Intermolecular Hydrogen Bonding Between Neutral Transition Metal Hydrides $(\eta^5\text{-}C_5H_5)M(CO)_3H$ (M = Mo, W) and Bases

Natalia V. Belkova[a], Evgenii I. Gutsul[a], Oleg A. Filippov[a], Vladislava A. Levina[a], Dmitry A. Valyaev[a], Lina M. Epstein[a], Agusti Lledos[b], Elena S. Shubina[a]*

[a] *A.N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, 28 Vavilov Str., 119991 Moscow, Russia.* [b] *Departament de Química, Edifici Cn, Universitat Autònoma de Barcelona, 08193 Bellaterra, Spain*

Supporting information

Experimental details

All manipulations were carried out under an argon atmosphere using standard Schlenk technique. The $(\eta^5\text{-}C_5H_5)Mo(CO)_3H$ and $(\eta^5\text{-}C_5H_5)W(CO)_3H$ hydrides were prepared according to the literature procedures.[1] All solvents used (CH_2Cl_2, hexane) and commercially available amines (Py, Et_3N) were freshly distilled under CaH_2 prior to use. $(n\text{-}C_8H_{17})_3PO$ purchased from ACROS and BH_3NEt_3 purchased from Fluka were used as received.

The IR measurements were performed on the Infralum FT-801 (Lumex) FTIR spectrometer or Specord M82 (Carl Zeiss Jena) spectrometer using CaF_2 cells (0.12 or 0.22 cm path length). Low temperature measurements were carried out using a cryostat (Carl Zeiss Jena) in the 200-310 K temperature range. The accuracy of the temperature adjustment was ±0.5 K. The reagents were mixed at room temperature and transferred into the cryostat.

The ν_{CO} and ν_{MH} bands of the hydrides show thermochromic behavior, shifting gradually to the lower frequencies upon cooling. The temperature drift of 2 cm^{-1} for the temperature change from 290 to 200K in hexane is accompanied by 1.4-1.7 times increase of absorption intensity.

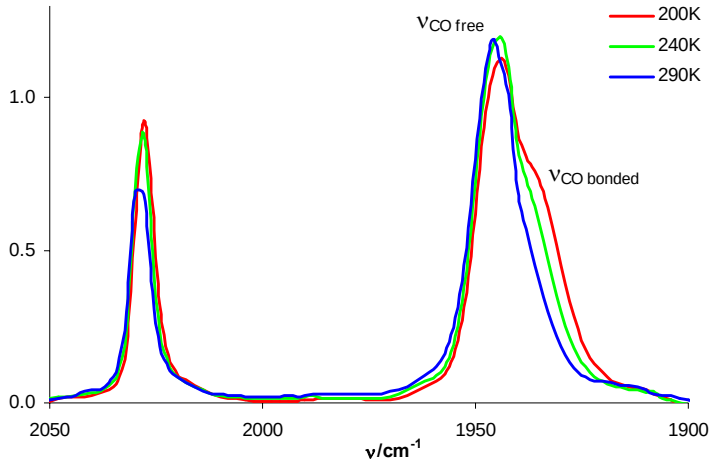

Figure S1. Variable temperature IR spectra of $CpMo(CO)_3H$ (0.001M) in hexane in the presence of 50 fold excess $(n\text{-}C_8H_{17})_3PO$.

Deprotonation of $CpMo(CO)_3H$ is complete in the neat pyridine as is evident from the absence of the ν_{CO} bands of the starting hydride. Since proton transfer from $CpM(CO)_3H$ takes place under large excess of base, other equilibrium participants (Equilibrium 1) must be considered. In particular the interaction of multiple bases with fully removed proton to give $[H(B)_n]^+$ can be envisaged.

Computational details.

