

Supplementary information

Exploring Phosphine Electronic Effects on Molybdenum Complexes: A Combined Photoelectron Spectroscopy and Energy Decomposition Analysis Study

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I- Synthetic procedure

a. General considerations

All reagents were obtained from commercial sources and used as received. Solvents (THF, DCM, toluene and Et₂O) were purified and dried over Braun solvent purification system (MB-SPS-800) or dried by standard procedures prior to use.¹ Analytical Thin Layer Chromatography (TLC) was carried out on Merck silica gel60 F₂₅₄. Products were revealed by ultraviolet light (254 or 366 nm) and stained with dyeing reagents solutions as 5% phosphomolybdic acid solution, potassium permanganate solution or *p*-anisaldehyde solution in ethanol followed by gentle heating. Flash chromatography was performed with Merck silica gel 60 (230-400 mesh). ¹H, ¹³C and ³¹P NMR spectra were recorded in CDCl₃ at ambient temperature on Bruker Avance III 300 or 400 spectrometers operating at 300 and 400 MHz respectively for ¹H. ¹³C nucleus was observed with ¹H decoupling. Solvent residual signals were used as internal standard.² Chemical shifts (δ) and coupling constants (*J*) are given in ppm and Hz respectively. The peaks patterns are indicated as the following format multiplicity (s: singlet; d: doublet; t: triplet; q: quartet; sept: septuplet; m: multiplet; dd: doublet of doublet; dt: doublet of triplet; dm: doublet of multiplet, etc.). The prefix br. indicates a broadened signal. IR spectra were recorded on a Bruker Alpha Platinum ATR.

b. Phosphines preparation

1-(Diphenylphosphino)-1*H*-pyrrole (PPh₂Pyrl)

Prepared according to Beller's procedure³ in 81% yield as a yellow light solid.

¹H NMR (300 MHz, CDCl₃): δ = 7.29-7.22 (m, 6H, *H*^{Ar}), 7.20-7.15 (m, 4H, *H*^{Ar}), 6.74 (br s, 2H, *H*^{Pyrl}), 6.22 (br s, 2H, *H*^{Pyrl}).

^{13}C NMR (100 MHz, CDCl_3): $\delta = 137.1$ (d, $J(^{13}\text{C}, ^{31}\text{P}) = 12.6$ Hz, C), 132.0 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 20.8$ Hz, CH), 129.8 (CH), 128.7 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 6.6$ Hz, CH), 125.6 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 12.5$ Hz, CH), 111.6 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 3.6$ Hz, CH).

^{31}P NMR (162 MHz, CDCl_3): $\delta = 47.8$.

1,1'-(Phenylphosphinediyl)bis(1*H*-pyrrole) (PPhPyr₂)

Prepared according to Beller's procedure³ in 66% yield as a white solid.

^1H NMR (300 MHz, CDCl_3): $\delta = 7.24$ - 7.18 (m, 3H, H^{Ar}), 6.98 - 6.93 (m, 2H, H^{Ar}), 6.80 (br s, 4H, H^{Pyr}), 6.19 (br s, 4H, H^{Pyr}).

^{13}C NMR (100 MHz, CDCl_3): $\delta = 136.6$ (d, $J(^{13}\text{C}, ^{31}\text{P}) = 5.6$ Hz, C), 130.5 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 18.7$ Hz, CH), 130.3 (CH), 128.8 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 5.1$ Hz, CH), 124.9 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 14.7$ Hz, CH), 112.5 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 4.3$ Hz, CH).

^{31}P NMR (162 MHz, CDCl_3): $\delta = 70.2$.

Tri(1*H*-pyrrol-1-yl)phosphine (PPyr₃)

Prepared according to Beller's procedure³ in 63% yield as a white solid.

^1H NMR (300 MHz, CDCl_3): $\delta = 6.81$ (br s, 6H, H^{Pyr}), 6.38 (br s, 6H, H^{Pyr}).

^{13}C NMR (100 MHz, CDCl_3): $\delta = 122.8$ (d, $J(^{13}\text{C}, ^{31}\text{P}) = 14.3$ Hz, CH), 113.1 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 4.5$ Hz, CH).

^{31}P NMR (162 MHz, CDCl_3): $\delta = 78.9$.

c. Molybdenum complexes synthesis

Me₃PMo(CO)₅⁴

In a Schlenk were introduced in turn Mo(CO)₆ (2.64 g, 10 mmol), Me₃NO·2H₂O (1.11 g, 10 mmol, 1 equiv.) and 50 mL of degassed acetonitrile (not necessarily dried and distilled). The mixture was stirred at 25 °C until the complete dissolution of the reactants (reaction mixture turned brown at that point). PMe₃ as a molar solution in THF (10 mL, 10 mmol, 1 equiv.) was added and the brown color disappeared rapidly. The reaction mixture was stirred 1 h at 25 °C. Volatiles were removed in vacuo and the residue was dissolved in Et₂O. After a filtration on a plug of Celite®, the evaporation gave to title product as a brown solid (2.85 g, 91% yield).

¹H NMR (400 MHz, CDCl₃): δ = 1.45 (d, *J*(H,P) = 7.3 Hz, 9H, CH₃).

¹³C NMR (100 MHz, CDCl₃): δ = 210.1 (d, *J*(¹³C, ³¹P) = 20.9 Hz, CO^{trans}), 205.9 (d, *J*(¹³C, ³¹P) = 9.7 Hz, CO^{cis}), 20.7 (d, *J*(¹³C, ³¹P) = 25.0 Hz, CH₃).

³¹P NMR (162 MHz, CDCl₃): δ = -14.9 (decup, *J*(H,P) = 7.3 Hz).

IR (ATR, cm⁻¹): 3764, 2976, 2911, 2070, 2013, 1931, 1842, 1423, 1287, 1105, 1065, 1002, 941, 851, 732, 674, 604, 574.

Et₃PMo(CO)₅

In a Schlenk were introduced in turn Mo(CO)₆ (2.64 g, 10 mmol), Me₃NO·2H₂O (1.11 g, 10 mmol, 1 equiv.) and 50 mL of degassed acetonitrile (not necessarily dried and distilled). The mixture was stirred at 25 °C until the complete dissolution of the reactants (reaction mixture turned brown at that point). PEt₃ as a molar solution in THF (10 mL, 10 mmol, 1 equiv.) was added and the brown color disappeared rapidly. The reaction mixture was stirred 1 h at 25 °C. Volatiles were removed in vacuo and the residue was dissolved in Et₂O. After a filtration on a plug of Celite®, the evaporation gave to title product as a brown oil (3.44 g, 91% yield).

¹H NMR (400 MHz, CDCl₃): δ = 1.45 (dd, $J(\text{H,H}) = 7.6$ Hz, $J(\text{H,P}) = 6.5$ Hz, 6H, CH₂), 1.07 (dt, $J(\text{H,H}) = 7.6$ Hz, $J(\text{H,P}) = 15.4$ Hz, 9H, CH₃).

¹³C NMR (100 MHz, CDCl₃): δ = 209.9 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 20.9$ Hz, CO^{trans}), 206.3 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 9.4$ Hz, CO^{cis}), 21.0 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 21.7$ Hz, CH₂), 7.8 (s, CH₃).

¹³P NMR (162 MHz, CDCl₃): δ = 20.1 (m).

IR (ATR, cm⁻¹): 2973, 2941, 2910, 2883, 2067, 1984, 1900, 1458, 1420, 1381, 1258, 1035, 1004, 929, 767, 717, 609, 582.

***i*Pr₃PMo(CO)₅**

In a Schlenk were introduced in turn Mo(CO)₆ (1.65 g, 6.25 mmol), Me₃NO·2H₂O (0.70 g, 6.25 mmol, 1 equiv.) and 50 mL of degassed acetonitrile (not necessarily dried and distilled). The mixture was stirred at 25 °C until the complete dissolution of the reactants (reaction mixture turned brown at that point). *Pi*Pr₃ (1 g, 6.25 mmol, 1 equiv.) was added and the brown color disappeared rapidly. The reaction mixture was stirred 1 h at 25 °C. Volatiles were removed in vacuo and the residue was dissolved in Et₂O. After a filtration on a plug of Celite®, the evaporation gave to title product as a brown solid (2.3 g, 96% yield).

¹H NMR (300 MHz, CDCl₃): δ = 2.12 (dsept, $J(\text{H,P}) = 7.2$ Hz, $J(\text{H,H}) = 7.1$ Hz, 3H, CH), 1.21 (dd, $J(\text{H,P}) = 13.7$ Hz, $J(\text{H,H}) = 7.1$ Hz, 18H, CH₃).

