

## Hydrogen bonding to carbonyl hydride complex $\text{Cp}^*\text{Mo}(\text{PMe}_3)_2(\text{CO})\text{H}$ and its role in proton transfer

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### Supplementary information

**Table S1.** Selected NMR (500 MHz) and IR data for  $\text{Cp}^*\text{MoH}(\text{PMe}_3)_2(\text{CO})$  in different solvents.

**Figure S1.** Potential energy curves for the proton transfer from  $\text{CF}_3\text{COOH}$  to **1** starting from the dihydrogen bonded complexes **B** (top) and **D** (bottom).

**Figure S2.** NMR spectra (hydride region on the left, phosphorus on the right) of  $\text{Cp}^*\text{MoH}(\text{PMe}_3)_2(\text{CO})$  in the presence of increasing amount of  $\text{CF}_3\text{COOH}$

**Figure S3.** IR spectra ( $\nu_{\text{CO}}$  region) of  $\text{Cp}^*\text{Mo}(\text{PMe}_3)_2(\text{CO})\text{H}$  (**1**, 0.07 M) at 200 K (a) and 250 K (b), and **1** in the presence of 5 equiv. PFTB at 200K (c), 230K (d), 250K (e).

**Figure S4.**  $^1\text{H}$  NMR (500.3 MHz) spectrum (hydride region) of **1** (a), and of **1** in the presence of 3 equiv (b) or 5 equiv PFTB (c). 200K, toluene- $d_8$ .

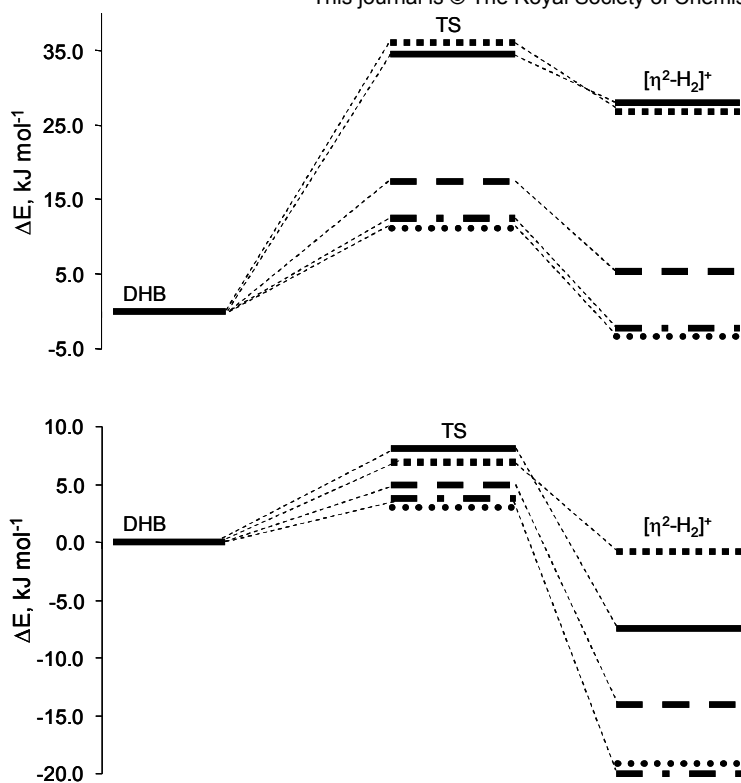
**Table S2.** Geometrical parameters (distances in Å, angles in degrees) for H-complexes between  $\text{Cp}^*\text{MoH}(\text{PMe}_3)_2(\text{CO})$  and proton donors.

**Table S3.** XYZ coordinates for all the optimized geometries

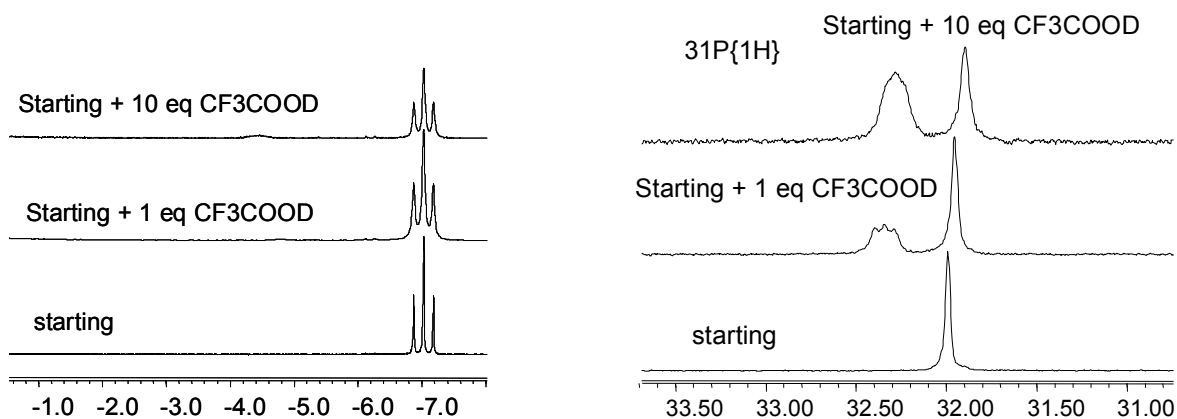
**Table S1.** Selected NMR (500 MHz) and IR data for compound **1** in different solvents.

T		toluene	CH <sub>2</sub> Cl <sub>2</sub> <sup>a</sup>	THF	hexane
200K	<sup>1</sup> H NMR/ppm	-6.85 (t, <sup>2</sup> J <sub>HP</sub> = 77Hz, 1H, MoH), 1.34 (d, <sup>2</sup> J <sub>P-H</sub> = 8 Hz, 18H), 1.96 (s, 15H, Cp*)	-6.98 (t, <sup>2</sup> J <sub>HP</sub> = 77Hz, 1H, MoH), 1.31 (d, <sup>2</sup> J <sub>P-H</sub> = 8 Hz, 18H), 1.89 (s, 15H, Cp*)	-7.03 (t, <sup>2</sup> J <sub>HP</sub> = 77Hz, 1H, MoH), 1.38 (d, <sup>2</sup> J <sub>P-H</sub> = 8 Hz, 18H), 1.95 (s, 15H, Cp*)	
	<sup>31</sup> P{ <sup>1</sup> H} NMR/ppm	31.9 (s)	31.4 (s)	32.0 (s)	
	<sup>13</sup> C{ <sup>1</sup> H} NMR/ppm	253.0 (t, <sup>2</sup> J <sub>CP</sub> = 28 Hz, <sup>13</sup> CO)	255.0 (t, <sup>2</sup> J <sub>CP</sub> = 28 Hz, <sup>13</sup> CO)	252.4 (t, <sup>2</sup> J <sub>CP</sub> = 28 Hz, <sup>13</sup> CO)	
	ν <sub>CO</sub> IR (ε/M <sup>-1</sup> ·cm <sup>-1</sup> )	1771 (1890)	1751 (1250)	1776 (2400)	1796 (3740)
298K	<sup>1</sup> H NMR/ppm	-6.88 (t, <sup>2</sup> J <sub>HP</sub> = 78Hz, H), 1.33 (d, <sup>2</sup> J <sub>P-H</sub> = 8 Hz, 18H), 1.93 (s, Cp*)			
	<sup>31</sup> P{ <sup>1</sup> H} NMR/ppm	30.3 (s)			
	<sup>13</sup> C{ <sup>1</sup> H} NMR/ppm	252.7 (vt, <sup>2</sup> J <sub>CP</sub> = 29 Hz, <sup>13</sup> CO)			
	ν <sub>CO</sub> IR (ε/M <sup>-1</sup> ·cm <sup>-1</sup> )	1778 (1060)		1788 (1556)	1800 (2253)
	[dv/dT] / cm <sup>-1</sup> K <sup>-1</sup> [dε/dT] / cm <sup>-1</sup> K <sup>-1</sup>	7.9·10 <sup>-2</sup> -8.7		1.2·10 <sup>-1</sup> -8.7	4.0·10 <sup>-2</sup> -14.7

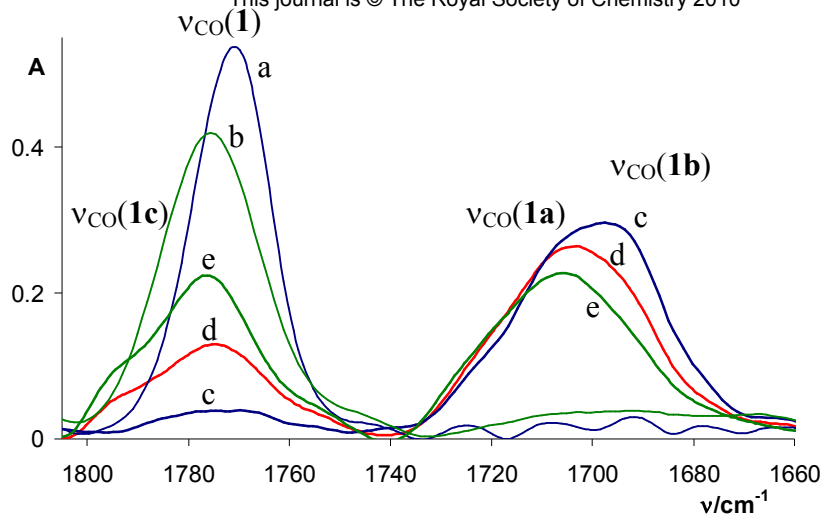
<sup>a</sup> complex **1** is not stable in this solvent at ambient temperatures and very slowly evolves into Cl-derivative.



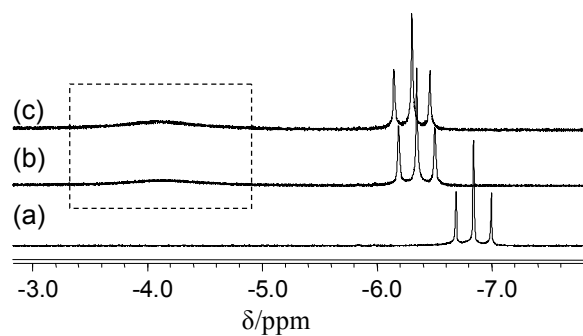
**Figure S1.** Potential energy curves for the proton transfer from  $\text{CF}_3\text{COOH}$  to **1** starting from the dihydrogen bonded complexes **B** (top) and **D** (bottom). Solid line -  $\Delta E$  gas phase, square dot -  $\Delta G$  gas phase, dash -  $\Delta G^{\text{solv}}$  toluene, dash dot -  $\Delta G^{\text{solv}}$   $\text{CH}_2\text{Cl}_2$ , dot -  $\Delta G^{\text{solv}}$  THF. Single point CPCM calculations.