Calculations were performed with the Gaussian 03[2] package at the DFT/B3LYP level.[3] As in the calculations of $CpM(CO)_3H$ (M = Mo, W) hydrides[4] and $[CpW(CO)_3H_2]^+$ [5] the effective core potentials (ECP) were used to represent the innermost electrons of the molybdenum and tungsten atoms.[6,7] The basis set for the Mo, W atoms was that associated with the pseudopotential,[7] with a standard double-ζ LANL2DZ contraction.[2] The carbon and hydrogen atoms of the Cp rings and carbon, oxygen atoms of carbonyl groups as well as the C, H, N atoms of the proton acceptor molecules were described with a 6-31G(d,p) set of basis functions.[8] Metal bound hydrogen was described with 6-311G(d,p) basis set.[9] The gas phase complexation energies were not corrected from the basis set superposition error.[10]

Frequency analyses performed showed that all the stationary points found are at least local minima.

The C_s symmetry was implied and found for free $CpM(CO)_3H$ hydrides, while no symmetry constraints were applied to $CpM(CO)_3H$·pyridine adducts.

Geometry of free $CpM(CO)_3H$ complexes obtained herein is in very good agreement with recently published results of microwave spectroscopic and DFT (B3PW91) studies.[11]

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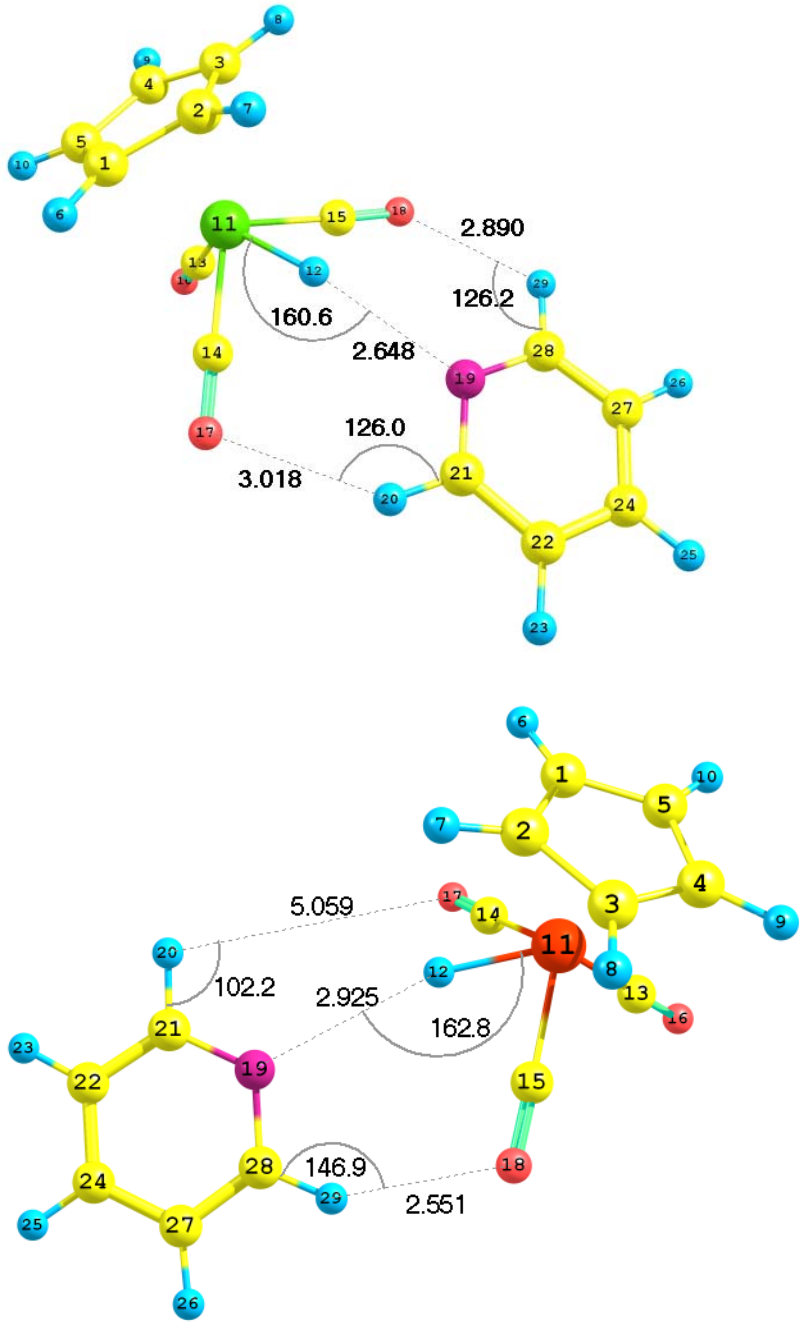

