-0.568011	0.714430
15	-1.610356	0.699074	-0.677143
15	1.544781	0.614239	-0.663982
6	0.347847	-1.667847	2.786040
6	-0.993971	-2.033960	2.411988
6	-0.939604	-2.746821	1.181316
6	0.456448	-2.843452	0.802826
6	1.253125	-2.203693	1.813459
6	0.738104	-0.993308	4.075292
6	-2.229726	-1.806760	3.241155
6	-2.093511	-3.428979	0.496259
6	0.994067	-3.683014	-0.328135
6	2.750754	-2.277283	1.947879
6	-3.183096	-0.124215	-1.251591
6	-4.317132	-0.090272	-0.413090
6	-5.479566	-0.791713	-0.746512
6	-5.534876	-1.545481	-1.926112
6	-4.415992	-1.594295	-2.763751
6	-3.250876	-0.892907	-2.428616
6	-2.264840	2.371907	-0.155834
6	-3.223458	3.048788	-0.938429
6	-3.659077	4.329644	-0.586674
6	-3.143810	4.957638	0.554993
6	-2.193076	4.296682	1.339138
6	-1.755087	3.013074	0.986309
6	-0.751749	1.184021	-2.293638
6	0.671033	1.687135	-1.981205
6	2.775547	1.850511	-0.000404
6	3.554733	2.618407	-0.891140
6	4.479556	3.551114	-0.412702
6	4.649497	3.727470	0.966640
6	3.889341	2.966147	1.860023
6	2.958293	2.035491	1.379852
6	2.680332	-0.442942	-1.708698
6	3.989238	-0.739706	-1.279259
6	4.811030	-1.598821	-2.018525
6	4.342721	-2.175449	-3.204597
6	3.044665	-1.889892	-3.643743
6	2.221245	-1.036663	-2.900600
1	-0.205632	-1.087235	-0.938025
1	-1.249541	0.268482	1.629242
1	0.538325	0.807636	1.531317
1	-0.003488	-0.249396	4.381100
1	1.699103	-0.479270	3.980891
1	0.831413	-1.725944	4.890224
1	-2.149728	-0.899622	3.846663
1	-2.394311	-2.652103	3.924887
1	-3.119815	-1.709362	2.613003
1	-2.240012	-4.448729	0.883239
1	-1.930213	-3.504946	-0.582507
1	-3.027873	-2.878713	0.640870
1	0.279926	-3.744936	-1.154084
1	1.197087	-4.707972	0.015385

1	1.925648	-3.277791	-0.732425
1	3.239876	-2.364717	0.974016
1	3.044555	-3.154344	2.544283
1	3.157190	-1.391117	2.445429
1	-4.288356	0.491723	0.502780
1	-6.342140	-0.746631	-0.088341
1	-6.437841	-2.088710	-2.186554
1	-4.446473	-2.176983	-3.679693
1	-2.394144	-0.959298	-3.089778
1	-3.640239	2.566714	-1.817295
1	-4.399876	4.834849	-1.199213
1	-3.482569	5.952218	0.828865
1	-1.789538	4.776551	2.225625
1	-1.015756	2.498943	1.590061
1	-0.711713	0.298139	-2.935593
1	-1.332319	1.954118	-2.814022
1	0.618230	2.690922	-1.542033
1	1.276747	1.753103	-2.892595
1	3.447467	2.480694	-1.962260
1	5.067603	4.135751	-1.113626
1	5.368303	4.450911	1.338977
1	4.015428	3.096305	2.930593
1	2.355092	1.456836	2.070517
1	4.371199	-0.290202	-0.369231
1	5.817012	-1.811556	-1.669556
1	4.981073	-2.838766	-3.779724
1	2.671330	-2.331898	-4.562672
1	1.212321	-0.843850	-3.249156

[Cp*W(dppe)H₄]⁺

-1478.17675672 h

74	-0.119800	-0.220793	0.991937
15	-1.822571	0.231302	-0.851493
15	1.426498	0.194797	-1.055631
6	-0.230110	-1.269773	3.114308
6	0.874133	-1.871385	2.419244
6	1.872549	-0.863354	2.215960
6	1.380891	0.373258	2.760983
6	0.085688	0.119860	3.327337
6	-1.391012	-2.009264	3.722750
6	1.038256	-3.346864	2.170380
6	3.280749	-1.123040	1.753863
6	2.173750	1.642861	2.920833
6	-0.698585	1.077174	4.184051
6	-3.207318	-0.980470	-0.967679
6	-4.452844	-0.690699	-0.378915
6	-5.484911	-1.634839	-0.406744
6	-5.287793	-2.875747	-1.021893
6	-4.048992	-3.175629	-1.601321
6	-3.011847	-2.238379	-1.569673
6	-2.656795	1.881265	-0.936657
6	-2.366342	2.921708	-0.037615
6	-2.991048	4.168915	-0.170209
6	-3.910167	4.391055	-1.199692
6	-4.209297	3.359957	-2.100374
6	-3.590151	2.114786	-1.971069
6	-0.964084	0.153163	-2.512213
6	0.359570	0.925926	-2.413775
6	2.224873	-1.220304	-1.947578
6	1.988042	-2.551934	-1.562053

6	2.543416	-3.614417	-2.286982	6	-1.355257	-2.354065	1.774614
6	3.338488	-3.360313	-3.408439	6	-0.729247	-2.927772	0.634573
6	3.575957	-2.038342	-3.807939	6	0.703573	-2.880745	0.835321
6	3.025117	-0.976375	-3.086101	6	0.947491	-2.334296	2.134417
6	2.763960	1.462661	-0.860116	6	-0.535454	-1.421653	4.089962
6	2.404400	2.809392	-0.645568	6	-2.831955	-2.340790	2.058260
6	3.386403	3.791197	-0.483126	6	-1.426217	-3.633680	-0.494591
6	4.742843	3.444418	-0.516602	6	1.725181	-3.539258	-0.051678
6	5.111389	2.109942	-0.715056	6	2.271300	-2.318679	2.848435
6	4.131391	1.124509	-0.887898	6	-3.111446	-0.074410	-1.254017
1	-1.377191	0.737779	1.572737	6	-4.304728	0.091737	-0.521617
1	-0.249077	-1.626480	0.016500	6	-5.463566	-0.602571	-0.885036
1	0.102609	1.450170	0.658463	6	-5.450446	-1.469616	-1.984149
1	-1.549788	-1.071364	1.221394	6	-4.270202	-1.644737	-2.715683
1	-1.124283	-2.356254	4.730186	6	-3.106244	-0.958105	-2.350870
1	-1.669504	-2.884070	3.130330	6	-2.206597	2.458152	-0.161252
1	-2.275020	-1.373448	3.812602	6	-3.050481	3.188040	-1.027874
1	0.094195	-3.818358	1.885647	6	-3.513721	4.454682	-0.665660
1	1.395174	-3.842547	3.083317	6	-3.147092	5.011368	0.567178
1	1.769182	-3.550214	1.384224	6	-2.317526	4.294635	1.434283
1	3.328154	-1.851260	0.939884	6	-1.847834	3.024852	1.073883
1	3.863575	-1.530688	2.590969	6	-0.666438	1.213249	-2.292413
1	3.779364	-0.209950	1.424900	6	0.742786	1.732767	-1.959688
1	2.854520	1.812558	2.084233	6	2.775690	1.946096	0.082753
1	2.775691	1.594792	3.838276	6	3.700905	2.601552	-0.759373
1	1.521910	2.516400	2.998347	6	4.541823	3.594820	-0.252146
1	-0.347240	1.022167	5.223082	6	4.476175	3.946688	1.102448
1	-1.765694	0.843081	4.179598	6	3.565823	3.301409	1.944669
1	-0.582085	2.110759	3.848768	6	2.717373	2.307451	1.439900
1	-4.619420	0.269495	0.096140	6	2.790480	-0.392567	-1.620979
1	-6.440817	-1.397515	0.048064	6	4.051539	-0.728741	-1.090182
1	-6.091017	-3.604288	-1.048532	6	4.903080	-1.597707	-1.781938
1	-3.889158	-4.137612	-2.076891	6	4.509260	-2.141669	-3.010140
1	-2.053884	-2.502406	-2.004318	6	3.257425	-1.815186	-3.544985
1	-1.656682	2.758356	0.763514	6	2.401461	-0.950666	-2.853914
1	-2.759235	4.961686	0.533282	1	-0.073543	-1.056867	-0.873473
1	-4.393744	5.356908	-1.300038	1	-1.383687	0.046965	1.553565
1	-4.925477	3.523948	-2.898516	1	1.399805	-0.192529	1.524727
1	-3.846039	1.321736	-2.666523	1	-1.438414	-0.809223	4.157178
1	-0.778669	-0.895528	-2.767320	1	0.303611	-0.810292	4.432784
1	-1.613107	0.577806	-3.284717	1	-0.646273	-2.257404	4.793687
1	0.172603	1.978337	-2.175030	1	-3.102714	-1.545535	2.757421
1	0.915345	0.889087	-3.355915	1	-3.133609	-3.295700	2.509209
1	1.353320	-2.757380	-0.708802	1	-3.422605	-2.202292	1.149164
1	2.350221	-4.635888	-1.976525	1	-1.600395	-4.684198	-0.224566
1	3.767671	-4.182917	-3.970337	1	-0.827824	-3.624631	-1.409266
1	4.188281	-1.834682	-4.679959	1	-2.396194	-3.186121	-0.722403
1	3.225801	0.040677	-3.406728	1	1.458664	-3.460071	-1.108604
1	1.359758	3.096694	-0.591547	1	1.806944	-4.606996	0.192675
1	3.092079	4.823948	-0.329048	1	2.716527	-3.096167	0.067952
1	5.503398	4.207202	-0.389445	1	3.108695	-2.214019	2.153912
1	6.159736	1.832161	-0.742054	1	2.406877	-3.264468	3.389906
1	4.437456	0.098767	-1.055177	1	2.333220	-1.507995	3.578506
[Cp*W(dppe)H₄]⁺				1	-4.334059	0.773828	0.321038
-1478.16247067				1	-6.375519	-0.458801	-0.315322
74	-0.040215	-0.588987	0.767723	1	-6.351947	-2.000700	-2.270001
15	-1.581300	0.806560	-0.709701	1	-4.253909	-2.311723	-3.571247
15	1.640354	0.693219	-0.665486	1	-2.202646	-1.120696	-2.927573
6	-0.315225	-1.937121	2.691752	1	-3.360645	2.762822	-1.977241
				1	-4.161857	5.003711	-1.340456