**Figure S2.** NMR spectra (hydride region on the left, phosphorus on the right) of  $\text{Cp}^*\text{MoH}(\text{PMe}_3)_2(\text{CO})$  in the presence of increasing amounts of  $\text{CF}_3\text{COOH}$ .



**Figure S3.** IR spectra ( $\nu_{\text{CO}}$  region) of  $\text{Cp}^*\text{Mo}(\text{PMe}_3)_2(\text{CO})\text{H}$  (**1**, 0.07 M) at 200 K (a) and 250 K (b), and **1** in the presence of 5 equiv. PFTB at 200K (c), 230K (d), 250K (e). Toluene,  $l = 0.04$  cm.



**Figure S4.**  $^1\text{H}$  NMR (500.3 MHz) spectrum (hydride region) of **1** (a), and of **1** in the presence of 3 equiv (b) or 5 equiv PFTB (c). 200K, toluene- $d_8$ .

**Table S2.** Geometrical parameters (distances in Å, angles in degrees) for H-complexes between **1** and proton donors.

Proton donor	H-complex notation	H-bond type	d(H...H)	d(Mo...H)	d(CO...H)	$\Delta$ d(OH)	H...HO	Mo...HO	CO...HO
CH <sub>3</sub> OH	<b>A</b>	CO...HOR			1.912	0.007			168.7
	<b>B</b>	H...HOR	1.694	3.245		0.012	170.4	169.0	
2CH <sub>3</sub> OH	<b>C</b>	CO...(HOR) <sub>2</sub>			1.860	0.036			176.1
	<b>D</b>	H...(HOR) <sub>2</sub>							
	<b>E</b>	CO...HO & H...HO	1.625	3.159	1.917	0.007 & 0.011	170.9	167.8	167.6
CF <sub>3</sub> OH	<b>A</b>	CO...HOR			1.615	0.029			179.3
	<b>B</b>	H...HOR	1.777	2.905		0.054	171.4	163.2	
CF <sub>3</sub> COOH	<b>A</b>	CO...HOR			1.638	0.028			170.4
	<b>B</b>	H...HOR	1.365	3.000		0.048	177.7	163.2	
2CF <sub>3</sub> COOH	<b>C</b>	CO...(HOR) <sub>2</sub>							
	<b>D</b>	H...(HOR) <sub>2</sub>	1.283	2.867		0.073	175.4	158.3	
	<b>E</b>	CO...HO & H...HO	1.391	2.981	1.660	0.025 & 0.043	176.8	161.3	170.8

**Table S3. XYZ coordinates for all the optimized geometries**

**a. free reactants**

1. **Cp\*MoH (CO) (PMe<sub>3</sub>)<sub>2</sub>** E = -824.080464629

6	-1.699568000	-1.411627000	0.196502000
6	-1.050375000	-1.376007000	1.478522000
6	0.362707000	-1.257838000	1.249614000
6	0.587838000	-1.211520000	-0.162168000
6	-0.681686000	-1.315203000	-0.812271000
42	-0.769090000	0.763660000	0.470782000
15	-1.545652000	2.066590000	-1.450013000
15	0.267180000	2.162880000	2.188121000
1	0.412072000	1.897995000	-0.139318000
6	-2.344021000	1.580188000	1.235699000
8	-3.325673000	2.045437000	1.713957000
1	0.379024000	4.510388000	2.971999000
6	-1.766600000	3.898790000	-1.210591000
1	0.279345000	4.402159000	1.192962000
6	-0.095696000	3.987815000	2.132994000
6	1.933202000	-1.216138000	-0.842413000
1	2.682736000	-0.670632000	-0.260469000
1	2.306459000	-2.241959000	-0.980348000
1	1.887658000	-0.748928000	-1.831215000
6	1.437019000	-1.430790000	2.291917000
1	1.144973000	-1.022246000	3.264053000
1	1.651079000	-2.498923000	2.445742000
1	2.376803000	-0.955896000	1.993680000
6	-1.711716000	-1.656039000	2.804162000
1	-2.743125000	-1.290957000	2.824782000
1	-1.739682000	-2.736372000	3.012881000
1	-1.181453000	-1.177255000	3.633029000
6	-3.153066000	-1.733189000	-0.042918000
1	-3.514179000	-1.307896000	-0.984454000
1	-3.316043000	-2.820696000	-0.090363000
1	-3.788812000	-1.340367000	0.756431000
6	-0.887440000	-1.551460000	-2.286354000
1	-0.084774000	-1.112614000	-2.887048000
1	-0.898882000	-2.629899000	-2.503067000
1	-1.837917000	-1.144478000	-2.644489000
1	-0.807117000	4.346258000	-0.936640000
1	-1.177609000	4.143966000	-2.176502000
6	-0.178800000	1.817279000	3.968534000
1	0.320656000	2.516159000	4.650026000
1	-1.263137000	1.911745000	4.086609000
1	0.107676000	0.795780000	4.237164000
6	2.128125000	2.223018000	2.306966000
1	2.449653000	2.913731000	3.095581000
1	2.525821000	1.227712000	2.524419000
1	2.534073000	2.554351000	1.346126000
6	-3.222148000	1.648077000	-2.156801000
1	-3.478826000	2.306138000	-2.995431000
1	-3.234676000	0.610609000	-2.503927000
1	-3.975559000	1.755473000	-1.369736000
6	-0.509687000	2.074830000	-3.001324000
1	-0.957180000	2.710920000	-3.774347000
1	0.489544000	2.448208000	-2.756303000
1	-0.411428000	1.058123000	-3.392321000
1	-2.139040000	4.374324000	-2.125780000
1	-2.478144000	4.074908000	-0.398001000

2. **CH<sub>3</sub>OH** E = -115.713492021

8	0.759809000	0.121939000	-0.000002000
1	1.156143000	-0.758486000	0.000031000
6	-0.679629000	-0.020512000	-0.000003000
1	-1.082714000	0.993875000	-0.000354000
1	-1.037035000	-0.544235000	-0.895842000
1	-1.037091000	-0.543600000	0.896195000

3. **CF<sub>3</sub>OH** E = -413.382341244

8	-1.182580000	0.699312000	0.003810000
1	-1.918502000	0.066778000	0.004428000
6	-0.012063000	0.031488000	0.000078000
9	1.015217000	0.939704000	-0.004613000
9	0.132869000	-0.793753000	1.114805000
9	0.124306000	-0.795973000	-1.114123000

4. **CF<sub>3</sub>COOH** E = -526.692246015

1	-2.491064000	-0.920180000	0.000070000
8	-1.525823000	-1.046975000	-0.000038000
8	-1.497266000	1.237559000	-0.000036000
6	-0.941044000	0.166836000	-0.000091000
6	0.584132000	0.000025000	-0.000033000
9	0.997894000	-0.702835000	-1.120616000

9	0.997897000	-0.700509000	1.122048000
9	1.206124000	1.224938000	-0.001291000

**b. hydrogen bonded complexes**

5. **[Cp\*Mo (CO) (PMe<sub>3</sub>)<sub>2</sub>H] · CF<sub>3</sub>OH (B)** E = -1237.48594451

6	2.698215000	0.714322000	0.892139000
6	2.697047000	-0.723676000	0.888967000
6	1.651943000	-1.162412000	1.773007000
6	1.006705000	-0.006603000	2.314889000
6	1.653750000	1.150680000	1.778355000
42	0.701217000	-0.000278000	-0.152133000
15	-0.224517000	-2.004869000	-1.081763000
15	-0.235022000	-2.099031000	-1.087217000
1	-1.074946000	0.005455000	-0.109224000
6	1.440394000	-0.000399000	-1.933915000
8	1.954080000	-0.000621000	-3.001852000
1	-1.650593000	-2.883191000	-2.953617000
6	-1.305467000	1.922577000	-2.581643000
1	-2.195165000	-1.309638000	-2.313545000
6	-1.319225000	-1.906019000	-2.583299000
6	-0.048167000	-0.004816700	-3.391108000
1	-0.696363000	-0.886929000	3.327609000
1	0.412045000	-0.010719000	4.390265000
1	-0.694960000	0.871910000	3.331478000
6	1.446709000	-2.573904000	2.258608000
1	1.662585000	-3.317901000	1.485726000
1	2.118072000	-2.785939000	3.103584000
1	0.424185000	-2.739195000	2.611214000
6	3.768223000	-1.591940000	0.279775000
1	4.125396000	-1.186594000	-0.671833000
1	4.636016000	-1.672460000	0.951391000
1	3.409601000	-2.607510000	0.089233000
6	3.771013000	1.583264000	0.286888000
1	3.414014000	2.600077000	0.100204000
1	4.638718000	1.659730000	0.959088000
1	4.127810000	1.181054000	-0.666192000
6	1.450573000	2.560106000	2.270807000
1	0.426990000	2.726672000	2.619772000
1	2.118797000	2.765618000	3.119881000
1	1.672117000	3.307561000	1.502908000
1	-2.182791000	1.325002000	-2.318687000
1	-0.767374000	-1.388156000	-3.372899000
6	0.989896000	-3.355641000	-1.713818000
1	0.476106000	-4.201470000	-2.187432000
1	1.655772000	-2.883398000	-2.442518000
1	1.597146000	-3.734036000	-0.885853000
6	-1.331916000	-3.181030000	-0.040255000
1	-1.620608000	-4.081342000	-0.595535000
1	-0.813528000	-3.479774000	0.873998000
1	-2.235552000	-2.630391000	0.230833000
6	1.005215000	3.360661000	-1.700896000
1	0.494454000	4.204740000	-2.178525000
1	1.606688000	3.740072000	-0.869192000
1	1.675987000	2.888029000	-2.424817000
6	-1.319786000	3.185919000	-0.032272000
1	-1.601824000	4.091345000	-0.582608000
1	-2.227086000	2.638081000	0.232121000
1	-0.802764000	3.475651000	0.885643000
1	-1.634731000	2.902385000	-2.946401000
1	-0.752119000	1.409271000	-3.373324000
1	-2.020984000	-0.002159000	0.863323000
8	-2.836471000	-0.007629000	1.482547000
6	-3.954749000	0.002430000	0.784077000
9	-5.053877000	-0.007479000	1.619625000
9	-4.084545000	1.128541000	-0.056611000
9	-4.086271000	-1.101396000	-0.085513000

6. **[Cp\*MoH (PMe<sub>3</sub>)<sub>2</sub> (CO)] · CF<sub>3</sub>OH (A) · E** = -1237.48653197