¹³C NMR (75 MHz, CDCl₃): δ = 209.9 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 21.5$ Hz, CO^{trans}), 207.0 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 8.8$ Hz, CO^{cis}), 26.4 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 15.5$ Hz, CH), 19.8 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 1.7$ Hz, CH₃).

¹³P NMR (121.5 MHz, CDCl₃): δ = -14.9 (m).

IR (ATR, cm⁻¹): 2966, 2936, 2877, 2066, 2015, 1981, 1880, 1459, 1385, 1370, 1298, 1241, 1156, 1089, 1058, 1027, 927, 881, 650, 610, 580, 521.

Ph₃PMo(CO)₅

In a Schlenk were introduced in turn Mo(CO)₆ (1.85 g, 7 mmol), Me₃NO·2H₂O (0.78 g, 7 mmol, 1 equiv.) and 50 mL of degassed acetonitrile (not necessarily dried and distilled). The mixture was stirred at 25 °C until the complete dissolution of the reactants (reaction mixture turned brown at that point). PPh₃ (1.83 g, 7 mmol, 1 equiv.) was added and the brown color disappeared rapidly. The reaction mixture was stirred 1 h at 25 °C. Volatiles were removed in vacuo and the product was purified by crystallization for Et₂O and petroleum ether to afford a brown light solid (2.15 g, 63% yield).

¹H NMR (400 MHz, CDCl₃): δ = 7.49-7.43 (m, 15H, H^{Ar}).

¹³C NMR (100 MHz, CDCl₃): δ = 210.3 (d, *J*(¹³C,³¹P) = 22.9 Hz, CO^{trans}), 205.7 (d, *J*(¹³C,³¹P) = 8.8 Hz, CO^{cis}), 135.5 (d, *J*(¹³C,³¹P) = 35.4 Hz, C), 132.9 (d, *J*(¹³C,³¹P) = 12.5 Hz, CH), 130.1 (d, *J*(¹³C,³¹P) = 2.0 Hz, CH), 128.6 (d, *J*(¹³C,³¹P) = 9.5 Hz, CH).

¹³P NMR (162 MHz, CDCl₃): δ = 37.7 (m).

IR (ATR, cm⁻¹): 2976, 2911, 2071, 1845, 1423, 1287, 1002, 942, 851, 733, 675, 604, 576.

MePh₂PMo(CO)₅

In a Schlenk were introduced in turn Mo(CO)₆ (1.32 g, 5 mmol), Me₃NO·2H₂O (0.55 g, 5 mmol, 1 equiv.) and 50 mL of degassed acetonitrile (not necessarily dried and distilled). The mixture was stirred at 25 °C until the complete dissolution of the reactants (reaction mixture turned brown at that point). PMePh₂ (1 g, 5 mmol, 1 equiv.) was added and the brown color disappeared rapidly. The reaction mixture was stirred 1 h at 25 °C. Volatiles were removed in vacuo and the residue was dissolved in Et₂O. After a filtration on a plug of Celite®, the evaporation gave to title product as a yellow oil (2.10 g, 96% yield).

¹H NMR (400 MHz, CDCl₃): δ = 7.56-7.44 (m, 10H, H^{Ar}), 2.10 (d, *J*(H,P) = 6.0 Hz, 3H, CH₃).

¹³C NMR (100 MHz, CDCl₃): δ = 210.2 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 22.3$ Hz, CO^{trans}), 205.7 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 9.1$ Hz, CO^{cis}), 137.4 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 36.0$ Hz, C), 131.2 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 12.2$ Hz, CH), 130.0 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 2.0$ Hz, CH), 128.7 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 9.5$ Hz, CH), 19.7 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 24.6$ Hz, CH₃).

¹³P NMR (162 MHz, CDCl₃): δ = 15.7 (m).

IR (ATR, cm⁻¹): 3059, 2364, 2070, 1988, 1907, 1483, 1435, 1290, 1187, 1096, 1000, 891, 742, 725, 693, 607, 582, 507.

Me₂PhPMo(CO)₅

In a Schlenk were introduced in turn Mo(CO)₆ (1.91 g, 7.25 mmol), Me₃NO·2H₂O (0.81 g, 7.25 mmol, 1 equiv.) and 50 mL of degassed acetonitrile (not necessarily dried and distilled). The mixture was stirred at 25 °C until the complete dissolution of the reactants (reaction mixture turned brown at that point). PMe₂Ph (1 g, 7.25 mmol, 1 equiv.) was added and the brown color disappeared rapidly. The reaction mixture was stirred 1 h at 25 °C. Volatiles were removed in vacuo and the residue was dissolved in Et₂O. After a filtration on a plug of Celite®, the evaporation gave to title product as a brown oil (2.6 g, 96% yield).

¹H NMR (400 MHz, CDCl₃): δ = 7.46-7.33 (m, 5H, H^{Ar}), 1.74 (d, $J(\text{H}, \text{P}) = 6.8$ Hz, 6H, CH₃).

¹³C NMR (100 MHz, CDCl₃): δ = 210.2 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 21.4$ Hz, CO^{trans}), 205.7 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 9.4$ Hz, CO^{cis}), 139.1 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 35.7$ Hz, C), 129.5 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 2.0$ Hz, CH), 128.9 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 3.3$ Hz, CH), 128.8 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 1.4$ Hz, CH), 19.5 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 24.7$ Hz, CH₃).

¹³P NMR (162 MHz, CDCl₃): δ = -2.3 (m).

IR (ATR, cm⁻¹): 3061, 2977, 2912, 2070, 1887, 1488, 1435, 1423, 1301, 1285, 1097, 944, 905, 836, 741, 692, 606, 576.

Ph₂PyrlPMo(CO)₅

In a Schlenk were introduced in turn Mo(CO)₆ (528 mg, 2 mmol), Me₃NO·2H₂O (222 mg, 2 mmol, 1 equiv.) and 10 mL of degassed acetonitrile (not necessarily dried and distilled). The mixture was stirred at 25 °C until the complete dissolution of the reactants (reaction mixture turned brown at that point). PPh₂Pyrl (502 mg, 2 mmol, 1 equiv.) was added and the brown color disappeared rapidly. The reaction mixture was stirred 1 h at 25 °C. Volatiles were removed in vacuo and the residue was dissolved in Et₂O. After a filtration on a plug of Celite®, the evaporation gave a crude product which was further purified by silica gel chromatography (Hexane/Et₂O 95:5) to afford the title product as a white solid (725 mg, 74% yield).

¹H NMR (400 MHz, CDCl₃): δ = 7.48-7.45 (m, 6H, *H*^{Ar}), 7.35-7.30 (m, 4H, *H*^{Ar}), 6.89-6.86 (m, 2H, *H*^{Pyrl}), 6.37-6.36 (m, 2H, *H*^{Pyrl}).

¹³C NMR (100 MHz, CDCl₃): δ = 210.2 (d, *J*(¹³C, ³¹P) = 27.0 Hz, CO^{trans}), 204.9 (d, *J*(¹³C, ³¹P) = 9.3 Hz, CO^{cis}), 136.3 (d, *J*(¹³C, ³¹P) = 38.0 Hz, C), 131.02 (d, *J*(¹³C, ³¹P) = 1.8 Hz, CH), 131.01 (d, *J*(¹³C, ³¹P) = 13.8 Hz, CH), 128.8 (d, *J*(¹³C, ³¹P) = 9.6 Hz, CH), 125.8 (d, *J*(¹³C, ³¹P) = 6.4 Hz, CH), 112.6 (d, *J*(¹³C, ³¹P) = 5.1 Hz, CH).

¹³P NMR (162 MHz, CDCl₃): δ = 92.6 (m).

IR (ATR, cm⁻¹): 3137, 3100, 2925, 2079, 2038, 2005, 1920, 1572, 1528, 1480, 1449, 1434, 1286, 1231, 1177, 1100, 1079, 1055, 1038, 997, 931, 864, 844, 731, 702, 689, 603, 574, 540, 520.

PhPyrl₂PMo(CO)₅

In a Schlenk were introduced in turn Mo(CO)₆ (528 mg, 2 mmol), Me₃NO·2H₂O (222 mg, 2 mmol, 1 equiv.) and 10 mL of degassed acetonitrile (not necessarily dried and distilled). The mixture was stirred at 25 °C until the complete dissolution of the reactants (reaction mixture turned brown at that point). PPhPyrl₂ (480 mg, 2 mmol, 1 equiv.) was added and the brown color disappeared

rapidly. The reaction mixture was stirred 1 h at 25 °C. Volatiles were removed in vacuo and the residue was dissolved in Et₂O. After a filtration on a plug of Celite®, the evaporation gave a crude product which was further purified by silica gel chromatography (Hexane/Et₂O 95:5) to afford the title product as a white solid (630 mg, 66% yield).