Figure S2. Optimized geometries of hydrogen bonded complexes of $CpM(CO)_3H$ (molybdenum – top, tungsten – bottom) with pyridine. Relevant distances (in Å) and angles (in degrees) are given.

Structural data (interatomic distances, R, in Å; angles, A, and dihedral angles, D, in degrees) for the optimized hydrogen bonded complexes of $CpM(CO)_3H$ with pyridine.

For atom numbering scheme see Figure S2.

Table S1. $CpMo(CO)_3H$·Pyridine

R(1,2)	1.4321	R(4,11)	2.4092	R(15,18)	1.1795
R(1,5)	1.4303	R(5,10)	1.0793	R(19,21)	1.3532
R(1,6)	1.0797	R(5,11)	2.4095	R(19,28)	1.3533
R(1,11)	2.4309	R(9,11)	3.1159	R(20,21)	1.0843
R(2,3)	1.4322	R(10,11)	3.1163	R(21,22)	1.3983
R(2,7)	1.0794	R(11,12)	1.7288	R(22,23)	1.0845
R(2,11)	2.4408	R(11,13)	1.9958	R(22,24)	1.3996
R(2,12)	2.8514	R(11,14)	1.9811	R(24,25)	1.0852
R(3,4)	1.4305	R(11,15)	1.9807	R(24,27)	1.3995
R(3,8)	1.0797	R(12,19)	2.6479	R(26,27)	1.0845
R(3,11)	2.4305	R(13,16)	1.1778	R(27,28)	1.3984
R(4,5)	1.4397	R(14,17)	1.1796	R(28,29)	1.0841
R(4,9)	1.0793				
A(2,1,5)	108.0979	A(2,11,4)	57.0789	A(10,11,12)	145.4734
A(2,1,6)	125.8017	A(2,11,5)	57.0707	A(10,11,13)	81.7966
A(5,1,6)	126.0838	A(2,11,9)	73.278	A(10,11,14)	100.4607
A(6,1,11)	121.6936	A(2,11,10)	73.264	A(10,11,15)	149.3916
A(1,2,3)	108.0507	A(2,11,13)	152.3421	A(12,11,13)	123.204
A(1,2,7)	125.9871	A(2,11,14)	112.8241	A(12,11,14)	64.0256
A(1,2,12)	93.9025	A(2,11,15)	112.9634	A(12,11,15)	63.9191
A(3,2,7)	125.9495	A(3,11,5)	57.2874	A(13,11,14)	82.945
A(3,2,12)	93.5611	A(3,11,9)	45.643	A(13,11,15)	82.9948
A(7,2,11)	121.7559	A(3,11,10)	73.4651	A(14,11,15)	103.8345
A(7,2,12)	84.6389	A(3,11,12)	102.3206	A(2,12,19)	140.8366
A(2,3,4)	108.0928	A(3,11,13)	126.6132	A(12,19,21)	120.0595
A(2,3,8)	125.8327	A(3,11,14)	147.0186	A(12,19,28)	121.6146
A(4,3,8)	126.0581	A(3,11,15)	95.0421	A(21,19,28)	118.0352
A(8,3,11)	121.6696	A(4,11,10)	45.8994	A(19,21,20)	115.9027
A(3,4,5)	107.8737	A(4,11,12)	136.5976	A(19,21,22)	122.8334
A(3,4,9)	126.0161	A(4,11,13)	96.8011	A(20,21,22)	121.2616
A(5,4,9)	126.0462	A(4,11,14)	145.4618	A(21,22,23)	120.1518
A(1,5,4)	107.8843	A(4,11,15)	110.4322	A(21,22,24)	118.7188