6	-2.209999000	0.679475000	1.761467000
6	-2.183232000	-0.755995000	1.751003000
6	-2.910616000	-1.198614000	0.594068000
6	-3.379366000	-0.046599000	-0.113018000
6	-2.953733000	1.115870000	0.610962000
42	-0.892168000	-0.000468000	-0.106405000
15	0.021389000	2.078125000	-1.046609000
15	0.098627000	-2.031527000	-1.073280000
1	-0.708522000	0.014107000	-1.844722000
6	0.761014000	0.025664000	0.826513000
8	1.744011000	0.042693000	1.521674000
1	2.042935000	-2.788703000	-2.385588000
6	1.616352000	1.938487000	-1.986182000
1	1.533154000	-1.140630000	-2.843810000
6	1.691380000	-1.822806000	-2.003928000

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6	-4.297411000	-0.054937000	-1.309058000	1	2.032356000	4.058260000	0.228927000
1	-4.125532000	-0.928560000	-1.945384000	1	0.700956000	3.539846000	1.289496000
1	-5.352847000	-0.076653000	-0.999815000	1	2.193640000	2.589207000	1.235828000
1	-4.158186000	0.833570000	-0.132664000	6	0.281998000	-3.351270000	-1.738266000
6	-3.339635000	-2.618364000	0.329776000	1	0.984992000	-4.163260000	-1.960368000
1	-2.560530000	-3.344204000	0.582032000	1	-0.554569000	-3.756669000	-1.161176000
1	-4.219831000	-2.868546000	0.939814000	1	-0.111868000	-2.949443000	-2.677044000
1	-3.620335000	-2.772163000	-0.716117000	6	1.923987000	-2.953606000	0.580882000
6	-1.686282000	-1.632880000	2.871531000	1	2.579668000	-3.730604000	0.170285000
1	-0.824577000	-1.189160000	3.379012000	1	2.507322000	-2.280139000	1.215677000
1	-2.470402000	-1.790111000	3.627307000	1	1.162795000	-3.430504000	1.204719000
1	-1.379631000	-2.618931000	2.510094000	1	3.104894000	-2.612740000	-2.108028000
6	-1.746078000	1.557881000	2.894888000	1	2.240553000	-1.224056000	-2.826185000
1	-1.471732000	2.558335000	2.547325000	1	2.256821000	0.106683000	1.839120000
1	-2.537130000	1.678565000	3.650149000	8	2.887023000	0.097791000	2.587117000
1	-0.871346000	1.136672000	3.399255000	6	4.217793000	0.275362000	2.066957000
6	-3.435768000	2.518074000	0.368246000	1	4.894770000	0.239980000	2.924106000
1	-3.724207000	2.676678000	-0.674798000	1	4.497863000	-0.524252000	1.366662000
1	-4.323419000	2.726100000	0.983298000	1	4.339051000	1.245876000	1.565526000
1	-2.683786000	3.268669000	0.630261000				
1	1.474151000	1.272999000	-2.842262000				
1	2.458901000	-1.400466000	-1.350863000				
6	0.591874000	-3.392710000	0.103076000	6	-1.883245000	0.717150000	1.636568000
1	1.065453000	-4.225402000	-0.429969000	6	-1.882139000	-0.719693000	1.636180000
1	1.297477000	-2.988973000	0.836240000	6	-2.493776000	-1.157169000	0.412732000
1	-0.282955000	-3.769389000	0.641999000	6	-2.862548000	-0.001443000	-0.344746000
6	-0.881872000	-2.988849000	-2.336907000	6	-2.495307000	1.154447000	0.413306000
1	-0.292242000	-3.823126000	-2.734827000	42	-0.389399000	0.000133000	-0.079587000
1	-1.797838000	-3.386852000	-1.892228000	15	0.683581000	2.034937000	-0.932933000
1	-1.155720000	-2.316907000	-3.156275000	15	0.685782000	-2.033235000	-0.933639000
6	0.470555000	3.439953000	0.146538000	1	-0.077597000	0.000464000	-1.795391000
1	0.916441000	4.293956000	-0.376584000	6	1.184167000	0.000520000	1.009058000
1	-0.416024000	3.781679000	0.689501000	8	2.128079000	0.000414000	1.744202000
1	1.189037000	3.050914000	0.875081000	1	2.776211000	-2.835140000	-1.972094000
6	-0.997641000	3.017735000	-2.292757000	6	2.388659000	1.863691000	-1.651338000
1	-0.440098000	3.878604000	-2.680131000	1	2.345591000	-1.194554000	-2.521990000
1	-1.250176000	2.348432000	-3.121087000	6	2.389538000	-1.859284000	-1.654477000
1	-1.925618000	3.375254000	-1.838647000	6	-3.648409000	-0.001543000	-1.631473000
1	1.938977000	2.922934000	-2.345355000	1	-3.426282000	-0.882675000	-2.241693000
1	2.397642000	1.521118000	-1.346351000	1	-4.731148000	-0.002196000	-1.435895000
1	3.351295000	0.081292000	1.675194000	1	-3.427300000	0.880224000	-2.241149000
8	4.344565000	0.103312000	1.781414000	6	-2.913695000	-2.570653000	0.100827000
6	4.936440000	0.014481000	0.606503000	1	-2.213268000	-3.210563000	0.500423000
9	6.307071000	0.034741000	0.749968000	1	-3.895392000	-2.785153000	0.548516000
9	4.609423000	-1.163032000	-0.098415000	1	-3.008148000	-2.742787000	-0.975817000
9	4.596120000	1.062962000	-0.274047999	6	-1.525879000	-1.525879000	-2.810912000
				1	-0.707986000	-1.167244000	3.398494000
				1	-2.386486000	-1.721296000	3.485211000
				1	-1.211130000	-2.493837000	2.493837000
				6	-1.527968000	1.592372000	2.811891000
6	-2.413349000	-0.904388000	0.210928000	6	-1.216007000	2.592586000	2.495713000
6	-2.527007000	0.528259000	0.214983000	1	-2.388262000	1.715590000	3.487134000
6	-1.813227000	1.020043000	1.361234000	1	-0.708513000	1.165781000	3.398286000
6	-1.256647000	-0.097287000	2.059880000	1	-2.917449000	2.567480000	0.101937000
6	-1.630742000	-1.284268000	1.355000000	1	-3.008754000	2.740914000	-0.974758000
42	-0.255903000	-0.014005000	-0.210624000	1	-3.901136000	2.779011000	0.546641000
15	1.110174000	-1.978692000	-0.785861000	1	-2.220048000	3.300300000	0.504994000
15	0.802575000	2.141433000	-0.740822000	1	2.347524000	1.197404000	-2.517768000
1	1.397384000	0.109659000	0.379855000	1	3.076078000	-1.424219000	-0.922101000
6	-0.413129000	-0.007160000	-1.234922000	6	0.988001000	-3.419632000	-0.279028000
8	-0.557211000	-0.006052000	-3.312620000	1	1.503963000	-4.261376000	-0.197646000
1	2.653874000	3.092738000	-2.081940000	1	1.601427000	-3.042450000	1.103711000
6	2.577822000	-1.676778000	-1.888351000	1	0.038228000	-3.774252000	0.691433000
1	3.071001000	1.495029000	-1.401663000	6	-0.144275000	-2.958602000	-2.323392000
6	2.278553000	2.084115000	-1.871960000	1	0.453741000	-3.824199000	-2.632210000
6	-0.550958000	-0.047048000	3.390854000	1	-1.133642000	-3.304247000	-2.013042000
1	-0.000504000	0.888226000	3.526975000	1	-0.266425000	-2.281155000	-3.174344000
1	-1.270126000	-0.129740000	4.219611000	1	0.981608000	3.422008000	0.279905000
1	0.173609000	-0.858780000	3.502090000	6	1.495788000	4.265141000	-0.196225000
6	-1.862623000	2.431840000	1.886140000	1	0.030610000	3.774121000	0.691565000
1	-1.912174000	3.172970000	1.082304000	1	1.595333000	3.046197000	1.104998000
1	-2.757128000	2.575944000	2.509912000	6	-0.146558000	2.958163000	-2.323981000
1	-0.994787000	2.666327000	2.510158000	1	0.448067000	3.827090000	-2.629971000
6	-3.442457000	1.331183000	-0.674330000	1	-0.262942000	2.281179000	-3.176106000
1	-3.485101000	0.919033000	-1.687215000	1	-1.138540000	3.298250000	-2.015900000
1	-4.468855000	1.338238000	-0.277281000	1	2.773817000	2.839826000	-1.969924000
1	-3.120427000	2.373514000	-0.758775000	1	3.074974000	1.431135000	-0.917243000
6	-3.189692000	-1.837956000	-0.682808000	1	3.925099000	0.000633000	1.090787000
1	-2.698162000	-2.810479000	-0.780731000	6	4.756821000	0.001749000	0.585368000
1	-4.197976000	-2.020653000	-0.281292000	8	5.858637000	0.000159000	1.514302000
1	-3.306402000	-1.427951000	-1.690715000	6	6.773565000	0.001673000	0.916728000
6	-1.467767000	-2.687350000	1.878681000	1	5.853700000	0.893208000	2.153878000
1	-0.578798000	-2.784632000	2.508380000	1	5.854237000	-0.895581000	2.150144000
1	-2.334260000	-2.965947000	2.496450000				
1	-1.398359000	-3.427836000	1.075874000				
1	3.264351000	-0.982974000	-1.394949000				
1	1.996240000	1.599812000	-2.811373000				
6	-0.232016000	3.407928000	-1.639228000	6	1.242805000	-2.258152000	-0.765124000
1	0.346206000	4.314120000	-1.854752000	6	1.876414000	-1.278017000	-1.604215000
1	-0.588614000	2.974436000	-2.578993000	6	0.842757000	-0.573803000	-2.309689000
1	-1.102586000	3.678852000	-1.033922000	6	-0.422156000	-1.107691000	-1.909360000
6	1.502886000	3.188150000	0.635144000	6	-0.178364000	-2.148768000	-0.959352000

8. [Cp\*MoH (PMe<sub>3</sub>)<sub>2</sub>(CO)] · CH<sub>3</sub>OH (A) · E = -939.803648099

7. [Cp\*Mo(CO) (PMe<sub>3</sub>)<sub>2</sub>H] · CH<sub>3</sub>OH (B) E = -939.801647124

9. [Cp\*Mo(CO) (PMe<sub>3</sub>)<sub>2</sub>H] · (CH<sub>3</sub>OH)<sub>2</sub> (D) E = -1055.52783486