¹H NMR (400 MHz, CDCl₃): δ = 7.52-7.47 (m, 3H, *H*^{Ar}), 7.23-7.18 (m, 2H, *H*^{Ar}), 6.92-6.90 (m, 4H, *H*^{Pyrl}), 6.38-6.37 (m, 4H, *H*^{Pyrl}).

¹³C NMR (100 MHz, CDCl₃): δ = 208.0 (d, *J*(¹³C, ³¹P) = 32.5 Hz, CO^{trans}), 204.0 (d, *J*(¹³C, ³¹P) = 10.0 Hz, CO^{cis}), 137.3 (d, *J*(¹³C, ³¹P) = 48.8 Hz, C), 131.7 (d, *J*(¹³C, ³¹P) = 1.5 Hz, CH), 129.7 (d, *J*(¹³C, ³¹P) = 14.2 Hz, CH), 129.0 (d, *J*(¹³C, ³¹P) = 10.0 Hz, CH), 124.7 (d, *J*(¹³C, ³¹P) = 7.4 Hz, CH), 113.2 (d, *J*(¹³C, ³¹P) = 5.9 Hz, CH).

³¹P NMR (162 MHz, CDCl₃): δ = 116.2 (m).

IR (ATR, cm⁻¹): 3063, 2927, 2076, 2030, 2001, 1914, 1576, 1521, 1480, 1450, 1433, 1331, 1306, 1287, 1236, 1179, 1160, 1039, 998, 925, 867, 844, 735, 691, 606, 577, 534, 510.

Pyrl₃PMo(CO)₅

In a Schlenk were introduced in turn Mo(CO)₆ (528 mg, 2 mmol), Me₃NO·2H₂O (222 mg, 2 mmol, 1 equiv.) and 10 mL of degassed acetonitrile (not necessarily dried and distilled). The mixture was stirred at 25 °C until the complete dissolution of the reactants (reaction mixture turned brown at that point). PPyrl₃ (458 mg, 2 mmol, 1 equiv.) was added and the brown color disappeared rapidly. The reaction mixture was stirred 1 h at 25 °C. Volatiles were removed in vacuo and the residue was dissolved in Et₂O. After a filtration on a plug of Celite®, the evaporation gave a crude product which was further purified by silica gel chromatography (Hexane/Et₂O 95:5) to afford the title product as a white solid (613 mg, 66% yield).

¹H NMR (400 MHz, CDCl₃): δ = 6.74-6.71 (m, 6H, *H*^{Pyrl}), 6.41-6.40 (m, 6H, *H*^{Pyrl}).

^{13}C NMR (100 MHz, CDCl_3): $\delta = 206.6$ (d, $J(^{13}\text{C}, ^{31}\text{P}) = 39.5$ Hz, CO^{trans}), 203.3 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 11.2$ Hz, CO^{cis}), 123.2 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 8.2$ Hz, CH), 113.8 (d, $J(^{13}\text{C}, ^{31}\text{P}) = 6.5$ Hz, CH).

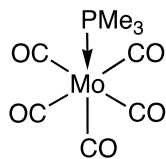
^{31}P NMR (162 MHz, CDCl_3): $\delta = 124.0$ (s).

IR (ATR, cm^{-1}): 3134, 2927, 2082, 2046, 1955, 1920, 1588, 1531, 1451, 1285, 1228, 1202, 1177, 1081, 1055, 1037, 932, 892, 865, 857, 730, 622, 612, 598, 573, 545, 529, 520.

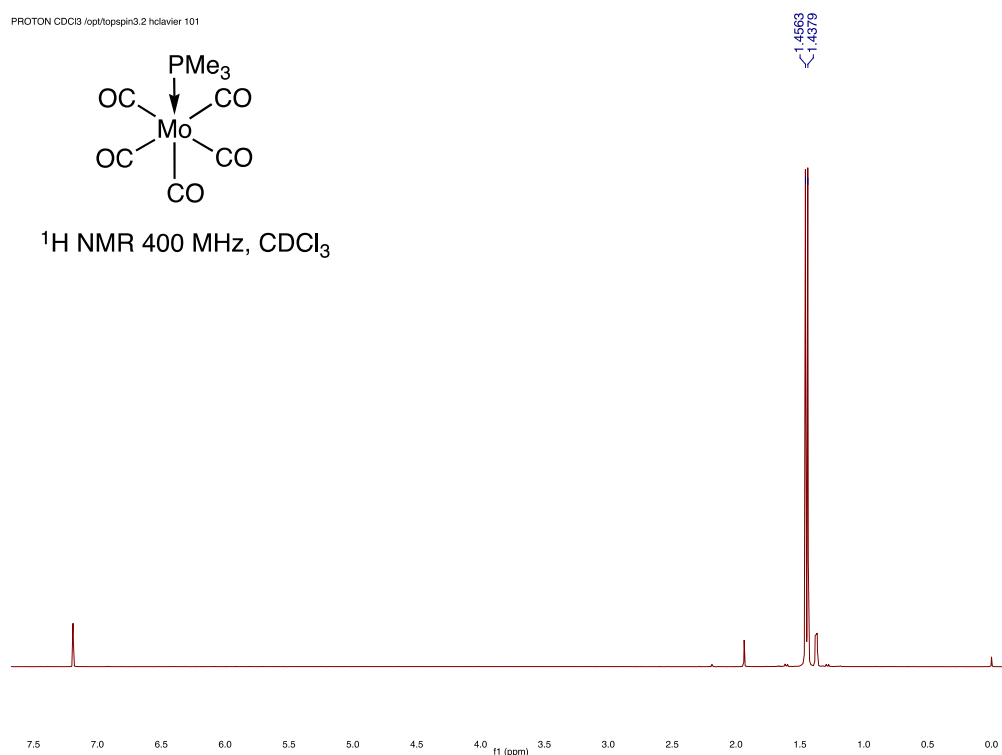
d. NMR spectra

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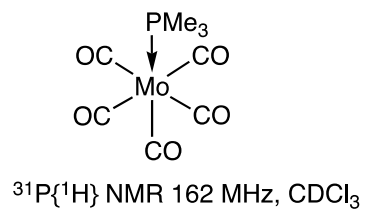
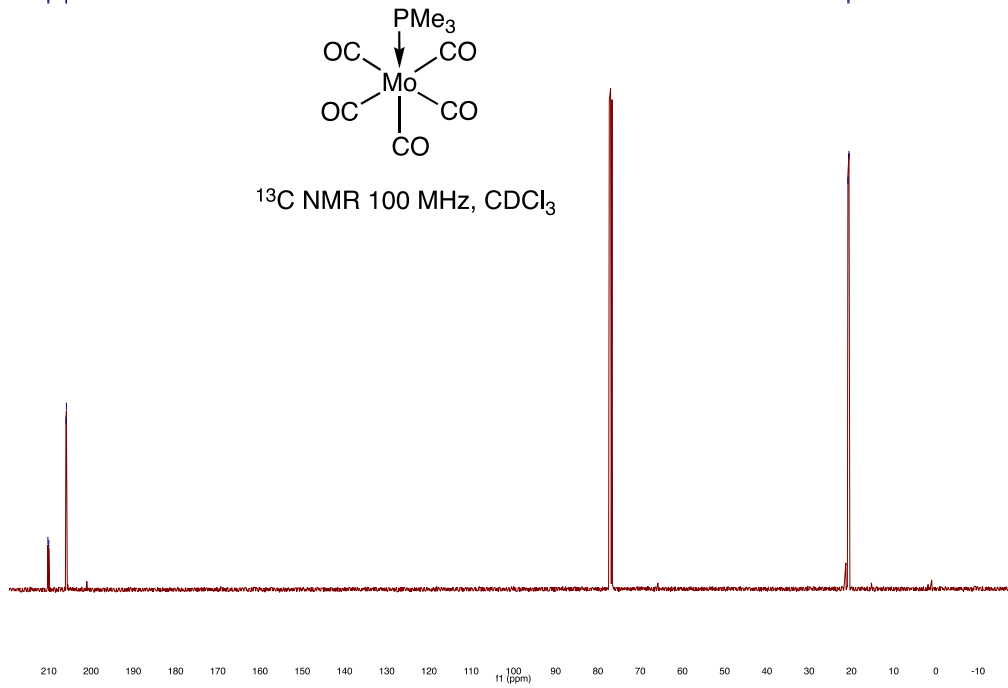