A(1,5,10)	126.0146	A(5,11,9)	45.9079	A(23,22,24)	121.1291
A(4,5,10)	126.0369	A(5,11,12)	136.8721	A(22,24,25)	120.5691
A(1,11,3)	56.9548	A(5,11,13)	96.6755	A(22,24,27)	118.8625
A(1,11,4)	57.2858	A(5,11,14)	110.7544	A(25,24,27)	120.568
A(1,11,9)	73.4697	A(5,11,15)	145.1245	A(24,27,26)	121.1188
A(1,11,10)	45.6313	A(9,11,10)	51.5456	A(24,27,28)	118.7391
A(1,11,12)	102.6377	A(9,11,12)	144.9893	A(26,27,28)	120.1418
A(1,11,13)	126.353	A(9,11,13)	81.9782	A(19,28,27)	122.8095
A(1,11,14)	95.1516	A(9,11,14)	149.8375	A(19,28,29)	115.8999
A(1,11,15)	147.1453	A(9,11,15)	100.0643	A(27,28,29)	121.2875

D(5,1,2,3)	0.2381	D(1,2,12,19)	-128.84	D(13,11,19,21)	-83.7832
D(5,1,2,7)	179.0019	D(3,2,12,19)	122.7738	D(13,11,19,28)	80.993
D(5,1,2,12)	-94.7938	D(7,2,12,19)	-3.0258	D(14,11,19,21)	-16.1877
D(6,1,2,3)	-178.352	D(2,3,4,5)	0.1483	D(14,11,19,28)	148.5885
D(6,1,2,7)	0.412	D(2,3,4,9)	177.3738	D(15,11,19,21)	-149.995
D(6,1,2,12)	86.6163	D(8,3,4,5)	-178.444	D(15,11,19,28)	14.7812
D(2,1,5,4)	-0.1462	D(8,3,4,9)	-1.2181	D(2,12,19,21)	94.0864
D(2,1,5,10)	-177.367	D(8,3,11,1)	159.2274	D(2,12,19,28)	-92.2284
D(6,1,5,4)	178.4386	D(8,3,11,5)	-159.577	D(12,19,21,20)	-5.1619
D(6,1,5,10)	1.2182	D(8,3,11,9)	-101.487	D(12,19,21,22)	174.2953
D(6,1,11,3)	-159.192	D(8,3,11,10)	-153.388	D(28,19,21,20)	-179.07
D(6,1,11,4)	159.601	D(8,3,11,12)	62.0423	D(28,19,21,22)	0.387
D(6,1,11,9)	153.4117	D(8,3,11,13)	-87.3429	D(12,19,28,27)	-174.223
D(6,1,11,10)	101.5193	D(8,3,11,14)	122.9017	D(12,19,28,29)	5.1407
D(6,1,11,12)	-62.5877	D(8,3,11,15)	-2.3325	D(21,19,28,27)	-0.4143
D(6,1,11,13)	86.9385	D(3,4,5,1)	-0.0013	D(21,19,28,29)	178.949
D(6,1,11,14)	1.9161	D(3,4,5,10)	177.2183	D(19,21,22,23)	-179.906
D(6,1,11,15)	-123.686	D(9,4,5,1)	-177.226	D(19,21,22,24)	-0.0804
D(1,2,3,4)	-0.2389	D(9,4,5,10)	-0.0061	D(20,21,22,23)	-0.477
D(1,2,3,8)	178.357	D(1,11,19,21)	65.9441	D(20,21,22,24)	179.3484
D(7,2,3,4)	-179.003	D(1,11,19,28)	-129.28	D(21,22,24,25)	-179.976
D(7,2,3,8)	-0.4073	D(3,11,19,21)	128.115	D(21,22,24,27)	-0.2075
D(12,2,3,4)	95.0398	D(3,11,19,28)	-67.1087	D(23,22,24,25)	-0.1519
D(12,2,3,8)	-86.3642	D(4,11,19,21)	131.4888	D(23,22,24,27)	179.6162
D(7,2,11,4)	-159.126	D(4,11,19,28)	-63.7349	D(22,24,27,26)	-179.605
D(7,2,11,5)	159.1705	D(5,11,19,21)	65.1608	D(22,24,27,28)	0.1823
D(7,2,11,9)	-152.976	D(5,11,19,28)	-130.063	D(25,24,27,26)	0.1636
D(7,2,11,10)	153.0205	D(9,11,19,21)	163.4091	D(25,24,27,28)	179.9504