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42	0.680524000	-0.123549000	0.091906000	1	-1.456225000	1.387214000	-3.232551000
15	-0.390753000	-0.653822000	2.254046000	6	1.476248000	-1.437048000	-2.173314000
15	1.298443000	2.240448000	-0.202133000	1	2.141789000	-1.856411000	-1.414269000
1	-0.663451000	0.963668000	0.453005000	1	1.571629000	-2.059933000	-3.075556000
6	2.188416000	0.007633000	1.290785000	1	1.865376000	-0.444743000	-2.419244000
8	3.139306000	0.050511000	1.998765000	6	-0.016479000	-3.595740000	-0.342779000
1	1.555392000	4.337320000	1.090831000	1	-0.510132000	-3.937557000	0.572386000
6	-0.234993000	0.642958000	3.578989000	1	-0.113770000	-4.404928000	-1.081499000
1	0.230479000	3.319941000	1.722916000	1	1.050547000	-3.483119000	-0.132746000
6	1.247215000	3.310193000	1.319960000	1	-0.092170000	1.020980000	3.759891000
6	-1.756523000	-0.768159000	-2.521993000	1	-0.652202000	3.269913000	1.872794000
1	-1.805438000	0.277904000	-2.840239000	6	-2.240738000	3.181000000	-0.798145000
1	-1.943063000	-1.389319000	-3.411262000	1	-2.836019000	4.047450000	-0.486366000
1	-2.583550000	-0.937251000	-1.826450000	1	-1.220046000	3.505055000	-1.025158000
6	1.058646000	0.368209000	-3.465740000	1	-2.678021000	2.760841000	-1.709252000
1	1.959723000	0.977285000	-3.344166000	6	-3.987994000	1.660895000	0.904357000
1	1.179866000	-0.198584000	-4.400705000	1	-4.469883000	2.624629000	1.107309000
1	0.208954000	1.042523000	-3.607834000	1	-4.487408000	1.186902000	0.055051000
6	3.356310000	-1.185406000	-1.875986000	1	-1.096779000	1.009104000	1.776866000
1	3.945736000	-1.426760000	-0.986277000	6	2.240074000	-1.442059000	1.839558000
1	3.654631000	-1.886459000	-2.670178000	1	2.743407000	-1.612094000	2.798949000
1	3.649853000	-0.182475000	-2.200575000	1	2.203497000	-2.388764000	1.293146000
6	1.954762000	-3.365783000	-0.030691000	1	2.830774000	-0.741323000	1.242727000
1	1.364992000	-3.741567000	0.810027000	6	-0.194695000	-2.114574000	3.198497000
1	2.150758000	-4.217545000	-0.699364000	1	0.489595000	-2.359920000	4.020513000
1	2.917637000	-3.032240000	0.367932000	1	-1.148751000	-1.767950000	3.607431000
6	-1.213155000	-3.129198000	-0.470584000	1	-0.380631000	-3.019745000	2.613208000
1	-2.207752000	-2.677614000	-0.412164000	1	1.448707000	0.126506000	4.203062000
1	-1.284791000	-3.981749000	-1.162219000	1	1.401678000	1.354095000	2.907117000
1	-0.965826000	-3.538941000	0.513663000	1	3.240837000	2.053079000	-0.236459000
1	-0.707353000	1.568085000	3.236314000	8	4.196302000	2.002960000	-0.430738000
1	1.917053000	2.894106000	2.078472000	1	4.191385000	3.880413000	-1.379290000
6	3.030690000	2.616189000	-0.783095000	1	3.935911000	2.482980000	-2.469657000
1	3.210413000	3.697155000	-0.819073000	6	4.468546000	2.838274000	-1.578898000
1	3.745933000	2.154427000	-0.095184000	1	5.544353000	2.784915000	-1.761103000
1	3.194517000	2.198122000	-1.781171000	1	4.664495000	0.248251000	-0.586463000
6	0.309657000	3.303600000	-1.373609000	8	4.903965000	-0.700662000	-0.637590000
1	0.648129000	4.345938000	-1.337775000	6	6.253559000	-0.849118000	-0.163519000
1	0.418564000	2.932858000	-2.396316000	1	6.973683000	-0.312366000	-0.797850000
1	-0.750204000	3.254719000	-1.106795000	1	6.489550000	-1.916308000	-0.199437000
6	0.262203000	-2.133479000	3.181414000	1	6.366033000	-0.498658000	0.872045000
1	-0.221002000	-2.230917000	4.160600000				
1	0.079589000	-3.046048000	2.606017000	11. [Cp*MoH (PMe <sub>3</sub> ) <sub>2</sub> (CO)] · (CH <sub>3</sub> OH) <sub>2</sub> (E) E =	-1055.52476928		
1	1.342115000	-2.022211000	3.319521000				
6	-2.222274000	-0.982625000	2.335502000	6	-1.622965000	-2.242838000	-0.125023000
1	-2.533708000	-1.177393000	3.368718000	6	-1.603232000	-1.702910000	-1.456483000
1	-2.774102000	-0.120988000	1.950378000	6	-2.340532000	-0.468777000	-1.437838000
1	-2.487188000	-1.844440000	1.718413000	6	-2.809895000	-0.243597000	-0.105761000
1	-0.712670000	0.316218000	4.510212000	6	-2.372925000	-1.340306000	0.702352000
1	0.823886000	0.843033000	3.767520000	42	-0.320159000	-0.252110000	-0.084599000
1	-2.121305000	1.410365000	-0.098297000	15	0.599249000	-0.114641000	2.198292000
8	-3.015554000	1.762752000	-0.308298000	15	0.738190000	1.295768000	-1.693422000
1	-2.663242000	3.573327000	0.709882000	1	-0.160296000	1.390847000	0.520582000
1	-3.443794000	2.295182000	1.691424000	6	1.352577000	-1.141897000	-0.347783000
6	-3.378643000	2.741638000	0.691282000	8	2.363699000	-1.755234000	-0.527148000
1	-4.361537000	3.126610000	0.410789000	1	2.712440000	2.754326000	-1.936519000
1	-4.181219000	0.342557000	-0.398072000	6	2.197562000	2.093320000	2.403617000
8	-4.774308000	-0.436107000	-0.402958000	1	2.126797000	2.698617000	-0.251536000
6	-5.751438000	-0.254497000	-1.443788000	6	2.320626000	2.101180000	-1.147354000
1	-6.381198000	0.628637000	-1.265724000	6	-3.740158000	0.860624000	0.326665000
1	-6.389185000	-1.142339000	-1.439912000	1	-3.548747000	1.793300000	-0.211495000
1	-5.283540000	-0.161806000	-2.433963000	1	-4.789574000	0.583380000	0.145946000
				1	-3.639829000	1.085132000	1.392485000
				6	-2.782991000	0.308481000	-2.650325000
				1	-2.043534000	0.278220000	-3.456651000
				1	-3.715039000	-0.113758000	-3.054148000
6	0.041393000	-1.370340000	-1.715701000	1	-2.982042000	1.357052000	-2.410652000
6	-0.950916000	-0.458546000	-2.212850000	1	-1.123376000	-2.433463000	-2.684922000
6	-2.224101000	-0.862233000	-1.680622000	6	-0.243376000	-3.047689000	-2.471069000
6	-2.020726000	-2.008580000	-0.850255000	1	-1.905703000	-3.101745000	-3.075513000
6	-0.625863000	-2.326543000	-0.878617000	1	-0.853318000	-1.743983000	-3.490463000
42	-0.788179000	-0.094989000	0.135267000	1	-1.155356000	-3.622360000	0.263185000
15	0.516139000	-0.785366000	2.102075000	6	-0.946284000	-3.694032000	1.334558000
15	-2.172619000	1.883463000	0.541722000	1	-1.920356000	-4.377482000	0.027510000
1	-1.682566000	-0.118376000	1.635533000	1	-0.240853000	-3.903985000	-0.267426000
6	0.557976000	1.259320000	0.090985000	1	-2.851351000	-1.633853000	2.100535000
8	1.398974000	2.110646000	0.015591000	6	-3.097426000	-0.720205000	2.649222000
1	-2.337574000	3.832815000	2.059425000	1	-3.765279000	-2.245034000	2.067191000
6	0.855805000	0.528352000	3.372968000	1	-2.115215000	-2.193959000	2.685223000
1	-1.777189000	2.365683000	2.907908000	1	2.055442000	1.848724000	2.091094000
6	-1.691942000	2.949547000	1.986988000	1	3.074582000	1.347379000	-0.901791000
6	-3.101603000	-2.836261000	-0.202918000	1	1.273941000	0.591814000	-3.334666000
1	-3.964443000	-2.225820000	0.081447000	6	1.784272000	1.249196000	-3.940958000
1	-3.464050000	-3.620140000	-0.884800000	1	1.953658000	-0.247915000	-3.160995000
1	-2.741996000	-3.333494000	0.703493000	1	0.404230000	0.222981000	-3.887199000
6	-3.566600000	-0.350401000	-2.135079000	1	-0.204977000	2.801106000	-2.262362000
1	-3.547690000	0.717074000	-2.375008000	6	-0.437719000	3.447737000	-2.871672000
1	-3.886495000	-0.877248000	-3.046246000	1	-1.069734000	2.503439000	-2.861114000
6	-4.342854000	-0.513376000	-1.381207000	1	-0.567163000	3.360314000	-1.394444000
1	-0.730551000	0.570528000	-3.292780000	1	-1.045123000	1.718899000	-3.038390000
1	0.267461000	1.014559000	-3.227174000	6	1.459020000	-1.541609000	4.037729000
1	-0.825382000	0.120390000	-4.292499000				



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1	0.161455000	-2.358219000	3.129634000	6	-1.796019000	1.128850000	1.944313000
1	1.787551000	-2.244233000	2.429202000	6	-1.070522000	-0.029219000	2.366737000
6	-0.418522000	0.706136000	3.527429000	6	-1.784812000	-1.183605000	1.915842000
0	0.139268000	0.753463000	4.470218000	42	-1.135233000	0.001262000	-0.112002000
1	-0.681424000	1.719773000	3.209689000	15	-0.296197000	-2.066294000	-1.191986000
1	-1.345987000	0.151924000	3.693166000	15	-0.310795000	2.099479000	-1.144849000
1	2.522255000	0.791057000	3.450752000	1	0.623075000	0.009199000	-0.295027000
1	2.979296000	0.368328000	1.778463000	6	-2.128485000	0.017435000	-1.769869000
1	-1.161213000	2.719224000	0.905961000	8	-2.790162000	0.026323000	-2.752241000
8	-1.602197000	3.561494000	1.132925000	1	0.884454000	2.888105000	-3.156135000
6	-0.594692000	4.521600000	1.504452000	6	0.603816000	-1.836508000	-2.800713000
1	-1.121827000	5.448229000	1.744422000	1	1.497851000	1.308664000	-2.592937000
1	-0.027149000	4.202230000	2.389530000	6	0.598153000	1.309533000	-2.753526000
1	0.108232000	4.720997000	0.683490000	6	0.140646000	-0.034094000	3.264397000
1	4.073465000	-0.933034000	-0.258760000	1	0.766963000	0.849691000	3.110438000
8	4.827386000	-0.351232000	-0.059285000	1	-0.155659000	-0.044891000	4.323694000
1	6.143731000	-1.964333000	0.290862000	1	0.772136000	-0.911074000	3.093793000
6	6.048017000	-1.066716000	-0.334799000	6	-1.529372000	2.537549000	2.405383000
6	6.870443000	-0.386489000	-0.100598000	1	-1.854722000	3.281975000	1.672230000
1	6.120267000	-1.356997000	-1.391621000	1	-2.075965000	2.744394000	3.337127000