1	-3.509023	5.994800	0.847581
1	-2.033275	4.718816	2.391391
1	-1.203057	2.478643	1.750624
1	-0.614073	0.301120	-2.894445
1	-1.226894	1.960035	-2.864417
1	0.677267	2.737171	-1.526147
1	1.360779	1.805666	-2.861215
1	3.775499	2.328586	-1.807123
1	5.247889	4.089610	-0.910566
1	5.131212	4.716637	1.495967
1	3.511740	3.568912	2.994672
1	2.010647	1.820969	2.100444
1	4.377380	-0.298406	-0.149228
1	5.875085	-1.840747	-1.365676
1	5.173336	-2.809677	-3.547978
1	2.949263	-2.227668	-4.500070
1	1.434291	-0.714080	-3.285469
1	0.093409	0.956320	1.500767

[Cp*W(dppe)H₃]HFIP

-2267.36156032 h

6	1.843598	-1.195275	2.667707
6	2.048496	0.135306	3.153093
6	0.760753	0.727862	3.414390
6	-0.247448	-0.202656	3.046290
6	0.423645	-1.394469	2.557039
74	0.973845	0.295322	1.030499
15	1.878196	-0.839044	-0.959500
6	1.367377	0.087926	-2.541727
6	0.050929	0.866123	-2.375628
15	0.015090	1.744871	-0.699237
1	-0.407512	-0.400106	0.207598
1	1.144703	1.940225	1.391913
1	2.494369	0.929899	0.531014
1	-0.059715	1.596522	-3.185686
1	-0.809270	0.191063	-2.410873
1	1.310254	-0.607975	-3.386641
1	2.189839	0.786369	-2.738564
1	-1.911372	-0.996441	0.251990
8	-2.704888	-1.576555	0.218237
6	-3.815027	-0.867346	-0.277920
1	-3.675602	0.217183	-0.280090
6	-4.061578	-1.284746	-1.727654
6	-5.001328	-1.158447	0.637094
9	-5.269127	-2.508073	0.753648
9	-4.745224	-0.667223	1.908452
9	-6.157207	-0.535037	0.183434
9	-5.112104	-0.587910	-2.304825
9	-2.925742	-1.003752	-2.491047
9	-4.318331	-2.634912	-1.867437
6	3.705667	-1.010770	-1.294293
6	4.153651	-1.602050	-2.494703
6	4.663421	-0.528175	-0.387141
6	5.519321	-1.704298	-2.775476
1	3.435195	-1.993907	-3.207406
6	6.032293	-0.633941	-0.666524
1	4.326512	-0.054805	0.527501
6	6.463345	-1.220996	-1.860182
1	5.845600	-2.161125	-3.704714
1	6.757560	-0.254566	0.046813

1	7.523816	-1.301612	-2.077782
6	1.285258	-2.581058	-1.262482
6	-0.042644	-2.808668	-1.672942
6	2.101436	-3.697958	-0.993504
6	-0.539588	-4.107816	-1.816041
1	-0.708576	-1.976801	-1.860498
6	1.603064	-4.999260	-1.135280
1	3.129725	-3.553990	-0.681821
6	0.282272	-5.208649	-1.547273
1	-1.571146	-4.250962	-2.121772
1	2.248775	-5.846161	-0.923668
1	-0.103856	-6.217498	-1.652946
6	-1.776008	2.274623	-0.593371
6	-2.267123	2.675094	0.664631
6	-2.662640	2.275422	-1.689405
6	-3.600210	3.067623	0.824751
1	-1.595278	2.654876	1.516909
6	-4.002841	2.657090	-1.527559
1	-2.322376	1.966592	-2.670867
6	-4.474211	3.055351	-0.271351
1	-3.959567	3.372781	1.802473
1	-4.674484	2.634197	-2.379793
1	-5.511954	3.346471	-0.145708
6	0.839314	3.368979	-1.137350
6	0.192397	4.316644	-1.957010
6	2.147286	3.645961	-0.699614
6	0.836738	5.500182	-2.330846
1	-0.823112	4.141998	-2.295345
6	2.791686	4.831452	-1.075442
1	2.652302	2.930099	-0.062563
6	2.140390	5.761121	-1.892028
1	0.318819	6.218604	-2.959055
1	3.801322	5.025649	-0.726371
1	2.639728	6.680741	-2.181190
6	-1.715891	-0.078902	3.352567
1	-2.332122	-0.657467	2.662954
1	-1.931697	-0.445093	4.367620
1	-2.053761	0.960359	3.301987
6	-0.240175	-2.720004	2.278405
1	-0.292448	-3.318663	3.199643
1	-1.259882	-2.600446	1.906254
1	0.311208	-3.305146	1.537274
6	2.898722	-2.260286	2.526242
1	3.086166	-2.745014	3.495916
1	2.589482	-3.040769	1.825994
1	3.850344	-1.854204	2.171843
6	3.374024	0.749428	3.520139
1	3.604778	0.573511	4.580785
1	4.191020	0.322393	2.931344
1	3.378476	1.830906	3.354715
6	0.534591	2.049892	4.097646
1	0.529952	1.920010	5.189391
1	1.316742	2.773254	3.851210
1	-0.425848	2.490555	3.814965

[Cp*W(dppe)H₄]⁺[(CF₃)₂CHO]⁻

-2267.34768306 h

6	1.172094	-1.817465	2.595181
6	2.039169	-0.796440	3.106720
6	1.222976	0.291574	3.563735

6	-0.153427	-0.054375	3.321849	6	2.186873	3.191689	-2.697606
6	-0.185326	-1.355846	2.716922	6	3.535719	2.373869	-0.860230
74	0.913162	0.151665	1.215891	6	3.329866	3.717895	-3.305455
15	1.010851	-1.351524	-0.884584	1	1.223343	3.331186	-3.176361
6	0.566382	-0.331863	-2.419477	6	4.679929	2.906022	-1.468831
6	-0.149415	0.990107	-2.098865	1	3.618845	1.852934	0.085492
15	0.725104	1.830747	-0.693035	6	4.581339	3.574221	-2.692754
1	-0.188861	1.378898	1.495046	1	3.242674	4.241688	-4.252071
1	1.664530	1.620165	1.602309	1	5.645167	2.795573	-0.984688
1	2.532309	0.211946	0.658508	1	5.468905	3.982944	-3.165292
1	-0.164063	1.636466	-2.983574	6	-1.433584	-2.163397	2.482933
1	-1.191070	0.818674	-1.777637	1	-1.264011	-2.990089	1.791287
1	-0.058929	-0.959701	-3.062564	1	-1.780277	-2.589551	3.435000
1	1.512079	-0.144671	-2.940517	1	-2.243399	-1.559474	2.069511
1	-0.610788	-0.053054	0.464553	6	-1.364664	0.705502	3.792771
8	-2.751027	0.367358	-0.672605	1	-2.207320	0.581058	3.108573
6	-4.089748	0.506141	-0.731381	1	-1.674385	0.339402	4.781752
1	-4.473780	1.553958	-0.669138	1	-1.160700	1.775804	3.879282
6	-4.660542	-0.005623	-2.068849	6	1.699409	1.487643	4.343841
6	-4.761811	-0.197319	0.464699	1	1.055133	2.355045	4.180079
9	-4.436592	-1.550882	0.564366	1	1.694636	1.263297	5.419579
9	-4.333707	0.390749	1.658382	1	2.717251	1.772839	4.065332
9	-6.155387	-0.122091	0.477111	6	3.525369	-0.918051	3.316117
9	-6.031928	0.216081	-2.219435	1	4.027729	0.048646	3.221517
9	-4.040284	0.646473	-3.127530	1	3.737505	-1.306062	4.322271
9	-4.457978	-1.371995	-2.270429	1	3.982318	-1.604292	2.598242
6	-0.168137	-2.780379	-0.955267	6	1.605478	-3.212963	2.234101
6	0.278682	-4.118195	-0.932498	1	2.564618	-3.227665	1.708278
6	-1.551614	-2.514153	-1.021023	1	1.723582	-3.808135	3.150318
6	-0.641056	-5.171718	-0.983250	1	0.871505	-3.719799	1.605904
1	1.337783	-4.342650	-0.884306	[Cp*W(dppe)H₃](HFIP)₂			
6	-2.461840	-3.578213	-1.080940	-3056.99455697 h			
1	-1.945246	-1.494425	-0.993708	6	0.849773	-2.092974	2.249311
6	-2.012659	-4.903057	-1.061975	6	2.222875	-1.783354	2.565046
1	-0.283340	-6.196784	-0.966292	6	2.250910	-0.452825	3.138932
1	-3.519476	-3.351551	-1.130873	6	0.881715	0.035887	3.165552
1	-2.725348	-5.720922	-1.105372	6	0.037011	-0.989156	2.636557
6	2.623981	-2.100101	-1.431213	74	1.670281	-0.192009	0.981922
6	2.688184	-2.798774	-2.656635	15	1.953174	-1.639495	-1.085053
6	3.803101	-1.950089	-0.682263	6	2.871508	-0.606614	-2.371381
6	3.897319	-3.330840	-3.112211	6	2.277188	0.810332	-2.433711
1	1.791027	-2.934747	-3.251379	15	2.320670	1.530494	-0.700522
6	5.013858	-2.489253	-1.137107	1	0.225081	0.441835	0.189948
1	3.775761	-1.386984	0.242923	1	1.931272	1.427283	1.478895
6	5.064071	-3.179837	-2.351393	1	3.374509	-0.235899	0.743879
1	3.928115	-3.862626	-4.057833	1	2.824472	1.434142	-3.148719
1	5.914710	-2.361819	-0.545064	1	1.227384	0.762201	-2.748728
1	6.002418	-3.594448	-2.705635	1	2.811806	-1.101324	-3.345882
6	-0.265199	3.346958	-0.335371	1	3.926023	-0.565236	-2.078702
6	0.344551	4.606811	-0.196153	1	-1.101610	0.644458	0.180634
6	-1.657286	3.217240	-0.148771	8	-2.084862	0.844187	0.050518
6	-0.428156	5.731370	0.116539	6	-2.248408	2.177245	-0.368918
1	1.414501	4.716799	-0.332074	1	-1.295931	2.712742	-0.398441
6	-2.418411	4.351643	0.156352	6	-2.811278	2.167943	-1.786846
1	-2.129061	2.233293	-0.237748	6	-3.132843	2.894765	0.645478
6	-1.810691	5.606553	0.289351	9	-4.396527	2.323547	0.743937
1	0.051283	6.699726	0.222135	9	-2.549047	2.831843	1.899667
1	-3.490531	4.251308	0.293210	9	-3.304088	4.232695	0.329689
1	-2.410146	6.479889	0.527909	9	-3.073176	3.441623	-2.264022
6	2.275341	2.503120	-1.468240				