^1H NMR 400 MHz, CDCl_3

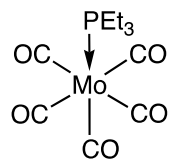


h59.333
C13

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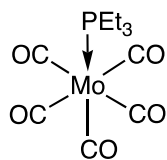
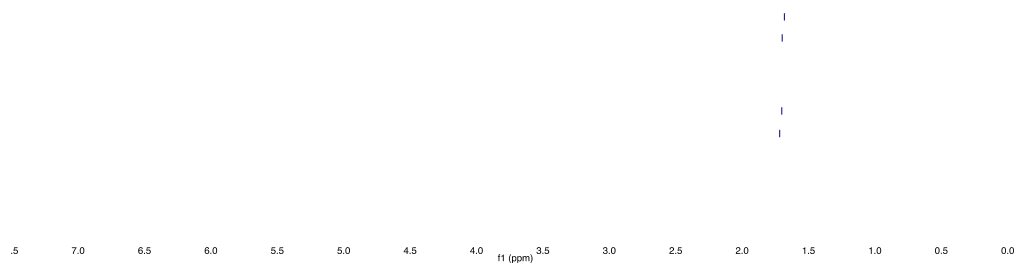


L = PEt₃



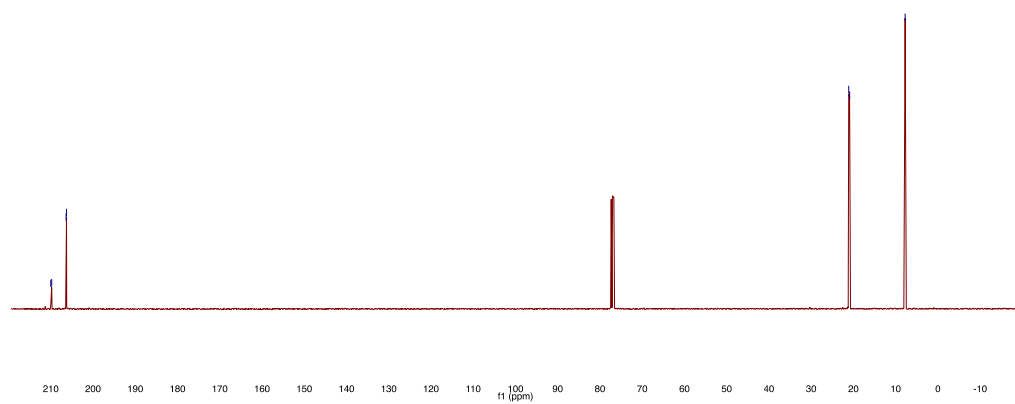
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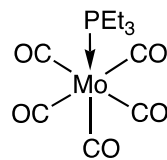
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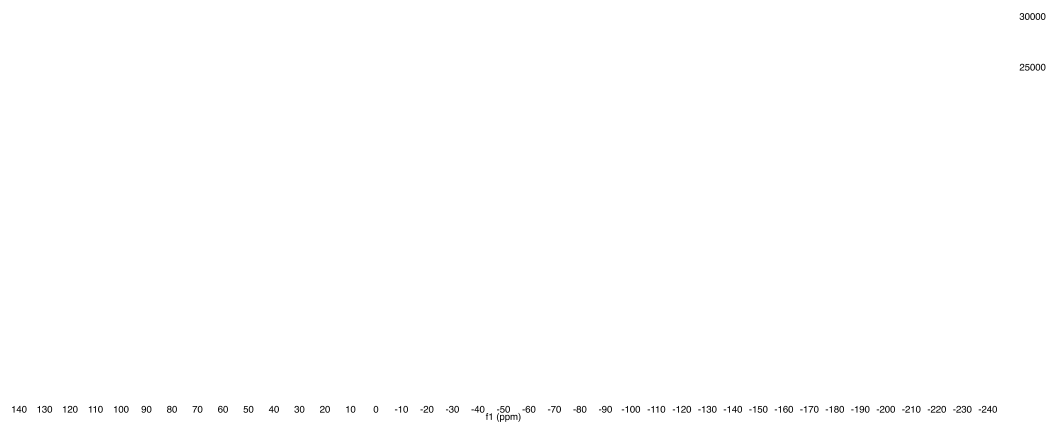
21.1225
20.9079
-7.7580

¹³C NMR 100 MHz, CDCl₃

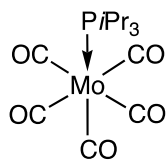




$^{31}\text{P}\{^1\text{H}\}$ NMR 162 MHz, CDCl_3

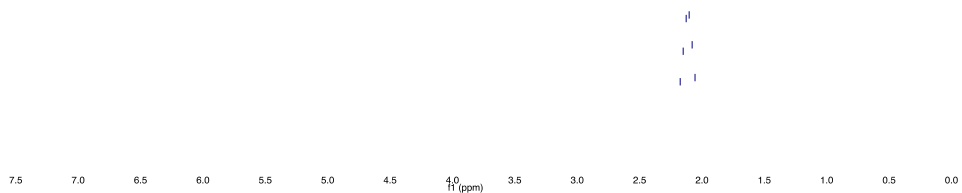


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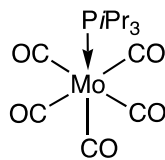


^1H NMR 300 MHz, CDCl_3

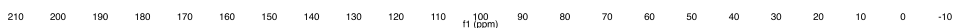
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2.0793
2.0556



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209.7274
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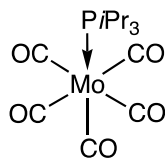