12. [Cp\*Mo(CO)(PMe<sub>3</sub>)<sub>2</sub>H]·CF<sub>3</sub>COOH (A) E = -1350.79302651

6	-0.544666000	-0.731890000	-2.059776000	1	-4.625733000	1.154973000	-0.082351000
6	-0.540763000	0.704200000	-2.068380000	1	-4.854123000	1.663918000	1.597149000
6	-1.907683000	1.145018000	-2.026619000	6	-3.781793000	2.577255000	0.529679000
6	-2.754104000	-0.007233000	-1.982963000	1	-4.095732000	-1.616159000	0.750972000
6	-1.914004000	-1.164531000	-2.013444000	1	-3.756458000	-2.617626000	0.470612000
42	-1.348402000	0.001329000	0.065123000	1	-4.840131000	-4.840131000	1.552437000
15	-1.607446000	-2.046667000	1.390121000	6	-4.610285000	-1.190457000	-0.115608000
15	-1.596412000	2.066021000	1.367524000	1	-1.505005000	-2.600753000	2.342631000
1	-2.707050000	0.010860000	1.166057000	1	-0.443000000	-2.762695000	2.548551000
6	0.310887000	0.002816000	0.986782000	1	-2.053189000	-2.836535000	3.266499000
8	1.372723000	0.003788000	1.559244000	1	-1.819577000	-3.329875000	1.589661000
1	-1.509426000	2.880822000	3.699393000	1	1.496901000	-1.227472000	-2.634298000
6	-1.424613000	-1.865559000	3.230151000	6	-0.043071000	1.397750000	-3.477069000
1	-2.187637000	1.232605000	3.591951000	1	-1.575657000	3.379829000	-1.626830000
6	-1.414593000	1.904824000	3.209483000	1	-1.100619000	4.225317000	-2.137642000
6	-4.259574000	-0.003659000	-2.066085000	1	-2.311822000	2.922920000	-2.295370000
1	-4.689870000	0.882011000	-1.588244000	6	-2.098921000	3.752047000	-0.714077000
1	-4.599451000	-0.009602000	-3.112311000	1	-0.910015000	3.150109000	-0.213401000
1	-4.694895000	-0.880484000	-1.576628000	1	1.235056000	4.005132000	-0.830105000
6	-2.376541000	2.555544000	-2.274481000	1	0.458801000	3.545141000	0.704482000
1	-1.715185000	3.303157000	-1.826326000	1	1.784173000	2.560085000	0.057374000
1	-2.401890000	2.759998000	-3.354831000	6	-1.552873000	-3.346825000	-1.695044000
1	-3.388264000	2.724639000	-1.893546000	1	-1.073133000	-4.179714000	-2.221925000
6	0.660592000	1.579056000	-2.322549000	1	-2.072371000	-3.738247000	-0.814870000
1	1.577083000	1.134313000	-1.926055000	6	-2.293239000	-2.882721000	-2.353894000
1	0.809868000	1.732518000	-3.401858000	1	0.936544000	-3.134680000	-0.286676000
1	0.547578000	2.567929000	-1.866593000	1	1.2656771000	-3.923322000	-0.921332000
6	0.651867000	-1.616519000	-2.302929000	1	1.806862000	-2.534880000	-0.005623000
1	0.532283000	-2.599872000	-1.836761000	1	0.491097000	-3.542289000	0.624552000
1	0.801742000	-1.782243000	-3.380341000	1	0.899782000	-2.804575000	-3.221772000
1	1.570475000	-1.173219000	-1.909780000	1	-0.046922000	-1.320237000	-3.512431000
6	-2.390370000	-2.575276000	-2.245152000	8	1.830504000	0.011220000	0.342428000
1	-3.403108000	-2.734840000	-1.862765000	6	2.752556000	-0.004324000	0.782749000
1	-2.416340000	-2.792095000	-3.323075000	6	3.713686000	0.029650000	-0.131615000
1	-1.733065000	-3.321016000	-1.788075000	6	5.087645000	-0.007447000	0.558876000
1	-2.194762000	-1.185809000	3.605041000	9	5.214960000	1.025835000	1.477149000
1	-0.434679000	1.478325000	3.442798000	9	6.109039000	0.108603000	-0.356322000
6	-0.372600000	3.436253000	1.046820000	9	5.259208000	-1.204018000	1.243851000
1	-0.551387000	4.294109000	1.705573000	8	3.605405000	0.072977000	-1.340304000

14. [Cp\*Mo(CO)(PMe<sub>3</sub>)<sub>2</sub>H]·(CF<sub>3</sub>COOH)<sub>2</sub> (D) E = -1877.49936439

1	0.638687000	3.054181000	1.219670000	6	4.440268000	0.267223000	-0.760122000
1	-0.438474000	3.769277000	0.006737000	6	4.431984000	0.504041000	0.658864000
6	-3.208411000	2.997002000	1.282217000	6	3.536231000	1.599230000	0.915224000
1	-3.190275000	3.873694000	1.940065000	6	2.993731000	2.036661000	-0.333640000
1	-3.400142000	3.326022000	0.257469000	6	3.549403000	1.218909000	-1.367215000
1	-4.020053000	2.329868000	1.588788000	6	2.304605000	-0.319298000	0.056141000
6	-0.391338000	-3.427040000	1.084285000	15	1.261669000	-1.442508000	-1.897848000
1	-0.574091000	-4.276176000	1.753202000	15	1.209164000	-0.75729000	2.248408000
1	-0.460176000	-3.771626000	0.048181000	1	0.555308000	0.009161000	-0.032807000
1	0.622101000	-3.048231000	1.251578000	1	2.769579000	-2.167419000	0.374332000
6	-3.224665000	-2.969469000	1.315766000	8	3.117364000	-3.282470000	0.566459000
1	-3.210805000	-3.839064000	1.983103000	6	-0.502590000	-2.241890000	3.238679000
1	-4.032285000	-2.294524000	1.615861000	1	-0.016286000	-2.733066000	-1.507383000
1	-3.419253000	-3.308469000	0.294821000	1	-0.887504000	-1.808085000	1.550548000
1	-1.523694000	-2.835515000	3.731125000	6	-0.084224000	-2.090619000	2.237016000
1	-0.442863000	-1.440755000	3.458617000	6	2.129948000	3.253583000	-0.541318000
8	2.972419000	0.004478000	1.206714000	1	1.483816000	3.448943000	0.318891000
6	4.400841000	0.006806000	1.158145000	1	2.749884000	4.148814000	-0.696621000
6	5.938244000	-0.002373000	-0.118967000	6	1.481214000	3.151446000	-1.416218000
9	6.440034000	1.134553000	0.500335000	1	3.395135000	2.332130000	2.242280000
9	6.416146000	-0.025986000	-1.410811000	1	3.505477000	1.665717000	3.085723000
9	6.453148000	-1.106829000	0.546157000	1	4.172066000	3.104306000	2.314702000
8	3.746420000	-0.027449000	-1.118681000	1	2.427942000	2.307253000	2.307253000

13. [Cp\*MoH(PMe<sub>3</sub>)<sub>2</sub>(CO)]·CF<sub>3</sub>COOH (B)·E = -1350.79060546

6	-2.953386000	-0.743377000	1.203919000	1	5.602536000	-1.156753000	1.408266000
6	-2.960558000	0.694708000	1.222085000	1	6.345902000	1.429984000	1.655341000
				1	4.992684000	-0.084205000	2.668249000