9	-1.899151	1.576613	-2.645907	1	4.614211	1.305445	1.186415
9	-3.992500	1.438725	-1.873618	6	5.684567	3.799371	-1.589538
1	-3.243051	-0.487062	0.017419	1	3.732810	3.480663	-2.421968
8	-3.819328	-1.278987	0.054900	6	6.572705	3.493478	-0.550307
6	-5.155225	-0.852716	0.172483	1	6.863005	2.363921	1.265188
1	-5.303125	0.179181	-0.158492	1	5.974521	4.500081	-2.366280
6	-5.997834	-1.735542	-0.740477	1	7.555324	3.953854	-0.520924
6	-5.580095	-0.910717	1.639393	6	1.290161	3.073475	-0.836473
9	-7.339377	-1.382310	-0.691673	6	0.737448	3.514376	-2.054805
9	-5.902916	-3.078156	-0.429784	6	1.074339	3.852641	0.319374
9	-5.576989	-1.581600	-2.054671	6	-0.019860	4.693555	-2.112506
9	-5.555542	-2.191083	2.159631	1	0.877735	2.942553	-2.963971
9	-4.713446	-0.134517	2.398303	6	0.323847	5.031083	0.258388
9	-6.858874	-0.403396	1.824267	1	1.483886	3.524112	1.267983
6	-1.466365	-0.964471	2.641259	6	-0.230462	5.453534	-0.957778
1	-1.867248	0.045460	2.537714	1	-0.450842	5.007175	-3.057455
1	-1.903201	-1.579351	1.850519	1	0.166118	5.614185	1.159907
1	-1.835943	-1.363715	3.596789	1	-0.823760	6.360587	-1.001754
6	0.332896	-3.432190	1.794270	[Cp*W(dppe)H₄]⁺[(CF₃)₂CHOHOCH(CF₃)₂]⁻			
1	0.081451	-4.053948	2.665503	-3057.00640564 h			
1	-0.572452	-3.339751	1.187846	6	-2.254839	-2.257937	-2.256932
1	1.076548	-3.979483	1.209983	6	-3.032135	-1.270602	-2.947484
6	3.356475	-2.772760	2.611478	6	-2.127280	-0.396078	-3.637843
1	3.389908	-3.268325	3.593312	6	-0.784984	-0.836048	-3.357396
1	3.256198	-3.551186	1.852140	6	-0.863696	-1.985000	-2.499327
1	4.322342	-2.285343	2.452726	74	-1.729982	-0.088916	-1.320354
6	3.413787	0.163824	3.869968	15	-1.880111	-1.098629	1.057519
1	3.416504	-0.131421	4.930139	6	-1.283333	0.182048	2.319604
1	4.367707	-0.151675	3.436488	6	-0.462282	1.327816	1.704905
1	3.378830	1.256825	3.828778	15	-1.300493	1.933991	0.164923
6	0.401297	1.282533	3.860544	1	-0.543804	0.941466	-1.892765
1	0.105614	1.058990	4.896127	1	-2.364440	1.330273	-1.989424
1	1.186408	2.043101	3.897151	1	-3.312609	0.244612	-0.757662
1	-0.464297	1.723429	3.357349	1	-0.339639	2.138831	2.430155
6	0.532518	-2.265487	-2.122142	1	0.544034	0.986686	1.430675
6	-0.789129	-2.034758	-1.706754	1	-0.687797	-0.337115	3.076735
6	0.747022	-2.925740	-3.351572	1	-2.188623	0.569590	2.800224
6	-1.875095	-2.439790	-2.495262	1	-0.202574	-0.289654	-0.575131
1	-0.960962	-1.524445	-0.767307	8	2.882933	-0.495771	-1.255320
6	-0.333417	-3.332037	-4.139006	6	4.123734	-0.910711	-1.691786
1	1.757255	-3.135531	-3.689368	1	4.080230	-1.154445	-2.763058
6	-1.646359	-3.086778	-3.713094	6	5.197412	0.183020	-1.582768
1	-2.885735	-2.243782	-2.155460	6	4.550096	-2.213516	-1.002928
1	-0.152182	-3.838388	-5.082246	9	4.566427	-2.114204	0.385726
1	-2.484412	-3.399930	-4.327672	9	3.651056	-3.224800	-1.320420
6	3.062659	-3.133601	-0.984147	9	5.808640	-2.652687	-1.397614
6	4.436878	-2.952511	-0.727202	9	6.334094	-0.136222	-2.320497
6	2.570590	-4.447539	-1.102974	9	4.715865	1.380713	-2.080877
6	5.294961	-4.050576	-0.617328	9	5.618243	0.411414	-0.275695
1	4.834238	-1.952739	-0.587660	1	2.811439	-0.204637	-0.180640
6	3.429649	-5.547175	-0.977256	8	2.457062	0.176185	1.033587
1	1.518893	-4.616358	-1.303033	6	3.433905	0.458088	1.961118
6	4.794102	-5.352829	-0.740717	1	4.417132	0.019579	1.733224
1	6.351580	-3.889378	-0.427358	6	3.671427	1.972179	2.052162
1	3.029586	-6.552058	-1.069838	6	3.039136	-0.126563	3.322106
1	5.460032	-6.204979	-0.649680	9	4.722520	2.315991	2.896597
6	4.021548	2.294031	-0.628281	9	2.548995	2.667015	2.499772
6	4.916817	2.002243	0.414054	9	3.987971	2.480372	0.798485
6	4.417897	3.210146	-1.624613	9	1.765421	0.264100	3.735598
6	6.183777	2.599230	0.451632				

9	3.028048	-1.515401	3.261153
9	3.914301	0.216876	4.348002
6	-0.173178	3.198899	-0.563457
6	-0.670015	4.422221	-1.049952
6	1.195504	2.899989	-0.708663
6	0.191825	5.334667	-1.668966
1	-1.721499	4.666303	-0.947550
6	2.051012	3.820012	-1.323675
1	1.605319	1.961374	-0.352330
6	1.552183	5.035688	-1.806077
1	-0.201202	6.276136	-2.040285
1	3.102076	3.573582	-1.418905
1	2.219468	5.745824	-2.284535
6	-2.729519	2.933956	0.798205
6	-2.493911	3.896935	1.803233
6	-4.034528	2.785672	0.299065
6	-3.540949	4.674764	2.304206
1	-1.490240	4.051896	2.184884
6	-5.081923	3.569956	0.799806
1	-4.228171	2.056261	-0.477691
6	-4.839434	4.511342	1.804470
1	-3.342334	5.408647	3.078639
1	-6.084272	3.442337	0.403312
1	-5.652232	5.116307	2.193580
6	-0.823954	-2.585903	1.378826
6	-1.378597	-3.866924	1.579174
6	0.576942	-2.438405	1.381275
6	-0.547111	-4.976121	1.772242
1	-2.453566	-4.002549	1.594662
6	1.401482	-3.552810	1.578032
1	1.050130	-1.472013	1.228251
6	0.844224	-4.821651	1.769251
1	-0.988587	-5.955690	1.928022
1	2.475490	-3.412710	1.576024
1	1.487934	-5.682727	1.918192
6	-3.522359	-1.570800	1.788390
6	-3.582992	-2.037099	3.120002
6	-4.722056	-1.427163	1.071147
6	-4.810449	-2.351821	3.709209
1	-2.671212	-2.161776	3.694898
6	-5.951455	-1.748015	1.662032
1	-4.693650	-1.041609	0.058779
6	-5.998551	-2.210841	2.980073
1	-4.838872	-2.706225	4.734566
1	-6.868134	-1.629808	1.092898
1	-6.950875	-2.456696	3.438789
6	0.483833	-0.320375	-3.983155
1	1.307461	-0.326352	-3.263169
1	0.763653	-0.952421	-4.837700
1	0.365382	0.703569	-4.347072
6	-2.509122	0.663397	-4.636557
1	-1.779490	1.476656	-4.656300
1	-2.558182	0.230895	-5.645450
1	-3.485928	1.099054	-4.410636
6	-4.530357	-1.270695	-3.094380
1	-4.927044	-0.257079	-3.196854
1	-4.824313	-1.835460	-3.990131
1	-5.021606	-1.738273	-2.237013
6	-2.817619	-3.492088	-1.604867
1	-3.723276	-3.283471	-1.027801