^{13}C NMR 75 MHz, CDCl_3

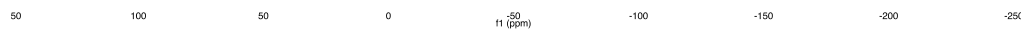


hc9-140_13.fid
P31CPD-jour CDCl3 /opt/topspin3.2/hclavier 23

-57.0935

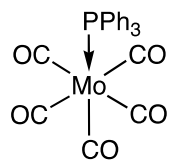


$^{31}\text{P}\{^1\text{H}\}$ NMR 121.5 MHz, CDCl_3

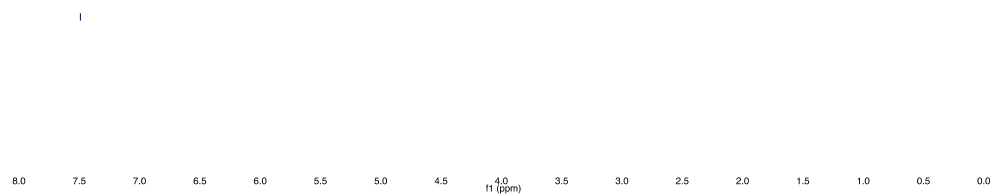


L = PPh₃

7.4912

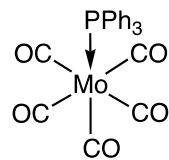


¹H NMR 400 MHz, CDCl₃

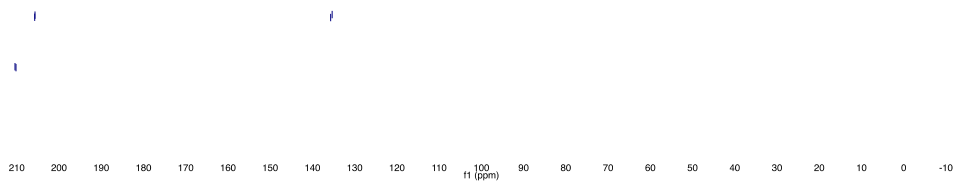


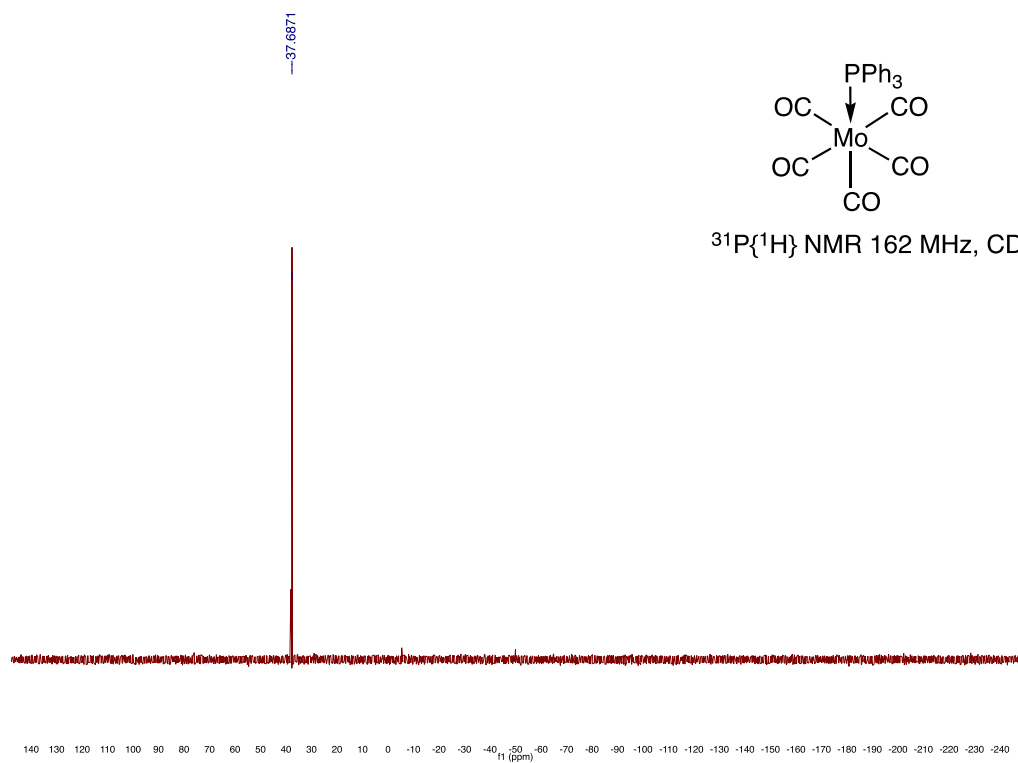
210.4190
210.1913
205.7715
205.6835

135.6060
135.5444



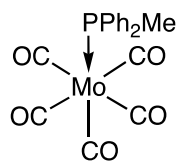
¹³C NMR 100 MHz, CDCl₃



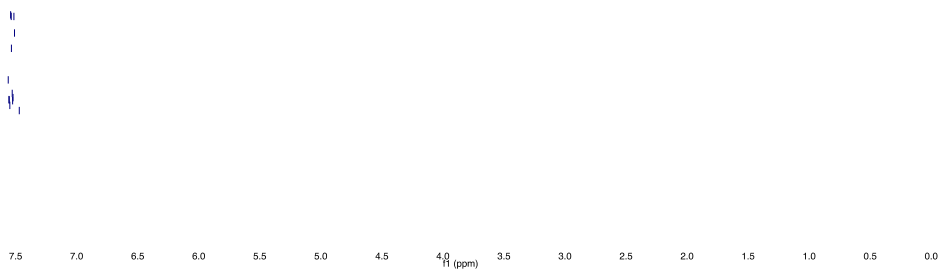


L = PPh₂Me

7.6604
7.6590
7.6478
7.6407
7.6383
7.6340
7.6283
7.6219
7.6211
7.6139
7.6081
7.4701

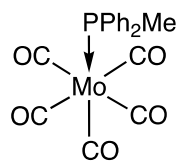


^1H NMR 400 MHz, CDCl_3

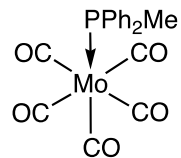
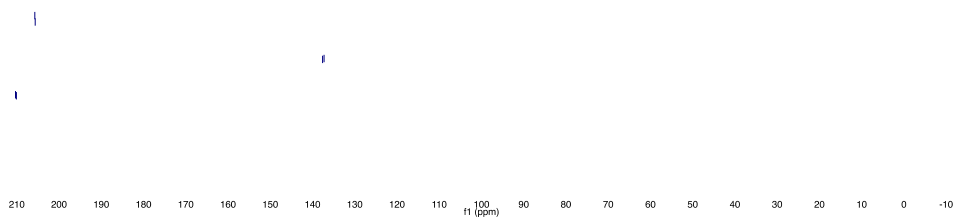