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6	5.407858000	-0.632209000	-1.485742000	1	4.567318000	-0.516917000	3.112306000
1	5.025561000	-0.937276000	-2.463826000	6	2.779995000	1.903556000	-2.975764000
1	6.366421000	-0.119379000	-1.654356000	1	3.457005000	2.567378000	-3.525952000
1	5.618443000	-1.543246000	-0.917542000	1	2.506426000	1.064435000	-3.621920000
6	3.429254000	1.492548000	-2.844218000	1	1.867587000	2.451365000	-2.719454000
1	2.473828000	1.962714000	-3.096584000	6	5.185890000	0.616527000	-2.052374000
1	4.223407000	2.180294000	-3.169346000	1	5.707243000	1.367545000	-2.657349000
1	3.528236000	0.584376000	-3.446284000	1	5.816443000	0.331798000	-1.204479000
1	-0.852126000	-2.263305000	-0.981455000	1	5.007802000	-0.271013000	-2.664898000
1	0.359827000	-3.026250000	1.885661000	1	4.713721000	3.474676000	-1.424586000
6	2.295032000	-1.343882000	3.642502000	1	3.289006000	3.474918000	-0.346835000
1	1.698522000	-1.578734000	4.531412000	1	-1.012501000	2.813053000	0.161997000
1	2.840098000	-2.238993000	3.327588000	8	-1.955152000	2.182003000	0.270238000
1	3.023395000	-0.569759000	3.902105000	8	-2.685814000	1.419670000	-0.970607000
6	0.264577000	0.604476000	3.100855000	6	-4.268223000	3.005107000	-0.069185000
1	-0.197898000	0.233533000	4.021966000	9	-4.573037000	3.047055000	1.277951000
1	0.933344000	1.432519000	3.349204000	9	-5.219561000	2.226990000	-0.705740000
1	-0.519036000	0.984186000	2.438741000	9	-4.366883000	4.292341000	-0.573275000
6	2.383007000	-2.414207000	-3.023635000	6	-2.860195000	2.435217000	-0.308185000
1	1.799896000	-2.951337000	-3.780318000	1	-3.871786000	0.156492000	-1.218020000
1	3.086771000	-1.747583000	-3.531391000	8	-4.311832000	-0.732072000	-1.259680000
1	2.954705000	-3.135032000	-2.431271000	8	-4.524480000	-0.480670000	1.002762000
6	0.308676000	-0.432683000	-3.141297000	6	-4.631300000	-1.114202000	-0.025195000
1	-0.074441000	-1.074890000	-3.943027000	6	-5.128980000	-2.566431000	-0.037413000
1	-0.538306000	0.044747000	-2.640842000	9	-5.720314000	-2.900151000	1.159654000
1	0.943082000	0.341178000	-3.580561000	9	-4.052346000	-3.429928000	-0.237140000
1	-0.388588000	-3.201035000	-2.426161000	9	-6.044066000	-2.798161000	-1.050072000
1	0.420254000	-3.501695000	-0.863082000				
1	-0.221042000	1.028744000	-0.100472000	16.	[Cp*MoH (PMe <sub>3</sub> ) <sub>2</sub> (CO)] · (CF <sub>3</sub> COOH) <sub>2</sub> (E) E=-1877.50097522		
8	-0.901183000	1.824966000	-0.096040000				
8	-2.475325000	0.342462000	-0.804298000	6	-0.987958000	2.464932000	0.116314000
6	-2.108760000	1.452479000	-0.435589000	6	-1.065519000	2.039928000	-1.253815000
6	-3.096322000	2.626693000	-0.310245000	6	0.254999000	2.130008000	-1.815565000
9	-2.607398000	3.759215000	-0.940611000	6	1.146764000	2.602061000	-0.801580000
9	-4.309747000	2.308706000	-0.890712000	6	0.380683000	2.813048000	0.388084000
9	-3.316723000	2.939050000	1.019714000	42	0.206676000	0.421327000	-0.071283000
1	-4.109775000	-0.260180000	-0.926562000	15	0.717755000	-0.151621000	2.290786000
8	-5.001030000	-0.693763000	-0.957709000	15	0.537173000	-1.391463000	-1.738214000
8	-5.192384000	0.044633000	1.196802000	1	1.765104000	-0.395788000	0.104438000
6	-5.615044000	-0.520953000	0.211663000	6	-1.241116000	-0.374393000	0.347393000
6	-7.006220000	-1.168828000	0.166794000	8	-2.171618000	-1.450339000	0.608406000
9	-7.671477000	-0.996106000	1.359138000	1	0.898861000	-3.830307000	-1.801026000
9	-6.905944000	-2.532773000	-0.075590000	6	0.980734000	-1.959937000	2.614164000
9	-7.781201000	-0.617308000	-0.842889000	1	1.738633000	-3.065109000	-0.423958000
				6	0.815874000	-3.075168000	-1.011022000
				6	2.592435000	-2.979118000	-0.999920000
				1	3.079762000	2.354301000	-1.754201000
				1	2.681285000	4.023523000	-1.333085000
				1	3.171708000	2.881167000	-0.077034000
				6	0.586566000	2.022036000	-3.280768000
				1	-0.028314000	1.275369000	-3.791841000
				1	0.400901000	3.780386000	-3.780364000
				1	1.638181000	1.771120000	-3.447117000
				6	-2.340630000	1.801071000	-2.021416000
				1	-3.133611000	1.414259000	-1.375964000
				1	-2.707086000	2.739124000	-2.463941000
				1	-2.200038000	1.089227000	-2.840237000
				6	2.168561000	2.745520000	1.010932000
				1	-1.908976000	2.663150000	2.070778000
				1	-2.542827000	3.768190000	0.846631000
				1	-2.997469000	2.059298000	0.818104000
				6	0.868457000	3.537058000	1.615444000
				1	1.937348000	3.380669000	1.787498000
				1	0.713713000	4.619740000	1.501482000
				1	0.329224000	3.232527000	2.517045000
				1	1.842726000	-2.303737000	2.038786000
				1	-0.018947000	-3.333303000	-0.353310000
				6	-0.865155000	-1.742198000	-2.911012000
				1	-0.633414000	-2.599633000	-3.553186000
				1	-1.770251000	-1.960137000	-2.335419000
				1	-1.061222000	-0.871058000	-3.543529000
				6	1.974933000	-1.302460000	-2.920169000
				1	2.045821000	-2.225267000	-3.507219000
				1	1.857909000	-0.458101000	-3.604169000
				1	2.903263000	-1.167048000	-2.358067000
				6	-0.579270000	0.242107000	3.566577000
				1	-0.277552000	-0.123613000	4.554816000
				1	-0.743080000	1.322415000	3.624687000
				6	-1.522003000	-0.233910000	3.279705000
				6	2.237370000	0.552415000	3.109074000
				1	2.370414000	0.114385000	4.104937000
				1	3.120677000	0.333320000	2.502781000
				1	2.150171000	1.636942000	3.211188000
				1	1.159721000	-2.146790000	3.680288000
				1	0.096482000	-2.521071000	2.298134000
				1	3.130821000	-0.151059000	0.002986000
				8	4.138917000	-0.025444000	-0.053910000
				8	4.289841000	-2.249506000	0.464447000
				6	4.770158000	-1.166665000	0.200178000
				6	6.289867000	-0.944937000	0.120115000
				9	6.700295000	-0.009560000	1.061228000
15.	[Cp*MoH (PMe <sub>3</sub> ) <sub>2</sub> (CO)] · (CF <sub>3</sub> COOH) <sub>2</sub> (C) · E =-1877.50320187						
6	0.818856000	-1.418456000	-1.385800000				
6	0.451079000	-1.735270000	-0.034949000	1	3.171708000	2.881167000	-0.077034000
6	1.552398000	-2.437146000	0.565931000	6	0.586566000	2.022036000	-3.280768000
6	2.601230000	-2.543290000	-0.400368000	1	-0.028314000	1.275369000	-3.791841000
6	2.143981000	-1.925115000	-1.607251000	1	0.400901000	3.780386000	-3.780364000
42	2.218068000	-0.131594000	0.069301000	1	1.638181000	1.771120000	-3.447117000
15	3.572177000	1.283911000	-1.405824000	6	-2.340630000	1.801071000	-2.021416000
15	2.402162000	0.414139000	2.457840000	1	-3.133611000	1.414259000	-1.375964000
1	3.843840000	0.176472000	0.634129000	1	-2.707086000	2.739124000	-2.463941000
1	1.174461000	1.444125000	0.105209000	1	-2.200038000	1.089227000	-2.840237000
8	0.496516000	2.448492000	0.112296000	6	2.168561000	2.745520000	1.010932000
1	3.016925000	2.290097000	3.942109000	1	-1.908976000	2.663150000	2.070778000
6	4.152424000	2.893664000	-0.683547000	1	-2.542827000	3.768190000	0.846631000
1	4.012167000	2.257981000	2.459999000	1	-2.997469000	2.059298000	0.818104000
6	3.002407000	2.126042000	2.858453000	6	0.868457000	3.537058000	1.615444000
6	3.882709000	-3.320350000	-0.235799000	1	1.937348000	3.380669000	1.787498000
1	4.225247000	-3.321657000	0.803614000	1	0.713713000	4.619740000	1.501482000
1	3.752233000	-4.369551000	-0.539184000	1	0.329224000	3.232527000	2.517045000
1	4.691475000	-2.903083000	-0.843900000	1	1.842726000	-2.303737000	2.038786000
6	1.505141000	-3.179549000	1.876210000	1	-0.018947000	-3.333303000	-0.353310000
1	0.902084000	-2.663970000	2.629189000	6	-0.865155000	-1.742198000	-2.911012000
1	1.052778000	-4.171220000	1.731029000	1	-0.633414000	-2.599633000	-3.553186000
1	2.504083000	-3.341523000	2.292315000	1	-1.770251000	-1.960137000	-2.335419000
6	-0.926597000	-1.581019000	0.556508000	1	-1.061222000	-0.871058000	-3.543529000
1	-1.426978000	-0.686764000	0.175447000	6	1.974933000	-1.302460000	-2.920169000
1	-1.560750000	-2.445072000	0.310539000	1	2.045821000	-2.225267000	-3.507219000
1	-0.896437000	-1.499889000	1.647075000	1	1.857909000	-0.458101000	-3.604169000
6	-0.106557000	-0.874654000	-2.444172000	1	2.903263000	-1.167048000	-2.358067000
1	0.443304000	-0.360197000	-3.238459000	6	-0.579270000	0.242107000	3.566577000
1	-0.679059000	-1.686938000	-2.916025000	1	-0.277552000	-0.123613000	4.554816000
1	-0.827017000	-0.164598000	-2.029180000	1	-0.743080000	1.322415000	3.624687000
6	2.819114000	-2.041787000	-2.949361000	6	-1.522003000	-0.233910000	3.279705000
1	3.902120000	-2.164351000	-2.854441000	6	2.237370000	0.552415000	3.109074000
1	2.441496000	-2.925331000					

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9	6.976845000	-2.113805000	0.352585000	1	3.673232000	-0.818196000	-0.549128000
9	6.656121000	-0.471903000	-1.132792000	1	3.260597000	-2.359176000	-1.305189000
1	-3.829192000	-1.502741000	0.533401000	1	2.830055000	-0.841536000	-2.097449000
8	-4.808792000	-1.693184000	0.499620000	6	2.492141000	-1.632878000	2.016927000
8	-5.092023000	0.549909000	0.156232000	1	2.246935000	-1.235278000	3.004687000
6	-5.503773000	-0.585200000	0.279374000	1	2.671228000	-2.709374000	2.145700000
6	-6.997481000	-0.923015000	0.150551000	1	3.437566000	-1.192109000	1.690870000
9	-7.767417000	0.219219000	0.166075000	6	-0.624385000	-1.895103000	2.619870000
9	-7.431046000	-1.745237000	1.178234000	1	-1.690315000	-1.652098000	2.648827000
9	-7.235902000	-1.583550000	-1.049317000	1	-0.529734000	-2.962713000	2.840826000
				1	-0.138814000	-1.350944000	3.434296000
				6	-2.144517000	-1.985895000	-0.196345000
				1	-2.555710000	-1.518351000	-1.095060000
				1	-2.261344000	-3.072458000	-0.309958000
				1	-2.766115000	-1.680646000	0.650267000
				6	0.063659000	-1.802216000	-2.477231000
				1	0.824161000	-1.353674000	-3.121191000
				1	0.117463000	-2.888599000	-2.633803000
				1	-0.920725000	-1.483648000	-2.828409000
				1	0.247706000	4.062417000	-1.224422000
				1	-0.126815000	3.833010000	2.177693000
				6	1.406814000	1.455620000	3.826091000
				1	1.548716000	2.129666000	4.498696000
				1	-0.066533000	1.554176000	4.015723000
				1	1.304893000	0.427942000	4.048356000
				6	3.213411000	1.935862000	2.004900000
				1	3.596268000	2.585955000	2.799095000
				1	3.631259000	0.936062000	2.139018000
				1	3.540246000	2.323633000	1.035625000
				6	-2.081265000	1.343376000	-2.602381000
				1	-2.262833000	1.974742000	-3.479109000
				1	-2.086316000	0.297565000	-2.918377000
				1	-2.892412000	1.493857000	-1.883421000
				6	0.723477000	1.760731000	-3.228875000
				1	0.360213000	2.401026000	-4.040051000
				1	1.698613000	2.126089000	-2.893295000
				1	0.844106000	0.745704000	-3.613450000
				1	-0.991463000	4.089580000	-2.505284000
				1	-1.459385000	3.801508000	-0.808887000
				1	-3.026488000	1.511765000	1.778854000