1	-3.081834	-4.226987	-2.377834
1	-2.095417	-3.962701	-0.936424
6	0.305605	-2.855652	-2.126090
1	0.082050	-3.499790	-1.274008
1	0.565852	-3.504889	-2.974130
1	1.187191	-2.264235	-1.868054

[CpW(dhpe)H₃]

-1145.61164812 h

6	1.842534	-1.665022	-1.724245
6	3.081523	-1.365964	-1.087256
6	3.001856	-1.779651	0.280200
6	1.712110	-2.340019	0.512720
6	1.007522	-2.249974	-0.724724
74	1.423722	-0.040701	-0.029897
15	0.812745	2.107550	-1.075499
6	0.280975	3.398082	0.208758
6	-0.405912	2.720014	1.413322
15	0.551113	1.174407	1.934723
1	2.622241	0.344522	1.094870
1	2.735348	0.881005	-0.569564
1	-0.388230	0.591877	2.833344
1	1.457875	1.704205	2.894989
1	1.742687	2.870627	-1.833858
1	-0.291202	2.144302	-1.970598
1	-0.490106	3.410324	2.259375
1	-1.408334	2.377827	1.142561
1	-0.373342	4.148923	-0.247123
1	1.201340	3.903043	0.530358
1	3.947781	-0.925611	-1.560121
1	3.799974	-1.702525	1.004665
1	1.350427	-2.779836	1.430006
1	-0.002042	-2.600586	-0.880760
1	1.605146	-1.520735	-2.768449
8	-0.756782	0.130321	-0.109390
6	-1.838201	-0.654103	-0.414343
1	-1.652799	-1.469111	-1.133041
6	-2.378954	-1.338149	0.851630
6	-2.898667	0.230729	-1.087375
9	-4.046910	-0.472283	-1.427842
9	-2.387591	0.757230	-2.268126
9	-3.287595	1.301707	-0.294716
9	-2.700633	-0.431497	1.850021
9	-1.409821	-2.193526	1.372703
9	-3.505736	-2.114295	0.612444

CpW(dhpe)H₂(OCH(CF₃)₂)

-1145.62084130 h

6	-2.538561	-2.009177	-0.860809
6	-1.244711	-2.609308	-0.692668
6	-0.880652	-2.506486	0.673905
6	-1.916225	-1.839368	1.371520
6	-2.963284	-1.524517	0.430806
74	-1.181474	-0.294209	-0.262951
15	-0.736366	1.858781	-1.426298
6	-0.825490	3.358165	-0.287199
6	-1.836841	3.109634	0.850895
15	-1.587060	1.369541	1.520961
1	-2.499971	0.383119	-1.115541
1	-0.385987	-0.531596	-1.772159

1	-2.703350	1.225064	2.389185
1	-0.576257	1.618149	2.502771
1	0.522617	2.079381	-2.045686
1	-1.578604	2.214669	-2.507774
1	-1.722065	3.851710	1.647969
1	-2.866147	3.162757	0.477309
1	-1.070061	4.261169	-0.855821
1	0.184402	3.477450	0.120507
1	-0.642553	-3.060665	-1.467329
1	0.074370	-2.788512	1.092952
1	-1.925504	-1.640790	2.434974
1	-3.931272	-1.107271	0.666910
1	-3.121579	-2.002830	-1.768831
8	0.820525	0.115072	0.391208
6	1.999921	-0.079670	-0.292653
1	1.906663	-0.083622	-1.391315
6	2.956131	1.072020	0.049617
6	2.616462	-1.443636	0.066458
9	3.345815	1.080781	1.376755
9	2.539983	-1.728360	1.419249
9	1.931813	-2.464915	-0.596947
9	3.950486	-1.562951	-0.309827
9	4.107354	1.067050	-0.728601
9	2.330227	2.297499	-0.200475

CpW(dhpe)H₂(OCH(CF₃)₂)

-1145.61914519 h

6	1.629370	-2.051028	0.890796
6	1.137203	-2.448878	-0.395477
6	2.117835	-2.103481	-1.380280
6	3.209510	-1.489688	-0.726785
6	2.919703	-1.422920	0.668621
74	1.260719	-0.158936	-0.291085
15	1.107432	1.064241	1.888487
6	0.322311	2.752804	1.644316
6	0.879224	3.413035	0.365877
15	0.790918	2.172477	-1.045530
1	2.593960	0.775224	-0.815263
1	0.594086	-0.185161	-1.878062
1	1.607095	2.783209	-2.030788
1	-0.485618	2.456861	-1.590702
1	0.301136	0.553634	2.948066
1	2.269085	1.380537	2.652591
1	0.324858	4.324237	0.116856
1	1.933796	3.685269	0.497304
1	0.479483	3.383706	2.524856
1	-0.751384	2.561008	1.539827
1	0.200343	-2.950223	-0.585367
1	2.027092	-2.263047	-2.445422
1	4.092449	-1.095518	-1.209048
1	3.588125	-1.042045	1.428299
1	1.162966	-2.266273	1.841203
8	-0.821015	0.130313	0.232523
6	-1.924614	-0.435734	-0.362066
1	-1.716755	-0.959923	-1.308009
6	-2.944171	0.665779	-0.701434
6	-2.542995	-1.477157	0.585741
9	-1.581578	-2.399186	0.993434
9	-3.069272	-0.908327	1.735156
9	-3.555281	-2.213927	-0.019842

9	-4.207746	0.177764	-1.011200
9	-3.095717	1.585720	0.325258
9	-2.517218	1.381302	-1.821298

CpW(dhpe)H₂(OCH₂CF₃)

-808.658844674 h

6	1.024546	-2.307236	-0.992314
6	2.387278	-1.945041	-0.770957
6	2.593858	-1.774884	0.630218
6	1.364403	-2.055734	1.298827
6	0.408190	-2.374772	0.301068
74	1.037152	-0.111606	-0.062170
15	0.403653	1.742607	-1.532559
6	0.053682	3.342919	-0.570814
6	-0.527971	3.019671	0.820253
15	0.434016	1.596107	1.608141
1	2.389087	0.724982	0.555311
1	2.257039	0.314945	-1.147203
1	-0.436913	1.275402	2.689855
1	1.438667	2.282409	2.343379
1	1.257734	2.245836	-2.552456
1	-0.796125	1.679555	-2.308779
1	-0.510494	3.898112	1.473916
1	-1.560847	2.666531	0.738061
1	-0.617193	3.995965	-1.139697
1	1.018473	3.857333	-0.470171
1	3.143518	-1.830312	-1.534467
1	3.527157	-1.502472	1.102146
1	1.198247	-2.039458	2.366750
1	-0.635584	-2.580451	0.497380
1	0.579823	-2.574091	-1.940267
8	-1.073403	0.071651	0.111674
6	-2.004792	-0.458151	-0.788277
1	-1.702114	-1.415920	-1.236603
6	-3.295571	-0.717290	-0.043482
9	-3.803705	0.425951	0.561166
9	-3.144452	-1.676133	0.956889
9	-4.279637	-1.193262	-0.912465
1	-2.249158	0.220704	-1.621121

CpW(dhpe)H₂(OCH₂CF₃)

-808.660308200 h

6	0.520675	2.680466	-0.925165
6	-0.861590	2.368627	-0.701732
6	-1.036779	2.083077	0.676373
6	0.217415	2.197908	1.325907
6	1.203868	2.572985	0.341565
74	0.508894	0.497034	-0.284919
15	1.346347	-1.562186	-1.374818
6	2.185452	-2.735469	-0.161817
6	2.964642	-1.925921	0.894681
15	1.868252	-0.526193	1.508913
1	1.903360	0.742728	-1.241498
1	-0.342397	0.163893	-1.742173
1	2.785333	0.250689	2.270008
1	1.204528	-1.194186	2.587461
1	0.405621	-2.442475	-1.975952
1	2.284522	-1.486665	-2.437894
1	3.284351	-2.563131	1.725983
1	3.856480	-1.466578	0.451921

1	2.831799	-3.444825	-0.688747
1	1.377018	-3.299287	0.318001
1	-1.641950	2.345667	-1.447935
1	-1.951844	1.734751	1.132984
1	0.384894	2.065392	2.386597
1	2.235275	2.829659	0.532842
1	0.952934	3.009298	-1.857611
8	-0.718796	-1.108661	0.437132
6	-1.856166	-1.640122	-0.171127
1	-1.814683	-1.657406	-1.272672
6	-3.137155	-0.902096	0.180627
9	-3.267599	-0.655521	1.543141
9	-3.265191	0.338541	-0.453718
9	-4.252134	-1.649176	-0.211144
1	-2.019866	-2.674444	0.173808

CpW(dhpe)H₂(OCH₂CF₃)