D(7,2,11,13)	179.5435	D(9,11,19,28)	-31.8146	D(24,27,28,19)	0.134
D(7,2,11,14)	58.4809	D(10,11,19,21)	31.7823	D(24,27,28,29)	-179.196
D(7,2,11,15)	-58.9117	D(10,11,19,28)	-163.442	D(26,27,28,19)	179.923
				D(26,27,28,29)	0.5931

Table S2. $CpW(CO)_3H$·Pyridine

R(1,2)	1.4329	R(4,11)	2.3944	R(15,18)	1.1821
R(1,5)	1.4335	R(5,10)	1.0788	R(18,29)	2.5508
R(1,6)	1.0794	R(5,11)	2.3943	R(19,21)	1.3529
R(1,11)	2.4187	R(9,11)	3.1052	R(19,28)	1.3547
R(2,3)	1.4323	R(10,11)	3.1053	R(20,21)	1.0847
R(2,7)	1.079	R(11,12)	1.7384	R(21,22)	1.3983
R(2,11)	2.4336	R(11,13)	1.9923	R(22,23)	1.0846
R(2,12)	2.7743	R(11,14)	1.9807	R(22,24)	1.3996
R(3,4)	1.4327	R(11,15)	1.9766	R(24,25)	1.0852
R(3,8)	1.0794	R(12,15)	2.0349	R(24,27)	1.3993
R(3,11)	2.4208	R(12,19)	2.9248	R(26,27)	1.0845
R(4,5)	1.4406	R(13,16)	1.1804	R(27,28)	1.3988
R(4,9)	1.0787	R(14,17)	1.1802	R(28,29)	1.0837
A(2,1,5)	108.054	A(2,11,4)	57.4018	A(10,11,13)	81.8153
A(2,1,6)	125.8071	A(2,11,5)	57.4283	A(10,11,14)	98.1683
A(5,1,6)	126.1196	A(2,11,9)	73.587	A(10,11,15)	149.0281
A(6,1,11)	121.8965	A(2,11,10)	73.6194	A(12,11,13)	126.2238
A(1,2,3)	108.1403	A(2,11,13)	152.2437	A(12,11,14)	67.6542
A(1,2,7)	125.9859	A(2,11,14)	113.8157	A(12,11,15)	66.0628
A(1,2,12)	94.0063	A(2,11,15)	112.8812	A(13,11,14)	81.9027
A(3,2,7)	125.8708	A(3,11,5)	57.6895	A(13,11,15)	82.2099
A(3,2,12)	94.3148	A(3,11,9)	45.863	A(14,11,15)	105.6221
A(7,2,11)	121.6787	A(3,11,10)	73.8558	A(2,12,19)	121.421
A(7,2,12)	83.3801	A(3,11,12)	100.0162	A(15,18,29)	113.3652
A(2,3,4)	108.0673	A(3,11,13)	125.874	A(12,19,21)	126.284
A(2,3,8)	125.7885	A(3,11,14)	148.0624	A(12,19,28)	114.5953
A(4,3,8)	126.129	A(3,11,15)	94.6904	A(21,19,28)	117.8632
A(8,3,11)	121.8801	A(4,11,10)	46.1111	A(19,21,20)	115.9714
A(3,4,5)	107.9021	A(4,11,12)	134.4225	A(19,21,22)	123.0371
A(3,4,9)	126.0062	A(4,11,13)	96.1056	A(20,21,22)	120.9912
A(5,4,9)	126.0126	A(4,11,14)	143.7245	A(21,22,23)	120.2037
A(1,5,4)	107.8361	A(4,11,15)	109.9919	A(21,22,24)	118.6632