### c. Ionic species

17.  $[\text{Cp}^*\text{Mo}(\eta^2\text{-H}_2)(\text{CO})(\text{PMe}_3)_2]^+ \text{E} = -824.482747257$

6	0.719710000	1.787633000	1.060998000	1	0.824161000	-1.353674000	-3.121191000
6	-0.719637000	1.787628000	1.061068000	1	0.117463000	-2.888599000	-2.633803000
6	-1.157152000	2.030936000	-0.291950000	1	-0.920725000	-1.483648000	-2.828409000
6	-0.000068000	2.167580000	-1.121964000	1	0.247706000	4.062417000	-1.224422000
6	1.157101000	2.030924000	-0.292070000	1	-0.126815000	3.833010000	2.177693000
42	0.000004000	-0.085843000	-0.131571000	6	1.406814000	1.455620000	3.826091000
15	2.290017000	-1.251900000	-0.320945000	1	1.548716000	2.129666000	4.498696000
15	-2.290016000	-1.251852000	-0.321161000	1	-0.066533000	1.554176000	4.015723000
1	0.000068000	-0.734413000	-1.885399000	1	1.304893000	0.427942000	4.048356000
6	-0.000073000	-1.229613000	1.462146000	6	3.213411000	1.935862000	2.004900000
8	-0.000116000	-1.807433000	2.477401000	1	3.596268000	2.585955000	2.799095000
1	-3.149226000	-3.556312000	-0.374264000	1	3.631259000	0.936062000	2.139018000
6	2.157005000	-3.102401000	-0.278176000	1	3.540246000	2.323633000	1.035625000
1	-1.528136000	-3.455897000	-1.101389000	6	-2.081265000	1.343376000	-2.602381000
6	-2.157020000	-3.102356000	-0.278458000	1	-2.262833000	1.974742000	-3.479109000
6	-0.000136000	2.571503000	-2.573036000	1	-2.086316000	0.297565000	-2.918377000
1	-0.883453000	2.202867000	-3.102094000	1	-2.892412000	1.493857000	-1.883421000
1	-0.000139000	3.666498000	-2.664049000	6	0.723477000	1.760731000	-3.228875000
1	0.883137000	2.202867000	-3.102170000	1	0.360213000	2.401026000	-4.040051000
6	-2.557766000	2.383310000	-0.716924000	1	1.698613000	2.126089000	-2.893295000
1	-3.322011000	1.876907000	-0.122778000	1	0.844106000	0.745704000	-3.613450000
1	-2.718285000	3.462403000	-0.586143000	1	-0.991463000	4.089580000	-2.505284000
1	-2.737347000	2.159817000	-1.771876000	1	-1.459385000	3.801508000	-0.808887000
6	-1.575462000	1.846206000	2.299948000	1	-3.026488000	1.511765000	1.778854000
1	-1.192422000	1.199569000	3.094625000				
1	-1.595628000	2.871473000	2.694235000				
1	-2.609660000	1.555533000	2.103884000				
6	1.575636000	1.846269000	2.299810000	8	-1.541832000	-1.151303000	-0.000046000
1	2.609865000	1.555788000	2.103633000	8	-1.599350000	-1.147666000	-0.000037000
1	1.595665000	2.871513000	2.694159000	6	-1.070513000	0.011703000	0.000058000
1	1.192778000	1.199516000	3.094482000	6	0.502236000	0.011782000	-0.000013000
6	2.557661000	2.383329000	-0.717202000	9	1.038542000	-0.645840000	-1.118743000
1	2.737220000	2.159591000	-1.772107000	9	1.038451000	-0.645385000	-1.119042000
1	2.718081000	3.462470000	-0.586696000	9	1.094019000	1.278801000	-0.000255000
1	3.321981000	1.877152000	-0.122962000				
1	1.528103000	-3.455974000	-1.101079000				
1	-1.708556000	-3.426268000	0.664906000				
6	-3.557351000	-0.958587000	0.998183000				
1	-4.408434000	-1.631373000	0.848015000				
1	-3.122292000	-1.152445000	1.982956000				
1	-3.921854000	0.070814000	0.973027000	6	-2.695962000	-1.180167000	0.997502000
6	-3.254425000	-1.003863000	-1.888062000	6	-2.936995000	0.233742000	1.115941000
1	-4.158435000	-1.622661000	-1.880165000	6	-1.900393000	0.783669000	1.950792000
1	-3.545971000	0.042403000	-2.003997000	6	-1.024804000	-0.278404000	2.343404000
1	-2.640539000	-1.289779000	-2.748253000	6	-1.519249000	-1.490484000	-1.770101000
6	3.557292000	-0.958616000	0.998453000	42	-0.966275000	-0.054872000	-0.104860000
1	4.408290000	-1.631545000	0.848443000	15	0.184518000	-2.014664000	-1.259108000
1	3.921943000	0.070728000	0.973166000	15	-0.607435000	-2.342401000	-0.950774000
1	3.122133000	-1.152266000	1.983222000	1	0.884026000	0.198966000	-0.552572000
6	3.254513000	-1.003963000	-1.887802000	1	-1.833619000	-0.071017000	-1.844814000
1	4.158550000	-1.622721000	-1.879822000	8	-2.450127000	-0.101060000	-2.846242000
1	2.640691000	-1.289946000	-2.748016000	1	0.601217000	3.412326000	-2.799513000
1	3.546016000	0.042311000	-2.003768000	6	0.992729000	-1.568670000	-2.863281000
1	3.149208000	-3.556364000	-0.373980000	1	1.399291000	1.906156000	-2.248544000
1	1.708555000	-3.426273000	0.665208000	6	0.436265000	2.377893000	-2.476942000
1	0.000082000	-1.441482000	-1.431772000	6	0.140745000	-0.144883000	3.288813000
				1	0.720252000	0.763289000	3.099192000
				1	-0.207479000	-0.111960000	4.331010000
				1	0.833817000	-0.833817000	3.199993000
				6	-1.881454000	2.165936000	2.546620000
				1	-2.343676000	2.909433000	1.891336000
				1	-2.446238000	2.172612000	3.490003000
				1	-0.864268000	2.495381000	2.774082000
				6	-4.197554000	0.937757000	0.685996000
				1	4.581414000	0.545419000	-0.260323000
				1	-4.986940000	0.810287000	1.440917000
				1	-4.040956000	2.011950000	0.558326000
				6	-3.671614000	-2.175003000	0.422215000
				1	-3.181296000	-3.101431000	0.112534000
				1	-4.434144000	-2.441857000	1.168219000
				1	-4.193188000	-1.771059000	-0.450591000
				6	-1.047174000	-2.873226000	2.135320000
				1	0.021888000	-2.896145000	2.362894000
				1	-1.576819000	-3.221024000	3.033633000
				1	-1.242604000	-3.605238000	1.347122000

18.  $[\text{Cp}^*\text{MoH}(\text{COH})(\text{PMe}_3)_2]^+ \text{E} = -824.450090537$

6	-0.696100000	-1.628153000	0.015321000	6	-1.881454000	2.165936000	2.546620000
6	-0.015817000	-1.578288000	1.277923000	1	-2.343676000	2.909433000	1.891336000
6	1.390688000	-1.431097000	1.011140000	1	-2.446238000	2.172612000	3.490003000
6	1.577519000	-1.355298000	-0.404341000	1	-0.864268000	2.495381000	2.774082000
6	0.291625000	-1.502961000	-1.019597000	6	-4.197554000	0.937757000	0.685996000
42	0.159482000	0.598387000	0.290430000	1	4.581414000	0.545419000	-0.260323000
15	-0.465592000	1.796613000	-1.808099000	1	-4.986940000	0.810287000	1.440917000
15	1.362404000	1.891299000	2.055416000	1	-4.040956000	2.011950000	0.558326000
1	1.254739000	1.831003000	-0.259236000	6	-3.671614000	-2.175003000	0.422215000
6	-1.295789000	1.439813000	0.956601000	1	-3.181296000	-3.101431000	0.112534000
8	-2.33068						