-808.661031542 h

6	0.476444	-2.019049	1.437340
6	-0.424656	-2.419293	0.412475
6	0.325863	-2.732281	-0.752473
6	1.706377	-2.527861	-0.472447
6	1.819196	-2.073613	0.889756
74	0.728386	-0.437115	-0.229485
15	1.138219	1.138067	1.645533
6	1.307836	2.912746	1.038863
6	2.012919	2.950019	-0.332327
15	1.233157	1.649775	-1.443012
1	2.337400	-0.226021	-0.811757
1	0.145872	-0.510423	-1.851025
1	2.096569	1.657642	-2.567635
1	0.144105	2.389104	-1.992096
1	0.161658	1.330153	2.669352
1	2.283140	0.989497	2.481363
1	1.951057	3.945130	-0.786254
1	3.073295	2.688750	-0.231010
1	1.831976	3.525449	1.779126
1	0.281971	3.289506	0.950804
1	-1.503191	-2.392339	0.480083
1	-0.087415	-3.049410	-1.699756
1	2.523157	-2.712685	-1.153548
1	2.740977	-1.920331	1.431981
1	0.201235	-1.783669	2.456328
8	-1.064410	0.660896	0.055544
6	-2.168141	0.640512	-0.799781
1	-2.098075	-0.119324	-1.591634
6	-3.425071	0.336894	-0.010890
9	-3.403087	-0.931032	0.578015
9	-3.654919	1.245477	1.013883
9	-4.550601	0.365495	-0.840367
1	-2.346798	1.612770	-1.291509

A [CpW(dhpe)H₃]TFE

-809.852526795 h

6	-1.436772	-2.452382	0.915185
6	-1.552610	-2.709721	-0.478846
6	-0.272841	-2.487685	-1.075136
6	0.643186	-2.075199	-0.062206
6	-0.093182	-2.051228	1.171282
74	-1.022084	-0.397818	-0.230745

15	-2.749024	0.896139	0.856920
6	-2.708418	2.716354	0.333965
6	-1.257083	3.156477	0.056284
15	-0.345947	1.815069	-0.928841
1	-0.235356	0.525439	1.019751
1	-0.767271	-0.305189	-1.901740
1	-2.453153	-0.124578	-1.168491
1	0.976543	2.355938	-0.853618
1	-0.618658	2.241278	-2.260226
1	-4.138534	0.623802	0.697337
1	-2.766089	1.039100	2.281317
1	-1.226203	4.110531	-0.481464
1	-0.709156	3.283703	0.998866
1	-3.185557	3.348357	1.090763
1	-3.304620	2.779436	-0.585263
1	-2.449002	-3.024153	-0.995167
1	-0.036923	-2.626627	-2.120898
1	1.703904	-1.911695	-0.177017
1	0.320388	-1.798262	2.137675
1	-2.226596	-2.555364	1.647146
1	1.555410	0.275126	1.233618
8	2.330715	0.042713	1.781531
6	3.467784	0.767265	1.358880
1	4.272970	0.545293	2.063533
6	3.945089	0.363908	-0.020087
9	3.025347	0.708703	-1.011371
9	4.164551	-1.002438	-0.134100
9	5.140657	1.007633	-0.328419
1	3.315071	1.854725	1.344697

B [CpW(dhpe)H₃]TFE

-809.856001553 h

6	2.253187	-1.923241	1.231085
6	1.128746	-2.552951	0.626964
6	1.301697	-2.513004	-0.789207
6	2.528813	-1.848790	-1.081067
6	3.110956	-1.481470	0.176481
74	1.118913	-0.258078	-0.036563
15	0.731555	1.465211	1.628537
6	0.237640	3.116735	0.840288
6	0.908148	3.279804	-0.538530
15	0.846462	1.645099	-1.497533
1	2.403365	0.910215	0.005886
1	-0.134205	-0.515559	-1.162790
1	-0.412384	-0.379908	0.733343
1	1.772774	1.978469	-2.538200
1	-0.339913	1.820179	-2.263527
1	-0.267803	1.352147	2.633311
1	1.796135	1.893122	2.483451
1	0.425474	4.071669	-1.121149
1	1.968194	3.540471	-0.426755
1	0.477544	3.953199	1.505912
1	-0.851932	3.070920	0.723504
1	0.288207	-2.988125	1.149443
1	0.615562	-2.922702	-1.517246
1	2.966224	-1.708888	-2.059326
1	4.062508	-0.984403	0.306540
1	2.436821	-1.829057	2.292453
1	-1.642114	0.563859	-0.122261
8	-2.431949	1.115345	-0.307636

6	-3.386461	0.303657	-0.964206
1	-2.938798	-0.353465	-1.720037
6	-4.149166	-0.572739	0.005717
9	-4.846901	0.158628	0.954682
9	-5.080009	-1.354403	-0.681046
9	-3.309831	-1.443916	0.694312
1	-4.110597	0.957402	-1.457590

C [CpW(dhpe)H₃]TFE

-809.854659301 h

6	-1.315087	-2.813554	-0.138861
6	-0.331413	-2.520919	-1.131531
6	0.806738	-1.929499	-0.496222
6	0.504770	-1.867060	0.906851
6	-0.790918	-2.416179	1.122895
74	-1.013544	-0.452424	-0.220783
15	-2.519948	0.631140	1.342480
6	-2.984268	2.378836	0.791898
6	-1.798034	3.032363	0.056466
15	-1.018635	1.792130	-1.143834
1	1.505702	0.509750	-1.032121
1	-0.001076	0.649751	0.664442
1	-2.673939	-0.395704	-0.730665
1	0.135295	2.540645	-1.526447
1	-1.790003	2.044200	-2.313226
1	-3.811060	0.107810	1.642704
1	-2.115696	0.874280	2.693091
1	-2.109600	3.936961	-0.477163
1	-1.014848	3.315722	0.771111
1	-3.311381	2.978643	1.647805
1	-3.837715	2.266085	0.111616
1	-0.423355	-2.735830	-2.186810
1	1.757279	-1.704220	-0.954831
1	1.170843	-1.492356	1.670367
1	-1.290752	-2.520449	2.076834
1	-2.283868	-3.260663	-0.313004
1	-1.224598	-0.459960	-1.903243
8	2.344024	0.943618	-1.303591
6	2.987084	1.443483	-0.147405
1	2.288070	1.653763	0.670728
6	4.026388	0.478961	0.381079
9	5.020306	0.198880	-0.540781
9	4.645316	1.010862	1.512885
9	3.469597	-0.744737	0.762325
1	3.511005	2.369322	-0.405117

D [CpW(dhpe)H₃]TFE

-809.850595484 h

6	1.130499	-2.011891	1.478839
6	-0.211477	-1.892081	0.942828
6	-0.175734	-2.365786	-0.408517
6	1.153866	-2.764208	-0.707515
6	1.963180	-2.543642	0.443840
74	1.159950	-0.437576	-0.188792
15	0.858771	1.217601	1.588497
6	0.756039	2.984883	0.954431
6	1.778173	3.170384	-0.184906
15	1.713115	1.676071	-1.331762
1	1.849473	-0.591624	-1.762076
1	-0.172424	0.100389	-1.142959

1	-1.407538	0.948144	-0.396991
1	2.959594	1.790103	-1.998844
1	0.874364	2.136921	-2.381087
1	-0.268353	1.169361	2.465126
1	1.833834	1.395375	2.629199
1	1.594623	4.093190	-0.745313
1	2.797820	3.217558	0.217303
1	0.928905	3.699496	1.765962
1	-0.266512	3.110639	0.581496
1	-1.100906	-1.616711	1.489607
1	-1.016389	-2.397447	-1.085464
1	1.501644	-3.141940	-1.658614
1	3.022397	-2.742979	0.518873
1	1.434995	-1.823787	2.499191
1	2.836797	-0.032205	0.035499
8	-2.125582	1.618270	-0.300983
6	-3.140469	1.111623	0.540194
1	-3.827805	1.931786	0.763946
6	-3.948765	0.009678	-0.110930
9	-4.532482	0.395722	-1.303298
9	-3.169085	-1.118707	-0.379504
9	-4.971277	-0.401893	0.744184
1	-2.760765	0.713274	1.490608

A' [CpW(dhpe)H₃]HFIP

-1146.80474747 h

6	-3.478278	-1.466203	1.344265
6	-3.939583	-1.915788	.077092
6	-2.811567	-2.387838	-.663671
6	-1.637714	-2.217386	.125009
6	-2.062454	-1.633577	1.371536
74	-2.492442	-.055673	-.308578
15	-3.215533	2.039281	.666580
6	-2.550670	3.543005	-.275415
6	-1.184054	3.215966	-.910099
15	-1.224594	1.490137	-1.681754
1	-1.108929	.615754	.510851
1	-2.614530	-.403465	-1.961963
1	-3.864425	.658376	-1.091852
1	.149019	1.366203	-2.041376
1	-1.719368	1.792724	-2.982033
1	-4.586982	2.407375	.785715
1	-2.830424	2.373826	2.002968
1	-.906878	3.963499	-1.661452
1	-.395291	3.194865	-.148582
1	-2.492408	4.415286	.384345
1	-3.288647	3.760693	-1.057959
1	-4.964622	-1.904220	-.266806
1	-2.849963	-2.814325	-1.656282
1	-.640254	-2.550079	-.119908
1	-1.414430	-1.401233	2.205121
1	-4.095131	-1.077108	2.143019
1	.342758	-.258109	.710732
8	1.022960	-.692784	1.276024
6	2.308116	-.551379	.737908
1	3.000908	-1.063202	1.412192
6	2.444815	-1.242217	-.621679
6	2.727126	.920277	.713492
9	3.964135	1.110752	.119983
9	2.800082	1.409154	2.004063

9	1.806139	1.706610	.025395
9	1.753441	-.578514	-1.626513
9	1.938940	-2.530034	-.549023
9	3.770187	-1.339237	-1.014970