210.3166
210.0952
205.7310
205.6407

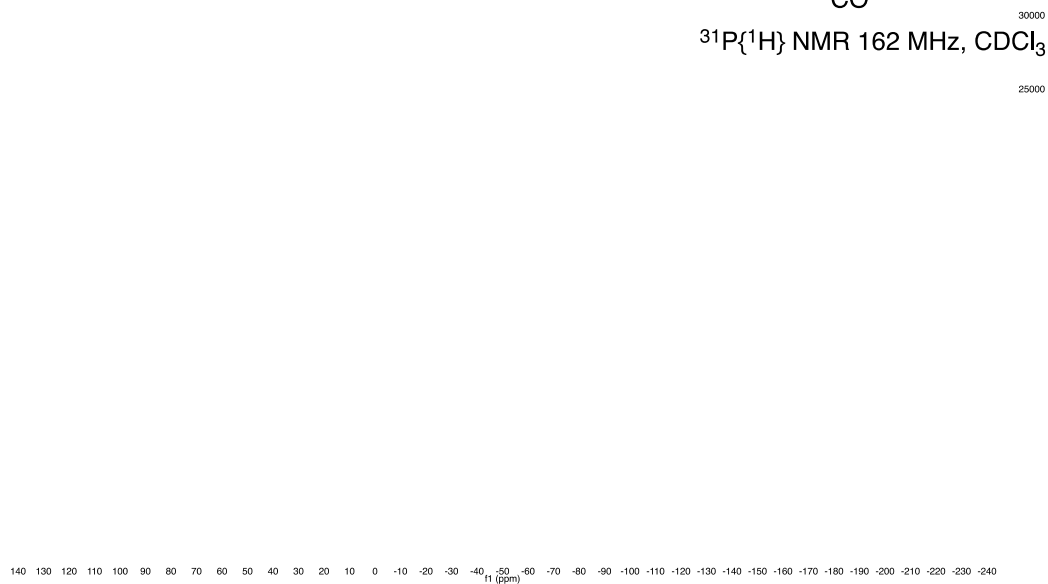
137.6134
137.2559



¹³C NMR 100 MHz, CDCl₃

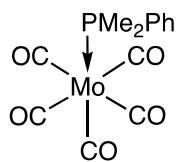


³¹P{¹H} NMR 162 MHz, CDCl₃

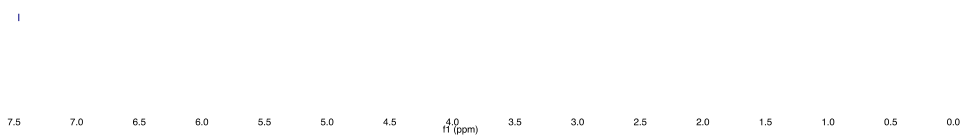


L = PPhMe₂

7.4626

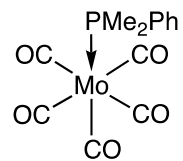


¹H NMR 400 MHz, CDCl₃

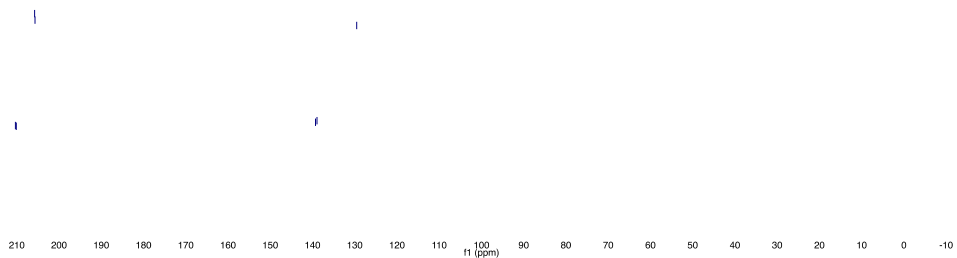


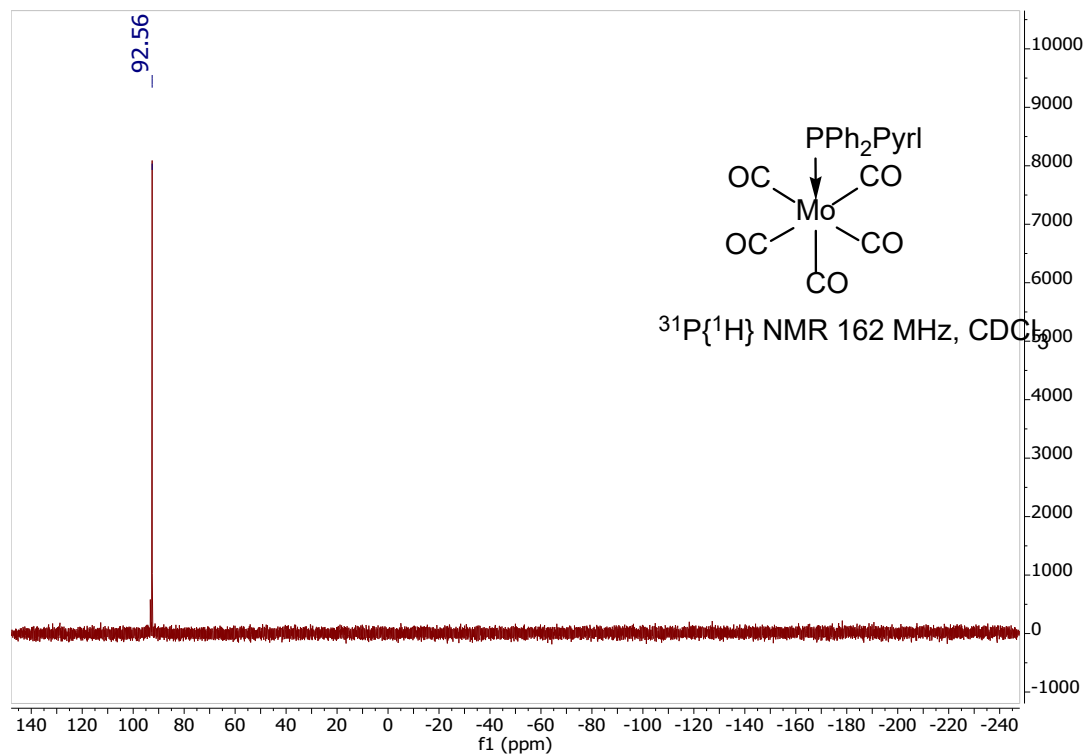
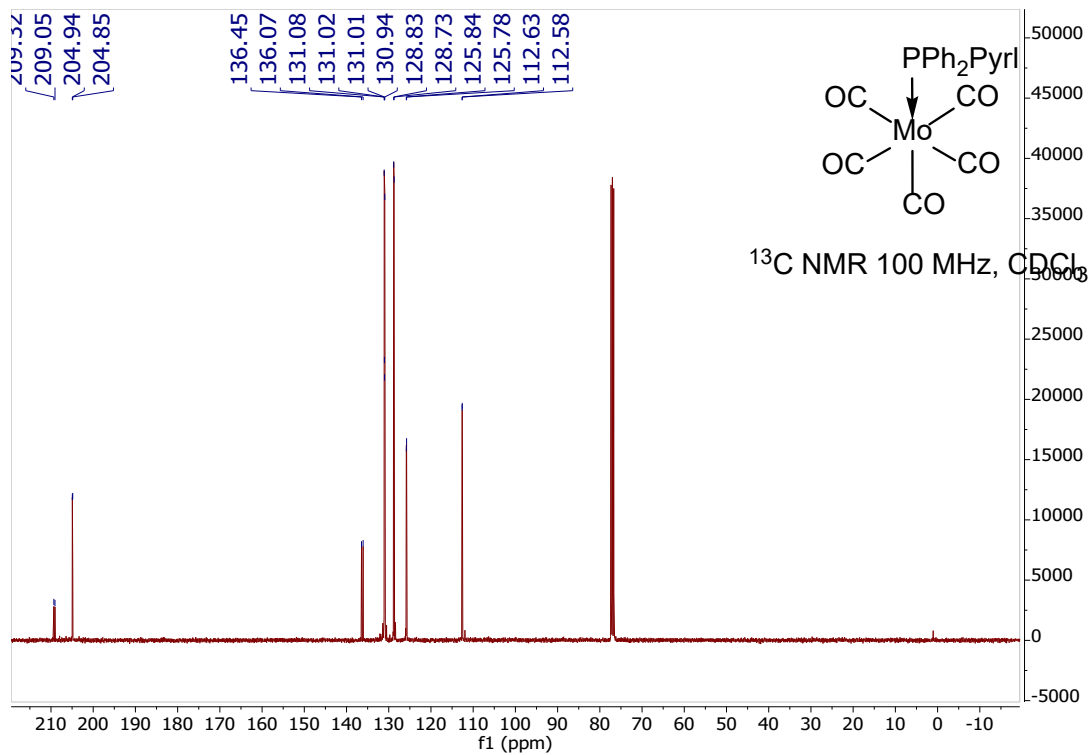
210.3260
210.1132
205.7818
205.6883

139.2856
138.8305
129.5365

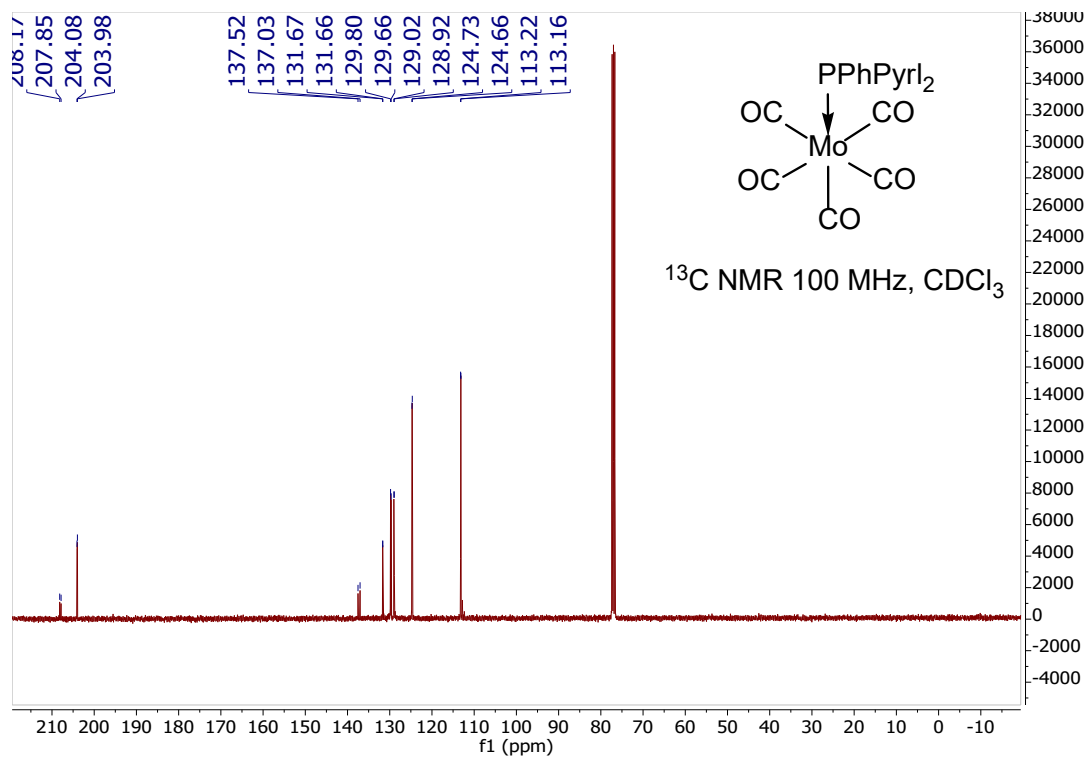
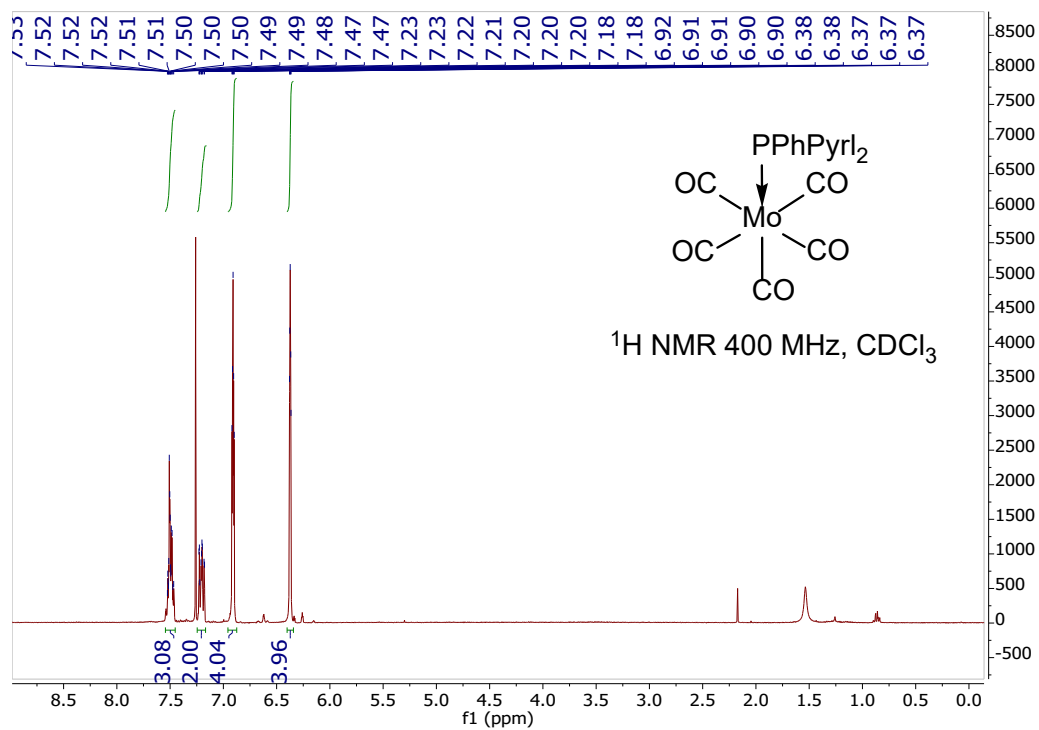