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1	1.786352000	-0.843458000	-2.657285000	6	1.667816000	2.363081000	0.564301000
1	-0.052784000	1.823199000	-3.282964000	6	2.487066000	3.151977000	-0.486800000
6	-2.108884000	3.310450000	-1.456103000	9	1.984186000	4.410879000	-0.746732000
1	-1.805167000	4.263703000	-1.903020000	9	3.820081000	3.440811000	-0.127131000
1	-2.694256000	2.743596000	-2.1866073000	9	2.471966000	2.448051000	-1.707479000
1	-2.739918000	3.516913000	-0.586623000	1	3.580768000	0.823158000	0.676632000
6	0.307843000	3.530837000	0.133894000	8	4.522930000	0.415547000	0.477446000
1	0.536519000	4.444020000	-0.427541000	8	3.552247000	-1.653471000	0.576124000
1	-0.285282000	3.794966000	1.012115000	6	4.496931000	-0.893258000	0.426637000
1	1.239740000	3.051817000	0.457023000	6	5.889940000	-1.446765000	0.076254000
6	-0.888130000	-3.448238000	-1.753178000	9	5.964874000	-2.806243000	0.308850000
1	-0.302132000	-4.171746000	-2.330974000	9	6.899143000	-0.839920000	0.805493000
1	-1.291388000	-3.951178000	-0.870201000	9	6.160929000	-1.237415000	-1.273706000
1	-1.722338000	-3.092937000	-2.365915000				
6	1.590399000	-2.841988000	-0.380427000				
1	1.998938000	-3.648876000	-0.999781000				
1	2.380190000	-2.110143000	-0.192977000				
1	1.262622000	-3.257930000	0.574785000				
1	1.428823000	-2.460633000	-3.327513000				
1	0.261408000	-1.126807000	-3.545709000				
1	0.815357000	0.480738000	0.211947000				
8	2.707715000	1.453103000	0.911839000	6	2.974746000	0.114749000	1.115503000
8	2.957127000	0.493479000	-1.153151000	6	2.635276000	-1.278267000	1.009217000
6	3.309276000	0.777949000	0.043723000	6	1.428954000	-1.491334000	1.769632000
6	4.616226000	0.089538000	0.522945000	6	1.031195000	-0.244534000	2.346481000
9	5.283804000	0.794936000	1.513919000	6	1.984975000	0.743521000	1.952827000
9	4.297937000	-1.174243000	1.075620000	42	0.996763000	-0.055367000	-0.127208000
9	5.519207000	-0.146996000	-0.469466000	15	0.699982000	2.346751000	-0.889917000
				15	-0.187727000	-1.953778000	-1.341121000
				1	-0.723915000	0.438316000	-0.569743000
				6	1.910646000	-0.081171000	-1.829381000
				8	2.555477000	-0.116588000	-2.817079000
				1	-1.558595000	-2.208203000	-3.373331000
				6	-0.238851000	2.500590000	-2.480833000
				1	-1.831789000	-0.633812000	-2.583253000
				6	-1.071455000	-1.368800000	-2.864119000
				6	-0.124739000	-0.051826000	3.291622000
				1	-1.028958000	-0.554911000	2.938781000
				1	0.121093000	-0.443433000	4.289048000
				1	-0.380656000	1.004931000	3.405080000
				6	0.836250000	-2.824436000	2.142310000
				1	1.021194000	-3.594744000	1.383629000
				1	1.286249000	-3.185187000	3.078645000
				1	-0.242770000	-2.756167000	2.306179000
				6	3.539964000	-2.348622000	0.454933000
				1	4.063063000	-2.014382000	-0.446108000
				1	4.303223000	-2.628583000	1.195581000
				1	2.989304000	-3.258043000	0.199405000
				6	4.281015000	0.725151000	0.677843000
				1	4.199502000	1.805981000	0.534639000
				1	5.060835000	0.554038000	1.434393000
				1	4.635426000	0.293965000	-0.263149000
				6	2.093906000	2.126931000	2.537779000
				1	1.125671000	2.507036000	2.873278000
				1	2.755388000	2.107589000	3.415697000
				1	2.518155000	2.849858000	1.835472000
				1	-1.254522000	2.125658000	-2.320116000
				1	-0.360828000	-0.893772000	-3.546253000
				6	0.858778000	-3.325247000	-2.026965000
				1	0.247668000	-4.00052000	-2.636746000
				1	1.659862000	-2.908400000	-2.644572000
				1	1.309555000	-3.901113000	-1.213840000
				6	-1.546705000	-2.886428000	-0.488646000
				1	-2.061638000	-3.535523000	-1.205910000
				1	-1.140749000	-3.503381000	0.316334000
				1	-2.259588000	-2.177959000	-0.056680000
				6	2.228346000	3.334894000	-1.262004000
				1	1.953079000	4.308032000	-1.684072000
				1	2.814809000	3.501412000	-0.353915000
				1	2.847696000	2.792980000	-1.983256000
				6	-0.296410000	3.478909000	0.186187000
				1	-0.380526000	4.467416000	-0.280422000
				1	-1.297957000	3.046123000	0.288937000
				1	0.158334000	3.587869000	1.173202000
				1	-0.294378000	3.550763000	-2.789677000
				1	0.246476000	1.917365000	-3.268105000
				1	-1.089152000	0.212868000	0.162631000
				8	-2.463372000	-0.020971000	0.971682000
				8	-3.152009000	1.705602000	-0.350665000
				6	-3.320392000	0.692912000	0.350092000
				6	-4.756149000	0.120843000	0.451454000
				9	-5.093456000	-0.257680000	1.745873000
				9	-5.732849000	0.997838000	0.016809000
				9	-4.859840000	-1.031164000	-0.344747000

**d. proton transfer transition states**

**22. [Cp\*MoH (PMe<sub>3</sub>)<sub>2</sub> (CO)] CF<sub>3</sub>COOH (B-TS) · E =**

-1350.77698017

6	2.974746000	0.114749000	1.115503000
6	2.635276000	-1.278267000	1.009217000
6	1.428954000	-1.491334000	1.769632000
6	1.031195000	-0.244534000	2.346481000
6	1.984975000	0.743521000	1.952827000
42	0.996763000	-0.055367000	-0.127208000
15	0.699982000	2.346751000	-0.889917000
15	-0.187727000	-1.953778000	-1.341121000
1	-0.723915000	0.438316000	-0.569743000
6	1.910646000	-0.081171000	-1.829381000
8	2.555477000	-0.116588000	-2.817079000
1	-1.558595000	-2.208203000	-3.373331000
6	-0.238851000	2.500590000	-2.480833000
1	-1.831789000	-0.633812000	-2.583253000
6	-1.071455000	-1.368800000	-2.864119000
6	-0.124739000	-0.051826000	3.291622000
1	-1.028958000	-0.554911000	2.938781000
1	0.121093000	-0.443433000	4.289048000
1	-0.380656000	1.004931000	3.405080000
6	0.836250000	-2.824436000	2.142310000
1	1.021194000	-3.594744000	1.383629000
1	1.286249000	-3.185187000	3.078645000
1	-0.242770000	-2.756167000	2.306179000
6	3.539964000	-2.348622000	0.454933000
1	4.063063000	-2.014382000	-0.446108000
1	4.303223000	-2.628583000	1.195581000
1	2.989304000	-3.258043000	0.199405000
6	4.281015000	0.725151000	0.677843000
1	4.199502000	1.805981000	0.534639000
1	5.060835000	0.554038000	1.434393000
1	4.635426000	0.293965000	-0.263149000
6	2.093906000	2.126931000	2.537779000
1	1.125671000	2.507036000	2.873278000
1	2.755388000	2.107589000	3.415697000
1	2.518155000	2.849858000	1.835472000
1	-1.254522000	2.125658000	-2.320116000
1	-0.360828000	-0.893772000	-3.546253000
6	0.858778000	-3.325247000	-2.026965000
1	0.247668000	-4.00052000	-2.636746000
1	1.659862000	-2.908400000	-2.644572000
1	1.309555000	-3.901113000	-1.213840000
6	-1.546705000	-2.886428000	-0.488646000
1	-2.061638000	-3.535523000	-1.205910000
1	-1.140749000	-3.503381000	0.316334000
1	-2.259588000	-2.177959000	-0.056680000
6	2.228346000	3.334894000	-1.262004000
1	1.953079000	4.308032000	-1.684072000
1	2.814809000	3.501412000	-0.353915000
1	2.847696000	2.792980000	-1.983256000
6	-0.296410000	3.478909000	0.186187000
1	-0.380526000	4.467416000	-0.280422000
1	-1.297957000	3.046123000	0.288937000
1	0.158334000	3.587869000	1.173202000
1	-0.294378000	3.550763000	-2.789677000
1	0.246476000	1.917365000	-3.268105000
1	-1.089152000	0.212868000	0.162631000
8	-2.463372000	-0.020971000	0.971682000
8	-3.152009000	1.705602000	-0.350665000
6	-3.320392000	0.692912000	0.350092000
6	-4.756149000	0.120843000	0.451454000
9	-5.093456000	-0.257680000	1.745873000
9	-5.732849000	0.997838000	0.016809000
9	-4.859840000	-1.031164000	-0.344747000

**23. [Cp\*Mo (CO) (PMe<sub>3</sub>)<sub>2</sub>H] (CF<sub>3</sub>COOH)<sub>2</sub> (D-TS) E =**

-1877.49626837

6	4.195936000	-0.201821000	-0.621999000
6	4.131528000	0.344047000	0.707233000
6	3.386201000	1.574407000	0.639637000

**21. [Cp\*Mo(η<sup>2</sup>-H<sub>2</sub>)(CO)(PMe<sub>3</sub>)<sub>2</sub>](CF<sub>3</sub>COOH)<sub>2</sub>(D') E =**

-1877.50247403

6	-4.114988000	0.007610000	0.300808000
6	-3.899987000	-0.325703000	-1.082235000
6	-3.162597000	0.758361000	-1.683541000
6	-2.912469000	1.744820000	-0.681397000
6	-3.497496000	1.287687000	0.541365000
42	-1.835041000	-0.377842000	0.001378000
15	-1.128393000	-0.468497000	2.482354000
15	-0.430460000	-1.414056000	-1.869546000
1	0.040836000	-0.061570000	0.170299000
1	-1.955685000	-2.272409000	0.419821000
8	-2.151787000	-3.407681000	0.650397000
1	1.455049000	-2.962892000	





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1	-3.499277000	0.948339000	-1.606650000	1	0.759031000	3.533197000	1.248831000
1	-4.450713000	1.360760000	-0.172409000	1	2.248782000	2.585431000	1.143720000
1	-3.112550000	2.397395000	-0.679073000	6	0.204083000	-3.334009000	-1.746755000
6	-3.202660000	-1.815253000	-0.605577000	1	0.897763000	-4.142452000	-2.006513000
1	-2.723962000	-2.793601000	-0.708522000	1	-0.608616000	-3.749136000	-1.143580000
1	-4.204320000	-1.984096000	-0.182283000	1	-0.228553000	-2.923878000	-2.664922000
1	-3.335064000	-1.409151000	-1.613153000	6	1.916961000	-2.958215000	0.509483000
6	-1.425917000	-2.674915000	1.913718000	1	2.534441000	-3.755689000	0.079224000
1	-0.525493000	-2.780603000	2.525675000	1	2.546687000	-2.296605000	1.111745000
1	-2.282544000	-2.943468000	2.549109000	1	1.174961000	-3.409578000	1.173728000
1	-1.379630000	-3.417801000	1.111372000	1	3.005102000	-2.619489000	-2.210244000
1	3.205326000	-0.997051000	-1.493401000	1	2.131072000	-1.218984000	-2.888164000
1	1.924766000	1.549845000	-2.863232000	1	2.299414000	0.100326000	1.813665000
6	-0.256582000	3.380353000	-1.656217000	8	2.933555000	0.089885000	2.558003000
1	0.313577000	4.287435000	-1.889382000	6	4.264093000	0.243062000	2.029492000
1	-0.631223000	2.941964000	-2.586734000	1	4.944165000	0.216938000	2.884519000
1	-1.117386000	3.653890000	-1.038333000	1	4.532722000	-0.573080000	1.343975000
6	1.534681000	3.178799000	0.564860000	1	4.393613000	1.202374000	1.509008000
1	2.048765000	4.048195000	0.137996000				