B1' [CpW(dhpe)H₃]HFIP

-1146.80863155 h

6	-3.781211	-1.184602	-1.594896
6	-2.852901	-2.116024	-1.048083
6	-3.141075	-2.278827	.339822
6	-4.248875	-1.446813	.672558
6	-4.638473	-.768732	-.528041
74	-2.487951	-.006967	.014394
15	-1.597282	1.895331	-1.215509
6	-.950169	3.246355	-.059861
6	-1.776415	3.288280	1.239710
15	-2.133015	1.529898	1.851403
1	-3.541431	1.373038	.047267
1	-1.409115	-.652553	1.167661
1	.206749	.050014	.743412
1	-3.154070	1.836878	2.806572
1	-1.077916	1.333372	2.785933
1	-.501627	1.782273	-2.111817
1	-2.450809	2.661370	-2.069656
1	-1.258103	3.854351	2.020829
1	-2.749140	3.765495	1.066210
1	-.941596	4.219724	-.562222
1	.086805	2.962709	.154896
1	-2.065843	-2.619420	-1.592100
1	-2.607177	-2.925633	1.021988
1	-4.735359	-1.383525	1.635601
1	-5.470491	-.084393	-.621198
1	-3.850801	-.885433	-2.631343
1	-.971246	-.340637	-.720512
8	1.147149	.282927	.926349
6	1.929903	-.295519	-.084716
6	2.833488	.786834	-.665078
6	2.692736	-1.489246	.486559
9	3.463756	-2.119023	-.484057
9	3.529685	-1.144860	1.529395
9	1.785874	-2.425562	.960742
9	3.615214	.303675	-1.704719
1	1.323839	-.678711	-.914873
9	2.049060	1.811577	-1.191346
9	3.675400	1.350730	.271510

B2' [CpW(dhpe)H₃]HFIP

-1146.80828237 h

6	3.500234	-1.520899	0.797488
6	2.429417	-2.406754	0.482690
6	2.184358	-2.340123	-0.921300
6	3.101187	-1.413613	-1.495621
6	3.909488	-0.905826	-0.429412
74	1.718937	-0.181983	-0.012913
15	1.235238	1.449926	1.723902
6	0.270175	2.934750	1.053949
6	0.678814	3.238186	-0.400095
15	0.859204	1.625757	-1.381847
1	2.720487	1.236228	-0.075067
1	0.245707	-0.624448	-0.771364

1	0.622917	-0.787824	1.149012
1	1.598328	2.131206	-2.497625
1	-0.401732	1.545887	-2.031803
1	0.449323	1.130595	2.863921
1	2.293565	2.116498	2.417805
1	-0.055679	3.885695	-0.889933
1	1.653078	3.741575	-0.435687
1	0.399654	3.811117	1.698241
1	-0.782865	2.631744	1.087901
1	1.892701	-3.026995	1.187022
1	1.431145	-2.900980	-1.456867
1	3.198552	-1.178858	-2.546359
1	4.722855	-0.201598	-0.538038
1	3.951828	-1.383419	1.769773
1	-0.959762	-0.271511	0.869620
8	-1.899838	-0.053246	1.072632
6	-2.664560	-0.382572	-0.057065
1	-2.040802	-0.617429	-0.928161
6	-3.490870	-1.633074	0.236662
6	-3.507551	0.831333	-0.431524
9	-4.375964	-1.462110	1.282999
9	-4.223495	-2.034094	-0.875145
9	-2.639930	-2.677065	0.565653
9	-4.352994	1.239167	0.579446
9	-2.667101	1.904388	-0.728355
9	-4.276374	0.597663	-1.562748

C1' [CpW(dhpe)H₃]HFIP

-1146.80783287 h

6	-2.853752	-2.357102	-0.074043
6	-1.900154	-2.462623	-1.131718
6	-0.583697	-2.363000	-0.580959
6	-0.748007	-2.198052	0.838240
6	-2.138726	-2.204393	1.145842
74	-1.661867	-0.298070	-0.214017
15	-2.434761	1.292274	1.456815
6	-2.168527	3.089376	0.925157
6	-0.940426	3.204490	-0.000199
15	-0.930386	1.785264	-1.242857
1	0.909624	-0.286372	-1.003481
1	-0.235843	0.332672	0.556877
1	-3.211673	0.392699	-0.573033
1	0.336129	2.018099	-1.852831
1	-1.739903	2.321396	-2.281572
1	-3.792251	1.351506	1.884336
1	-1.841111	1.300102	2.756695
1	-0.926513	4.168193	-0.520705
1	-0.007261	3.118524	0.569252
1	-2.075560	3.736854	1.803221
1	-3.077111	3.383887	0.385165
1	-2.136914	-2.617062	-2.174971
1	0.348759	-2.520317	-1.101688
1	0.057571	-2.129225	1.555316
1	-2.577870	-2.118244	2.130783
1	-3.929139	-2.387124	-0.181031
1	-2.009664	-0.218453	-1.871875
8	1.885745	-0.271337	-1.173958
6	2.537187	-0.042140	0.047496
1	1.829619	0.101721	0.873198
6	3.376784	-1.266025	0.399756

6	3.343918	1.247733	-0.058704
9	4.338756	-1.556429	-0.544801
9	4.272724	1.227846	-1.077107
9	4.014050	-1.120648	1.625374
9	4.013536	1.538369	1.122955
9	2.475538	2.311283	-0.301078
9	2.541055	-2.375271	0.508067

C2'[CpW(dhpe)H₃]HFIP

-1146.80561232 h

6	-2.508428	-1.749337	1.191675
6	-3.271210	-1.934047	-0.004067
6	-2.382042	-2.360256	-1.033244
6	-1.071845	-2.433337	-0.491704
6	-1.125256	-2.050569	0.887201
74	-1.755146	-0.174847	-0.305360
15	-1.499104	1.217793	1.695762
6	-1.170046	3.038578	1.325880
6	-0.409885	3.189457	-0.005157
15	-1.171499	2.023532	-1.261053
1	-0.191082	-0.124658	-1.038765
1	-2.202620	0.004954	-1.959780
1	-3.221218	0.751192	-0.333407
1	-0.250523	2.095185	-2.335815
1	-2.202994	2.827130	-1.822343
1	-2.584362	1.369364	2.617647
1	-0.508086	0.929348	2.684907
1	-0.429035	4.224206	-0.364317
1	0.635845	2.884027	0.107687
1	-0.617820	3.488529	2.156671
1	-2.149029	3.529260	1.268838
1	-4.335439	-1.781582	-0.111096
1	-2.656299	-2.566681	-2.058069
1	-0.180376	-2.726661	-1.026221
1	-0.299463	-2.085913	1.582741
1	-2.912847	-1.509370	2.165637
1	0.711077	0.083893	0.515102
8	1.633969	0.179031	0.882895
6	2.528573	-0.191012	-0.130925
1	2.024992	-0.333710	-1.095949
6	3.531320	0.940593	-0.322042
6	3.168975	-1.529370	0.226871
9	3.881563	-1.490905	1.408338
9	2.169019	-2.488927	0.369827
9	4.023315	-1.980493	-0.770292
9	4.464015	0.649666	-1.307378
9	2.853783	2.088167	-0.733020
9	4.219023	1.256253	0.831687

D' [CpW(dhpe)H₃]HFIP

-1146.80355325 h

6	-1.896900	-1.494495	-1.844092
6	-0.598783	-1.790243	-1.271114
6	-0.828509	-2.513060	-0.055242
6	-2.230206	-2.655973	0.125955
6	-2.892823	-2.026640	-0.966240
74	-1.691548	-0.334012	0.127240
15	-0.991494	1.522832	-1.306829
6	-0.510981	3.076220	-0.362744
6	-1.475199	3.259272	0.826415

15	-1.778083	1.597862	1.664506
1	-2.488203	-0.645444	1.622537
1	-0.323880	-0.350836	1.177494
1	1.030040	0.378277	0.824790
1	-2.983907	1.863488	2.362702
1	-0.884738	1.649015	2.767803
1	0.107559	1.376545	-2.200744
1	-1.892185	2.100036	-2.265677
1	-1.092695	3.987601	1.549291
1	-2.451320	3.616153	0.474950
1	-0.526448	3.948857	-1.024231
1	0.515684	2.919406	-0.015354
1	0.364090	-1.588461	-1.714598
1	-0.063260	-2.874880	0.615691
1	-2.714531	-3.133406	0.965740
1	-3.962624	-1.960170	-1.102515
1	-2.085903	-1.031908	-2.803153
1	-3.231485	0.464772	0.003037
8	1.807860	0.951592	1.074054
6	3.024852	0.468230	0.581473
1	3.822944	1.052611	1.050872
6	3.265997	-0.988391	0.979920
6	3.164842	0.711104	-0.924409
9	2.303995	-0.071163	-1.687495
9	2.873668	2.035481	-1.213491
9	4.453347	0.462225	-1.369135
9	3.214417	-1.115372	2.354190
9	2.310201	-1.844692	0.443812
9	4.509091	-1.439151	0.560833

[CpW(dhpe)H₄]⁺[(CF₃)₂CHCO]⁻

-1146.78440032 h

6	-2.705949	-1.705341	0.855736
6	-3.760355	-0.776401	0.611046
6	-3.933898	-0.676636	-0.801391
6	-2.985940	-1.546177	-1.425965
6	-2.224925	-2.181146	-0.400046
74	-1.779126	0.147641	-0.307559
15	-0.396005	0.345179	1.807572
6	0.293636	2.049452	2.140966
6	0.460629	2.903995	0.859071
15	-0.144991	2.035173	-0.680183
1	-1.362232	0.224621	-1.947150
1	-2.604834	1.362333	-1.150497
1	-2.291221	1.462102	0.684347
1	0.946182	1.864640	-1.550585
1	-0.798682	3.103789	-1.358542
1	-1.338053	0.269011	2.888764
1	0.487121	-0.647375	2.266733
1	-0.091749	3.845423	0.947430
1	1.516729	3.119152	0.686413
1	1.263571	1.898136	2.618227
1	-0.385280	2.537883	2.846584
1	-4.330138	-0.246685	1.361129
1	-4.665668	-0.066497	-1.310353
1	-2.874911	-1.703650	-2.488843
1	-1.425336	-2.893709	-0.542522
1	-2.343459	-2.012599	1.827405
1	-0.293245	-0.579473	-0.675797
8	1.696016	0.579086	0.515316