A(1,5,10)	126.0714	A(5,11,9)	46.1097	A(23,22,24)	121.133
A(4,5,10)	126.0163	A(5,11,12)	134.28	A(22,24,25)	120.5788
A(1,11,3)	57.2925	A(5,11,13)	96.5475	A(22,24,27)	118.8084
A(1,11,4)	57.7066	A(5,11,14)	108.9132	A(25,24,27)	120.6126
A(1,11,9)	73.8766	A(5,11,15)	144.9131	A(24,27,26)	121.1037
A(1,11,10)	45.9019	A(9,11,10)	51.7263	A(24,27,28)	118.8406
A(1,11,12)	99.8131	A(9,11,12)	143.5868	A(26,27,28)	120.0556
A(1,11,13)	126.784	A(9,11,13)	81.1694	A(19,28,27)	122.7872
A(1,11,14)	94.6062	A(9,11,14)	147.2538	A(19,28,29)	115.8845
A(1,11,15)	147.2226	A(9,11,15)	99.5918	A(27,28,29)	121.3274
		A(10,11,12)	143.336	A(18,29,28)	146.8594

D(5,1,2,3)	0.0828	D(8,3,4,5)	-178.52	D(13,11,19,21)	-121.613
D(5,1,2,7)	179.487	D(8,3,4,9)	-1.6055	D(13,11,19,28)	47.4138
D(5,1,2,12)	-95.7894	D(8,3,11,1)	159.0945	D(14,11,19,21)	-51.3882
D(6,1,2,3)	-178.397	D(8,3,11,5)	-159.551	D(14,11,19,28)	117.6389
D(6,1,2,7)	1.0069	D(8,3,11,9)	-101.51	D(15,11,19,21)	-171.62
D(6,1,2,12)	85.7305	D(8,3,11,10)	-153.366	D(15,11,19,28)	-2.5925
D(2,1,5,4)	-0.0061	D(8,3,11,12)	63.8005	D(2,12,19,21)	77.9073
D(2,1,5,10)	-176.976	D(8,3,11,13)	-86.4606	D(2,12,19,28)	-115.267
D(6,1,5,4)	178.4679	D(8,3,11,14)	127.281	D(15,18,29,28)	6.8093
D(6,1,5,10)	1.4981	D(8,3,11,15)	-2.6895	D(12,19,21,20)	-13.2388
D(6,1,11,3)	-159.12	D(3,4,5,1)	-0.0728	D(12,19,21,22)	166.5806
D(6,1,11,4)	159.5742	D(3,4,5,10)	176.8991	D(28,19,21,20)	-179.682
D(6,1,11,9)	153.4003	D(9,4,5,1)	-176.987	D(28,19,21,22)	0.1372
D(6,1,11,10)	101.5501	D(9,4,5,10)	-0.0153	D(12,19,28,27)	-168.137
D(6,1,11,12)	-63.4557	D(1,11,18,29)	66.1748	D(12,19,28,29)	11.5229
D(6,1,11,13)	87.9609	D(2,11,18,29)	65.2193	D(21,19,28,27)	-0.1305
D(6,1,11,14)	4.634	D(3,11,18,29)	95.3311	D(21,19,28,29)	179.529
D(6,1,11,15)	-123.986	D(4,11,18,29)	126.8482	D(19,21,22,23)	-179.933
D(1,2,3,4)	-0.1281	D(5,11,18,29)	128.8764	D(19,21,22,24)	-0.0369
D(1,2,3,8)	178.5219	D(9,11,18,29)	141.151	D(20,21,22,23)	-0.1225
D(7,2,3,4)	-179.533	D(10,11,18,29)	159.1724	D(20,21,22,24)	179.7737
D(7,2,3,8)	-0.8831	D(12,11,18,29)	-4.073	D(21,22,24,25)	-179.929
D(12,2,3,4)	95.5218	D(13,11,18,29)	-138.944	D(21,22,24,27)	-0.0727
D(12,2,3,8)	-85.8282	D(14,11,18,29)	-59.3825	D(23,22,24,25)	-0.034
D(7,2,11,4)	-159.011	D(1,11,19,21)	39.3133	D(23,22,24,27)	179.8225
D(7,2,11,5)	159.1528	D(1,11,19,28)	-151.66	D(22,24,27,26)	-179.814
D(7,2,11,9)	-152.871	D(3,11,19,21)	97.0469	D(22,24,27,28)	0.0786