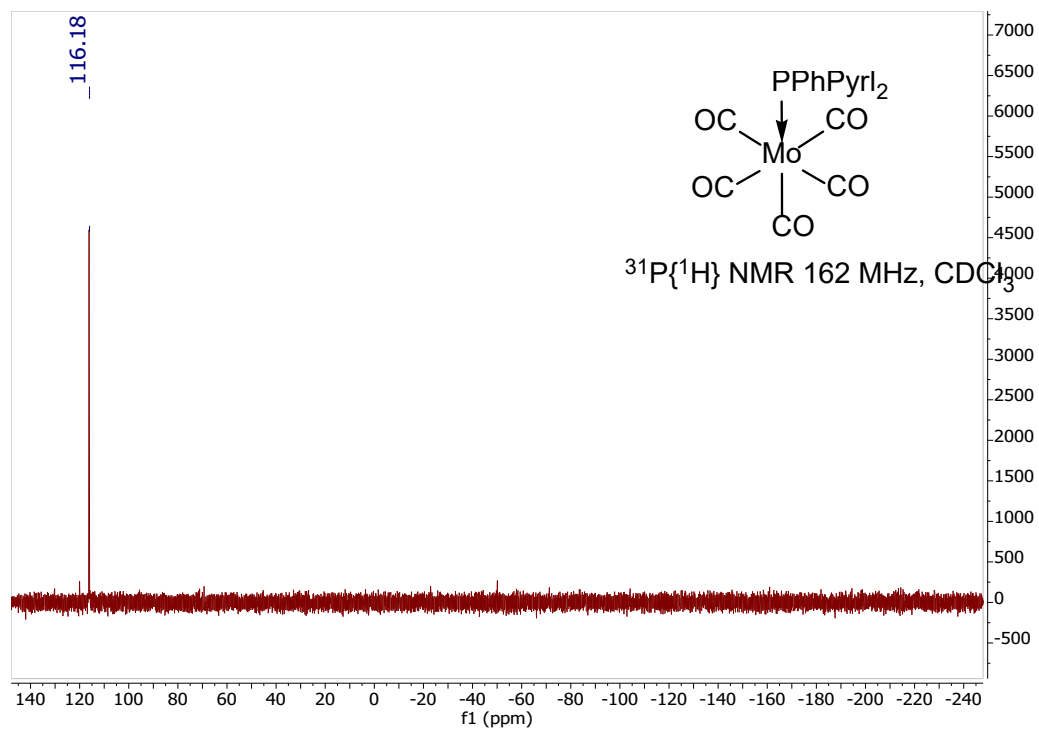
¹³C NMR 100 MHz, CDCl₃



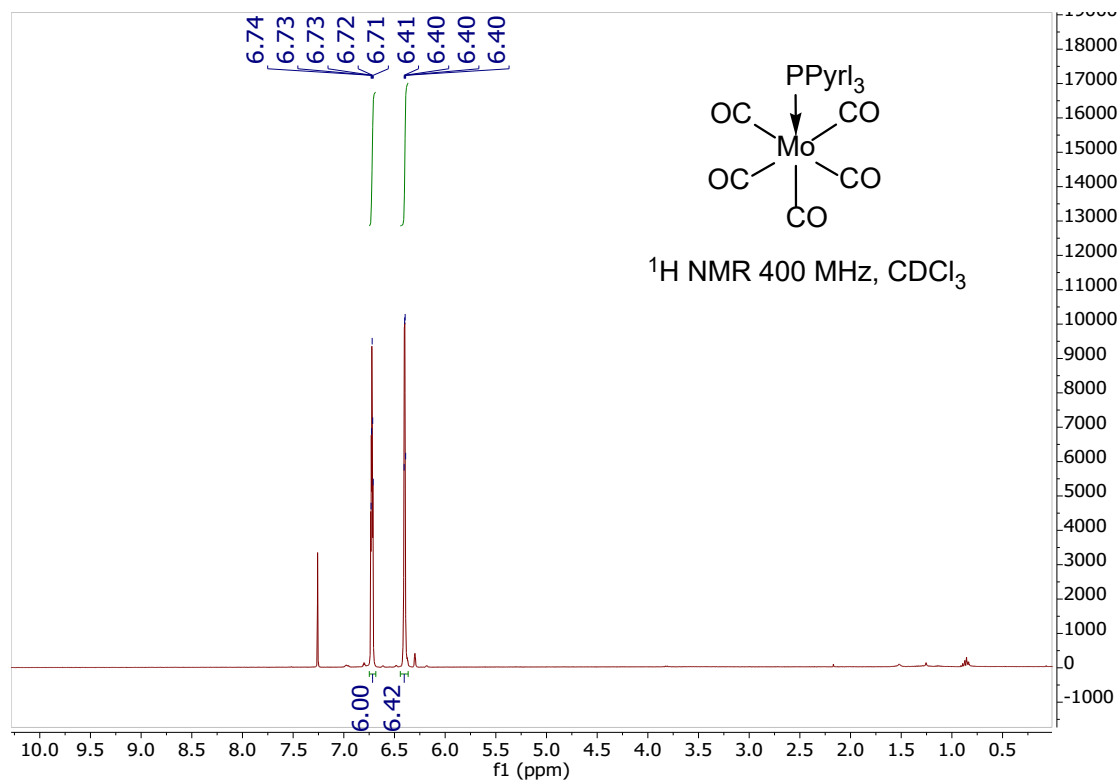


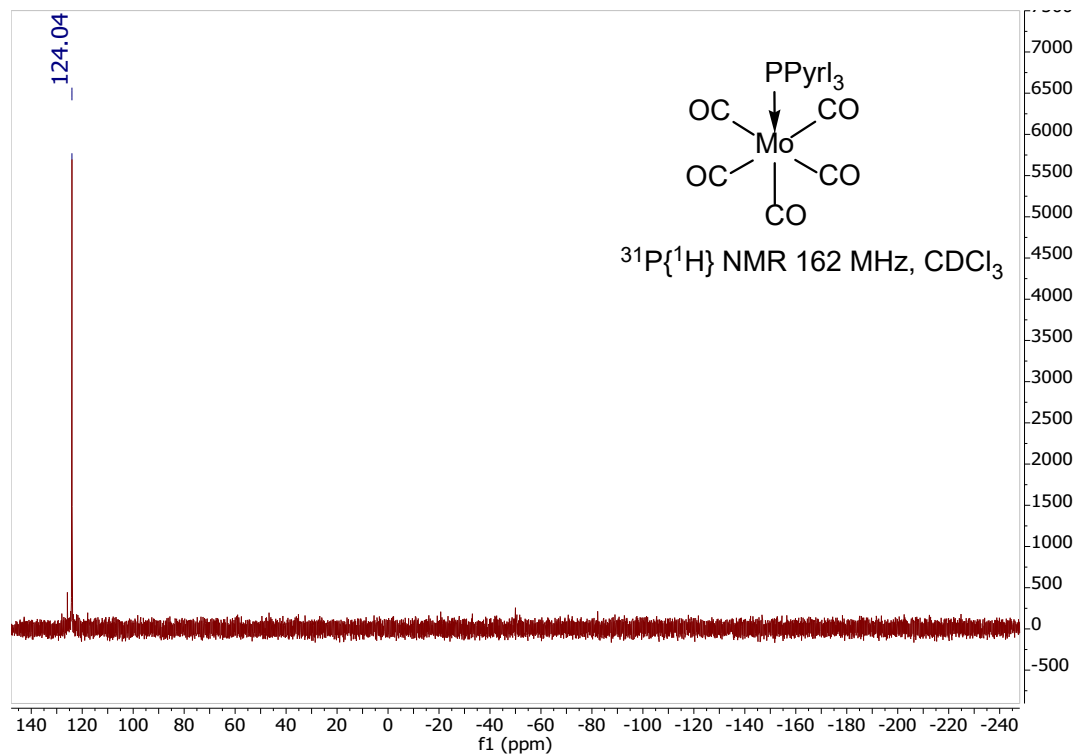
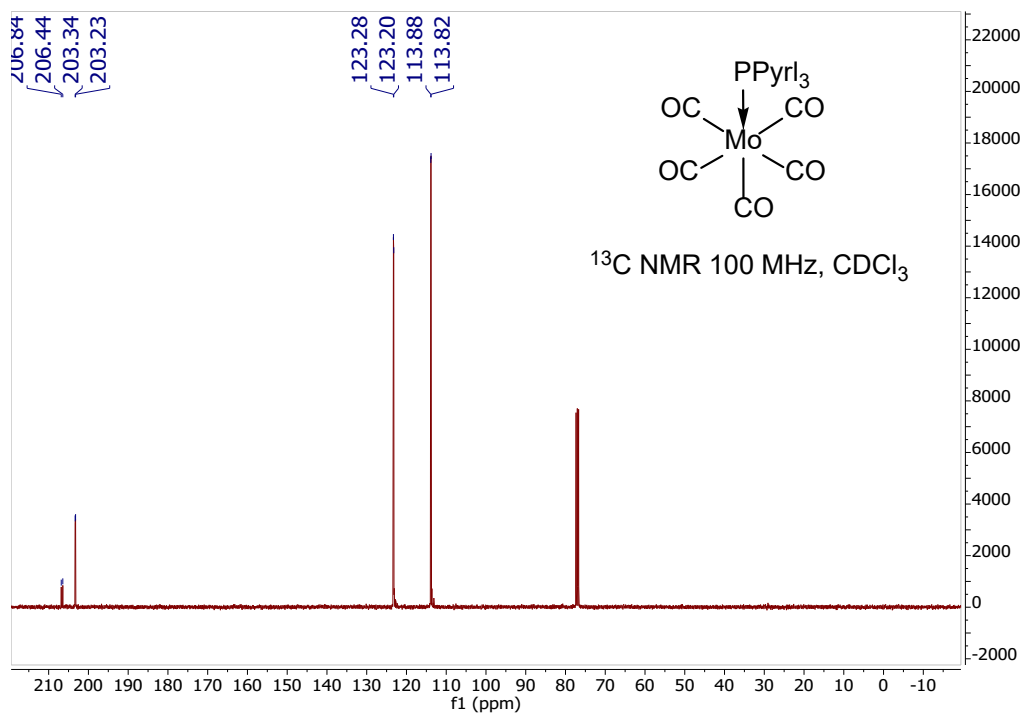
L = PPhPyr1₂





L = PPyrl₃





II- Computational data

a. DFT

Table S1. Calculated electronic and corrected zero-point energies (in hartrees, H) of optimized compounds studied in this work obtained at the LC- ω PBEh($\omega = 0.30$)/Def2-TZVP//PBE0/Def2-TZVP level of theory.

	Electronic energy	Zero-point energy	Vertical electronic energy ^a
Mo(CO)₆	-748.1373266	0.0499194	
Mo(CO)₆⁺⁺	-747.836366	0.0488003	-747.8266789
Mo(CO)₅PMe₃	-1095.815	0.1565263	
Mo(CO)₅PMe₃⁺⁺	-1095.5473	0.1556257	-1095.538395
Mo(CO)₅PEt₃	-1213.694	0.2431849	
Mo(CO)₅PEt₃⁺⁺	-1213.4302	0.2427619	-1213.419988
Mo(CO)₅PiPr₃	-1331.5646	0.3284392	
Mo(CO)₅PiPr₃⁺⁺	-1331.303	0.32806	-1331.293892
Mo(CO)₅PPh₃	-1670.7128	0.3182896	
Mo(CO)₅PPh₃⁺⁺	-1670.4538	0.3178484	-1670.444357
Mo(CO)₅PPh₂Me	-1479.0822	0.2644157	
Mo(CO)₅PPh₂Me⁺⁺	-1478.8195	0.2638452	-1478.81112
Mo(CO)₅PPhMe₂	-1287.4486	0.2105481	
Mo(CO)₅PPhMe₂⁺⁺	-1287.1835	0.2099735	-1287.175185
Mo(CO)₅PPh₂Pyrl	-1648.6692	0.300289	
Mo(CO)₅PPh₂Pyrl⁺⁺	-1648.3989	0.2994692	-1648.393199
Mo(CO)₅PPhPyrl₂	-1626.624	0.2822873	
Mo(CO)₅PPhPyrl₂⁺⁺	-1626.347	0.2810893	-1626.340244
Mo(CO)₅PPyrl₃	-1604.5768	0.2643055	
Mo(CO)₅PPyrl₃⁺⁺	-1604.2749	0.2620864	-1604.284412