6	2.326937	-0.324764	-0.276727
1	1.735385	-0.691552	-1.146515
6	3.587829	0.306732	-0.893472
6	2.680225	-1.603695	0.504485
9	3.338587	-1.352087	1.695573
9	1.499651	-2.284017	0.842792
9	3.452582	-2.512951	-0.213399
9	4.193038	-0.500211	-1.855634
9	3.251308	1.495690	-1.544492
9	4.556925	0.621903	0.044888

A1" [CpW(dhpe)H₃](HFIP)₂

-1936.43536894 h

6	-1.314866	-3.059211	-0.571627
6	-2.198430	-2.933561	-1.676713
6	-1.748303	-1.846954	-2.491083
6	-0.600889	-1.270038	-1.889647
6	-0.343355	-2.017567	-0.679216
74	-2.382195	-0.952947	-0.353917
15	-2.962771	-1.250669	1.980715
6	-3.979239	0.195344	2.655939
6	-3.572091	1.508745	1.958154
15	-3.376670	1.221212	0.099666
1	-1.310130	0.125657	0.505423
1	-3.460723	-0.460149	-1.563606
1	-4.016383	-1.468979	-0.080972
1	-2.840927	2.485425	-0.281310
1	-4.707969	1.446372	-0.348154
1	-3.747706	-2.347007	2.441054
1	-1.933399	-1.343141	2.968096
1	-4.303953	2.301636	2.147275
1	-2.597976	1.856590	2.321988
1	-3.870021	0.265573	3.743281
1	-5.028148	-0.041405	2.437248
1	-3.064146	-3.551546	-1.871525
1	-2.212301	-1.521493	-3.411802
1	-0.000582	-0.469861	-2.297231
1	0.486398	-1.873883	-0.001713
1	-1.361523	-3.816313	0.198941
1	-0.038678	0.808843	-0.084098
8	0.937266	1.000684	-0.158895
6	1.227326	2.371193	-0.324624
1	2.314330	2.459070	-0.384979
6	0.666793	2.898393	-1.644899
6	0.785349	3.165046	0.902882
9	1.068410	4.512268	0.780443
9	1.441954	2.686835	2.021508
9	-0.580248	3.038556	1.140305
9	-0.718760	2.966559	-1.648917
9	1.047590	2.057515	-2.678204
9	1.154236	4.162177	-1.927113
1	1.949469	-0.044317	0.869956
8	2.553941	-0.735541	1.210258
6	3.483026	-1.026020	0.196842
1	3.067801	-0.918211	-0.812455
6	3.878202	-2.490467	0.351956
6	4.664600	-0.059376	0.283403
9	4.821292	-2.857428	-0.598293
9	2.764930	-3.294175	0.161870
9	4.398593	-2.772891	1.597602

9	5.570545	-0.244300	-0.747618
9	5.347650	-0.133415	1.475305
9	4.176279	1.248605	0.161960

A2" [CpW(dhpe)H₃](HFIP)₂

-1936.43624496 h

6	-4.306943	0.034318	1.098385
6	-3.493120	1.132163	0.619404
6	-3.725556	1.242528	-0.792419
6	-4.658455	0.239239	-1.174706
6	-5.013971	-0.508635	-0.018374
74	-2.695147	-0.800517	-0.319277
15	-1.501149	-1.313151	1.754568
6	0.157698	-2.150308	1.486223
6	0.048670	-3.154239	0.321501
15	-0.957158	-2.397271	-1.077487
1	-2.860203	-1.353667	-1.943922
1	-1.440973	0.095708	-1.109979
1	-0.267173	0.743565	-0.497868
1	-1.368473	-3.550414	-1.791034
1	0.049273	-1.945792	-1.970735
1	-1.159438	-0.292088	2.688339
1	-2.068053	-2.213513	2.718643
1	1.040273	-3.444866	-0.035454
1	-0.482152	-4.058360	0.643365
1	0.499668	-2.642227	2.402391
1	0.870451	-1.358083	1.238136
1	-2.898362	1.804271	1.219205
1	-3.270702	1.966023	-1.451998
1	-5.015614	0.056259	-2.178194
1	-5.693211	-1.348505	0.006376
1	-4.427741	-0.273930	2.128018
1	-3.232592	-2.442563	-0.160108
8	0.703098	1.026261	-0.534056
6	0.971850	2.316278	-0.043782
1	2.004502	2.553697	-0.312549
6	0.097653	3.377473	-0.709584
6	0.912042	2.335682	1.483781
9	-0.360999	2.103791	1.983688
9	1.734369	1.325092	1.982449
9	1.361803	3.531071	2.009115
9	0.235402	3.308859	-2.079910
9	-1.251254	3.218898	-0.412376
9	0.465412	4.650650	-0.304560
1	1.926593	-0.173251	-0.888812
8	2.580960	-0.901463	-0.971991
6	3.646090	-0.647663	-0.091883
1	3.326912	-0.204418	0.859045
6	4.622623	0.347827	-0.720383
6	4.281116	-1.992384	0.240610
9	5.209756	-0.110768	-1.876735
9	5.626477	0.717742	0.159256
9	3.915874	1.513801	-1.042280
9	4.694621	-2.681945	-0.878862
9	3.357851	-2.788826	0.909691
9	5.374224	-1.838951	1.079769

B2" [CpW(dhpe)H₃](HFIP)₂

-1936.44015120h

6	3.326573	-2.411561	-1.307528
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6	2.585446	-1.631953	-2.241924
6	3.256901	-0.386665	-2.425292
6	4.426077	-0.379691	-1.611727
6	4.463971	-1.631156	-0.919333
74	2.566120	-0.496564	-0.142582
15	1.271324	-1.320047	1.750244
6	1.155827	-0.042325	3.143313
6	2.421813	0.834841	3.190916
15	2.956170	1.309277	1.437273
1	3.527490	-0.923722	1.236802
1	1.843013	0.964434	-0.696800
1	0.946220	-0.828923	-0.551880
1	4.276802	1.776323	1.725349
1	2.346798	2.584511	1.286210
1	-0.093866	-1.680370	1.615523
1	1.702759	-2.468963	2.482921
1	2.256395	1.738640	3.786481
1	3.260017	0.284805	3.636513
1	0.969759	-0.529879	4.106210
1	0.282861	0.577112	2.903073
1	1.668517	-1.932593	-2.729462
1	2.933541	0.413818	-3.076072
1	5.166629	0.406221	-1.563421
1	5.244631	-1.951823	-0.243272
1	3.100496	-3.421639	-0.996458
1	0.099952	0.555763	-0.246109
8	-0.797952	0.982828	-0.132922
6	-0.760650	2.302083	-0.617607
1	0.245283	2.575880	-0.954925
6	-1.684772	2.390402	-1.829263
6	-1.132602	3.246918	0.520192
9	-2.956440	1.907224	-1.548411
9	-1.818368	3.685747	-2.297428
9	-1.166874	1.620473	-2.857569
9	-2.413497	3.024815	0.989700
9	-0.256230	3.053347	1.583930
9	-1.033346	4.574846	0.143051
1	-2.077694	0.105544	0.760328
8	-2.676480	-0.574802	1.125106
6	-3.429069	-1.090056	0.053473
1	-3.439606	-0.425361	-0.816566
6	-2.818564	-2.412761	-0.408620
6	-4.873812	-1.221480	0.523939
9	-2.869266	-3.400205	0.557137
9	-3.436660	-2.902080	-1.550044
9	-1.478104	-2.210180	-0.725132
9	-4.994068	-1.983585	1.669262
9	-5.672254	-1.800597	-0.455747
9	-5.392964	0.032829	0.792712

B1" [CpW(dhpe)H₃](HFIP)₂

-1936.44126742 h

6	-4.911301	0.574467	-0.572833
6	-4.027253	1.038160	-1.589038
6	-3.565313	-0.086905	-2.334414
6	-4.151129	-1.263997	-1.785386
6	-4.981889	-0.849150	-0.694346
74	-2.770739	-0.344749	-0.098656
15	-2.336415	0.289724	2.213370
6	-0.970847	-0.762709	2.996174

6	-0.955193	-2.183776	2.397857
15	-1.253844	-2.135463	0.527850
1	-3.386162	-1.472284	1.065480
1	-1.391704	-0.376919	-1.103290
1	-0.279536	0.590000	-0.214650
1	-1.594858	-3.508334	0.322677
1	0.066739	-2.195246	0.012436
1	-1.895801	1.589870	2.579556
1	-3.368042	0.166690	3.194615
1	-0.002784	-2.684332	2.600167
1	-1.758473	-2.793148	2.829976
1	-1.076964	-0.790223	4.086038
1	-0.035017	-0.240179	2.764117
1	-3.758142	2.069311	-1.771324
1	-2.884339	-0.051301	-3.173346
1	-4.035239	-2.270989	-2.160752
1	-5.594700	-1.501835	-0.087869
1	-5.462153	1.189886	0.124632
1	-1.981532	1.181814	0.013890
8	0.671770	0.881089	-0.101068
6	0.739581	2.286770	-0.121156
6	1.466827	2.742887	1.138980
6	1.413545	2.722403	-1.419877
9	1.553905	4.097488	-1.497847
9	2.675613	2.160640	-1.568229
9	0.645188	2.315276	-2.495978
9	1.568719	4.120097	1.212217
1	-0.259598	2.736871	-0.105042
9	0.757252	2.317913	2.257292
9	2.739996	2.208510	1.225037
1	1.824810	-0.306081	0.546185
8	2.438769	-1.046120	0.716820
6	3.444933	-0.975429	-0.267307
1	3.371216	-0.071959	-0.880753
6	4.796264	-0.921407	0.438263
6	3.293195	-2.164368	-1.212488
9	4.870548	0.227366	1.207229
9	5.005515	-2.003089	1.272312
9	5.844543	-0.881009	-0.472913
9	4.199075	-2.112485	-2.261169
9	2.019081	-2.145130	-1.770637
9	3.449233	-3.381747	-0.577657