D(7,2,11,10)	153.0354	D(3,11,19,28)	-93.926	D(25,24,27,26)	0.0428
D(7,2,11,13)	-178.269	D(4,11,19,21)	100.6521	D(25,24,27,28)	179.935
D(7,2,11,14)	61.1939	D(4,11,19,28)	-90.3208	D(24,27,28,19)	0.0243
D(7,2,11,15)	-59.1887	D(5,11,19,21)	51.4887	D(24,27,28,29)	-179.617
D(1,2,12,19)	-145.509	D(5,11,19,28)	-139.484	D(26,27,28,19)	179.9177
D(3,2,12,19)	105.932	D(9,11,19,21)	123.1346	D(26,27,28,29)	0.2763
D(7,2,12,19)	-19.7167	D(9,11,19,28)	-67.8383	D(19,28,29,18)	-14.2966
D(2,3,4,5)	0.124	D(10,11,19,21)	29.634	D(27,28,29,18)	165.3683
D(2,3,4,9)	177.0388	D(10,11,19,28)	-161.339		

Tables of the optimized geometries (Cartesian coordinates) for the calculated species

Energies in Hartries in parenthesis.

Table S3. $CpMo(CO)_3H$·Pyridine (-849.76116057800)

6	-2.555382000	-0.245226000	-2.038147000
6	-1.920505000	-1.493039000	-1.737027000
6	-2.502480000	-2.008145000	-0.534019000
6	-3.493156000	-1.078448000	-0.086313000
6	-3.525929000	0.016437000	-1.020615000
1	-2.352212000	0.375550000	-2.897891000
1	-1.152945000	-1.972448000	-2.325439000
1	-2.252781000	-2.946895000	-0.062658000
1	-4.135886000	-1.200245000	0.772187000
1	-4.197701000	0.860520000	-0.986346000
42	-1.375403000	0.060173000	0.065158000
1	0.264240000	-0.274050000	-0.369022000
6	-1.883547000	1.309694000	1.536123000
6	-0.308272000	1.610539000	-0.553037000
6	-0.250305000	-0.756990000	1.475728000
8	-2.190717000	2.045493000	2.403023000
8	0.338511000	2.499793000	-0.980065000
8	0.429376000	-1.297992000	2.273547000
7	2.911646000	-0.275535000	-0.316378000
1	3.013843000	1.286317000	-1.672425000
6	3.604364000	0.639772000	-1.032985000
6	4.994883000	0.766998000	-0.958024000

1	5.505984000	1.517396000	-1.551116000
6	5.703295000	-0.086694000	-0.104645000
1	6.782947000	-0.013864000	-0.022874000
1	5.506165000	-1.707925000	1.322366000
6	4.994913000	-1.032613000	0.645123000
6	3.604271000	-1.092446000	0.510837000
1	3.013494000	-1.800248000	1.081195000

Table S4. $CpW(CO)_3H$·Pyridine (-850.06058918900)