C1" [CpW(dhpe)H₃](HFIP)₂

-1936.43991542 h

6	2.174197	-1.991345	-2.339742
6	0.768393	-1.881279	-2.122464
6	0.389622	-0.503050	-2.232683
6	1.591035	0.228738	-2.527548
6	2.678945	-0.686713	-2.601276
74	1.819288	-0.700776	-0.372613
15	4.011333	-0.094138	0.514947
6	4.014304	0.043223	2.395350
6	2.651288	0.563055	2.892941
15	1.250435	-0.313763	1.984728
1	-0.212058	0.778341	-0.070851
1	1.694262	1.007403	-0.057339
1	2.637294	-2.004994	0.431173
1	0.146359	0.448101	2.455631
1	1.060594	-1.462525	2.794323

1	5.147736	-0.926883	0.307809
1	4.623709	1.140561	0.139599
1	2.546249	0.427772	3.974712
1	2.540490	1.633116	2.677736
1	4.837958	0.681866	2.730206
1	4.196789	-0.969640	2.774960
1	0.092691	-2.703969	-1.936650
1	-0.617637	-0.116299	-2.253689
1	1.647941	1.293401	-2.704818
1	3.708980	-0.439443	-2.822359
1	2.753029	-2.904012	-2.314398
1	0.767444	-1.881710	0.242911
8	-1.039036	1.344957	0.034705
6	-0.710576	2.701384	-0.140946
1	0.368325	2.835291	-0.279520
6	-1.393477	3.210887	-1.406187
6	-1.096123	3.456607	1.126228
9	-2.765552	3.073034	-1.357697
9	-2.426342	3.290208	1.454458
9	-1.100612	4.542359	-1.653951
9	-0.843844	4.814797	1.021395
9	-0.334036	2.978683	2.188743
9	-0.930040	2.479063	-2.495979
1	-2.635080	0.484990	0.418273
8	-3.225509	-0.266111	0.615014
6	-2.498350	-1.444992	0.378960
1	-1.432133	-1.268100	0.187762
6	-2.560426	-2.302167	1.636967
6	-3.045869	-2.131716	-0.868199
9	-1.930528	-3.528256	1.459545
9	-1.886250	-1.645335	2.663946
9	-3.845803	-2.547462	2.069419
9	-2.287517	-3.252244	-1.213982
9	-4.356666	-2.538769	-0.744227
9	-2.969279	-1.253182	-1.943161

C2" [CpW(dhpe)H₃](HFIP)₂

-1936.43815890 h

6	2.617027	0.154260	-2.550943
6	1.789746	1.211769	-2.032667
6	2.646204	2.093234	-1.311485
6	3.980948	1.596653	-1.378799
6	3.969449	0.407783	-2.157571
74	2.662105	-0.042539	-0.236239
15	3.841741	-2.181604	-0.071144
6	3.040451	-3.385835	1.136624
6	2.446453	-2.603500	2.323285
15	1.534028	-1.070499	1.700603
1	3.846879	0.027874	1.035703
1	2.279785	1.159654	0.914274
1	1.454362	-1.175754	-0.708160
1	1.415412	-0.348287	2.915434
1	0.206284	-1.564556	1.617572
1	3.966216	-3.003010	-1.228852
1	5.204348	-2.228241	0.341116
1	1.773478	-3.230298	2.917665
1	3.246068	-2.243550	2.982398
1	3.765524	-4.135628	1.468800
1	2.248243	-3.901600	0.580499
1	0.742750	1.369248	-2.239475

1	2.337167	2.999684	-0.811496
1	4.847441	2.038589	-0.906667
1	4.837875	-0.179275	-2.424986
1	2.279733	-0.658041	-3.178918
1	0.242455	0.566740	-0.054968
8	-0.712502	0.891857	0.030469
6	-0.760980	2.041832	0.837362
1	0.234252	2.300326	1.218774
6	-1.245711	3.213844	-0.010681
6	-1.645852	1.756859	2.048065
8	-2.563008	-0.598445	-1.385784
1	-1.966049	0.014292	-0.912485
6	-3.686040	-0.834820	-0.576688
1	-3.969305	0.028397	0.034796
6	-3.394948	-1.977248	0.397423
6	-4.857331	-1.117585	-1.509881
9	-0.336160	3.445018	-1.037598
9	-2.476369	2.965962	-0.590571
9	-1.343593	4.385071	0.721632
9	-1.728319	2.845892	2.898985
9	-2.941565	1.409958	1.685268
9	-1.119156	0.701238	2.774044
9	-2.276931	-1.645603	1.162555
9	-4.439970	-2.192454	1.283830
9	-4.605593	-2.156251	-2.384598
9	-6.005271	-1.437726	-0.794065
9	-5.140599	0.010296	-2.260212
9	-3.121763	-3.175617	-0.232929

D" [CpW(dhpe)H₃](HFIP)₂

-1936.43828899 h

6	-0.582741	-2.215784	-0.858042
6	-1.759734	-3.004181	-0.588552
6	-2.724529	-2.707118	-1.612432
6	-2.132415	-1.745478	-2.499852
6	-0.820732	-1.460635	-2.035011
74	-2.441518	-0.835037	-0.350812
15	-1.589886	-0.900693	1.962323
6	-2.682118	0.067132	3.148888
6	-3.162509	1.368410	2.475022
15	-3.732602	0.975824	0.728292
1	-1.817140	0.710971	-0.855816
1	-3.753163	-0.188409	-1.267133
1	-3.842677	-1.463392	0.439398
1	-3.772258	2.266631	0.139917
1	-5.127835	0.781285	0.894127
1	-1.508023	-2.154742	2.638985
1	-0.298363	-0.434483	2.362725
1	-3.959760	1.851257	3.050295
1	-2.333734	2.080300	2.381518
1	-2.135615	0.276916	4.073933
1	-3.533418	-0.577853	3.395200
1	-1.865978	-3.742862	0.193020
1	-3.695383	-3.164638	-1.730034
1	-2.599234	-1.318913	-3.375955
1	-0.131656	-0.749189	-2.468611
1	0.338240	-2.223207	-0.291574
1	-0.480092	0.813097	-0.097953
8	0.388111	1.303301	0.084274
6	0.398850	2.490666	-0.666735

1	-0.510196	2.586399	-1.273225
6	0.426405	3.675791	0.293927
6	1.580089	2.445660	-1.631124
9	2.768580	2.138380	-0.976090
9	1.365403	1.462996	-2.584440
9	1.767167	3.641854	-2.298751
9	0.346299	4.886857	-0.373428
9	-0.675316	3.602741	1.140865
9	1.562289	3.693847	1.079975
1	1.633161	0.161094	0.624959
8	2.080590	-0.631661	0.987973
6	3.392152	-0.705257	0.485385
1	3.806073	0.271682	0.215928
6	4.268048	-1.269072	1.598533
6	3.400768	-1.549353	-0.788898
9	5.577230	-1.446027	1.171315
9	3.809984	-2.483909	2.070430
9	4.294718	-0.383375	2.662205
9	2.964890	-2.845859	-0.574197
9	2.536500	-0.971629	-1.715549
9	4.653134	-1.610759	-1.374945

[CpW(dhpe)H₄]⁺[(CF₃)₂CHOHOCH(CF₃)₂]⁻
-1936.43553284 h

6	-2.896651	-1.095118	-2.014126
6	-4.238425	-0.980169	-1.537416
6	-4.554105	0.407833	-1.462346
6	-3.405542	1.146917	-1.889829
6	-2.376489	0.217033	-2.226962
74	-2.824068	0.010053	0.087897
15	-1.351381	-1.974935	0.590017
6	-0.757355	-1.991902	2.360813
6	-0.502719	-0.557699	2.862413
15	-1.892826	0.567723	2.344337
1	-2.580560	1.668789	0.270661
1	-4.081002	0.726662	0.977290
1	-3.664912	-1.073177	1.133694
1	-1.358448	1.861210	2.522673

1	-2.809244	0.520377	3.426959
1	-1.956788	-3.250591	0.447535
1	-0.174631	-2.091889	-0.186534
1	-0.381546	-0.536895	3.950329
1	0.389619	-0.122538	2.398271
1	0.158554	-2.585980	2.416247
1	-1.533786	-2.489449	2.953456
1	-4.899776	-1.797824	-1.288051
1	-5.499837	0.828136	-1.152387
1	-3.333649	2.221928	-1.966927
1	-1.381000	0.468312	-2.565220
1	-2.370459	-2.019585	-2.213986
1	-1.186020	0.495884	0.005989
8	0.951345	1.206226	0.788546
6	1.410147	2.437915	0.410162
1	0.774370	3.266292	0.774106
6	2.791988	2.706467	1.028553
6	1.428968	2.609714	-1.116850
9	2.330582	1.766547	-1.749887
9	0.167735	2.327667	-1.645611
9	1.732611	3.909412	-1.511279
9	3.325537	3.945183	0.683759
9	2.693436	2.681839	2.412051
9	3.738751	1.747562	0.672514
1	1.300996	0.137441	0.068530
8	1.453141	-0.818609	-0.445153
6	2.774379	-1.233969	-0.348666
1	3.469101	-0.416753	-0.117361
6	2.901891	-2.248975	0.789272
6	3.196290	-1.810721	-1.697570
9	4.180428	-2.754269	0.954561
9	2.042329	-3.338805	0.635594
9	2.543105	-1.647378	1.996305
9	2.385489	-2.868578	-2.092726
9	3.119975	-0.842400	-2.679936
9	4.505915	-2.281337	-1.682766