6	2.113276000	-2.144777000	0.466984000
6	1.163899000	-2.295100000	-0.595730000
6	1.637081000	-1.551712000	-1.724897000
6	2.879418000	-0.936672000	-1.363003000
6	3.176291000	-1.305377000	-0.002376000
1	2.049586000	-2.606283000	1.440674000
1	0.255261000	-2.875787000	-0.556765000
1	1.151737000	-1.487801000	-2.686897000
1	3.507859000	-0.347120000	-2.011870000
1	4.066270000	-1.040675000	0.546786000
74	1.206496000	0.055290000	0.033662000
1	-0.479134000	-0.256851000	0.322400000
6	2.139295000	1.799021000	0.275795000
6	0.690725000	0.388474000	1.916767000
6	-0.012834000	1.165051000	-1.056514000
8	2.707261000	2.824741000	0.412045000
8	0.382179000	0.516369000	3.048768000
8	-0.764645000	1.764890000	-1.743762000
7	-3.385885000	-0.391781000	0.027584000
1	-3.778356000	-1.864543000	1.430873000
6	-4.235197000	-1.117435000	0.790751000
6	-5.621087000	-0.932036000	0.776132000
1	-6.259541000	-1.539508000	1.408337000
6	-6.158292000	0.049129000	-0.065009000
1	-7.229363000	0.220064000	-0.100141000
1	-5.665053000	1.579329000	-1.520087000
6	-5.289316000	0.807499000	-0.857331000
6	-3.915171000	0.556930000	-0.781760000
1	-3.205675000	1.124194000	-1.372673000

Table S5. $CpMo(CO)_3H$ (-601.54097773000)

6	-0.123942000	-2.063774000	1.159679000
6	-0.946888000	-2.235441000	0.000000000
6	-0.123942000	-2.063774000	-1.159679000
6	1.207305000	-1.778501000	-0.720258000
6	1.207305000	-1.778501000	0.720258000
1	-0.448839000	-2.159026000	2.184835000
1	-1.998302000	-2.479336000	0.000000000
1	-0.448839000	-2.159026000	-2.184835000
1	2.069036000	-1.639734000	-1.355323000
1	2.069036000	-1.639734000	1.355323000
42	-0.149384000	0.068115000	0.000000000
1	-1.836706000	0.420639000	0.000000000
6	1.334396000	1.411713000	0.000000000
6	-0.724167000	1.114308000	1.590351000
6	-0.724167000	1.114308000	-1.590351000
8	2.211758000	2.195072000	0.000000000
8	-1.091296000	1.682049000	2.553576000
8	-1.091296000	1.682049000	-2.553576000

Table S6. $CpW(CO)_3H$ (-601.84056048700)

6	-0.077591000	-2.070951000	1.160693000
6	-0.896332000	-2.258679000	0.000000000
6	-0.077591000	-2.070951000	-1.160693000
6	1.251745000	-1.764614000	-0.721052000
6	1.251745000	-1.764614000	0.721052000
1	-0.401427000	-2.171466000	2.185420000
1	-1.944924000	-2.513465000	0.000000000
1	-0.401427000	-2.171466000	-2.185420000
1	2.111342000	-1.616704000	-1.356464000
1	2.111342000	-1.616704000	1.356464000
74	-0.123181000	0.051082000	0.000000000
1	-1.832874000	0.349398000	0.000000000
6	1.337053000	1.410569000	0.000000000
6	-0.686005000	1.090272000	1.593168000
6	-0.686005000	1.090272000	-1.593168000
8	2.211389000	2.201936000	0.000000000
8	-1.044992000	1.648563000	2.568113000
8	-1.044992000	1.648563000	-2.568113000

Table S7. Pyridine (-248.21617745700)

6	0.000000000	1.157650000	0.723589000
6	0.000000000	1.204659000	-0.674563000
6	0.000000000	0.000000000	-1.386934000
6	0.000000000	-1.204659000	-0.674563000
6	0.000000000	-1.157650000	0.723589000
7	0.000000000	0.000000000	1.422453000
1	0.000000000	2.068857000	1.312758000
1	0.000000000	2.159723000	-1.188646000
1	0.000000000	0.000000000	-2.472107000
1	0.000000000	-2.159723000	-1.188646000
1	0.000000000	-2.068857000	1.312758000