^a corresponds to the energy of the ion which the geometry of the neutral.

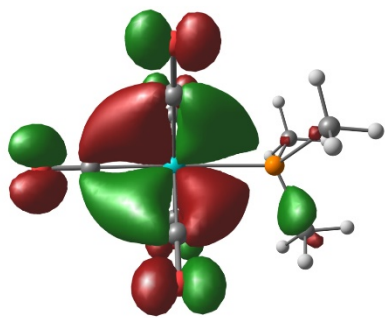
Table S2. Calculated energies (in H) of the first HOMOs of the complexes (-E_{MO}) obtained at the LC- ω PBEh($\omega = 0.30$)/Def2-TZVP//PBE0/Def2-TZVP level of theory.

L	-E _{MO}
PMe ₃	0.29752, 0.29766, 0.30476, 0.38071
PEt ₃	0.29635, 0.2968, 0.30432, 0.37229, 0.41848
PiPr ₃	0.29468, 0.2953, 0.30532, 0.36212, 0.39739
PPh ₃	0.29528, 0.2957, 0.30251, 0.34133, 0.35653, 0.3606, 0.36533, 0.36809, 0.37531
PPh ₂ Me	0.29613, 0.29733, 0.30402, 0.34572, 0.36302, 0.36679, 0.37084
PPhMe ₂	0.29668, 0.29755, 0.30458, 0.3529, 0.36681, 0.39675
PPh ₂ Pyr	0.30248, 0.30381, 0.30904, 0.32065, 0.34608, 0.35992, 0.36529, 0.37092, 0.37504
PPhPyr ₂	0.30952, 0.31121, 0.31471, 0.32357, 0.32819, 0.35019, 0.36719, 0.37235, 0.37403
PPyr ₃	0.31739, 0.31782, 0.32072, 0.32701, 0.32748, 0.34335, 0.35624, 0.37111, 0.37343

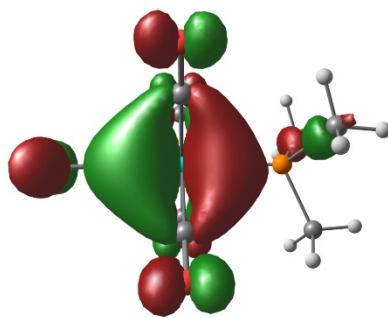
Table S3. Calculated electronic energies (in H) of the L moiety obtained at the PBE0/Def2-TZVP level of theory.

L	E _{el} (H)	
	L	L ⁺
PMe ₃	-460.87096	-460.5639024
PEt ₃	-578.69859	-578.4019186
PiPr ₃	-696.51526	-696.2382331
PPh ₃	-1035.589	-1035.314681
PPh ₂ Me	-844.01588	-843.7334703
PPhMe ₂	-652.44292	-652.1529302
PPh ₂ Pyr	-1013.5487	-1013.265685
PPhPyr ₂	-991.50976	-991.2266455
PPyr ₃	-969.46796	-969.1729658

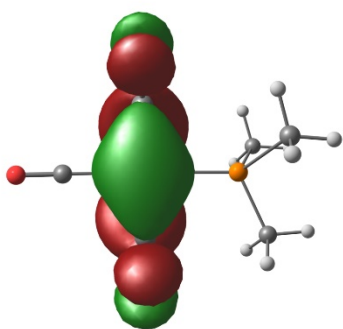
$L = \text{PMe}_3$



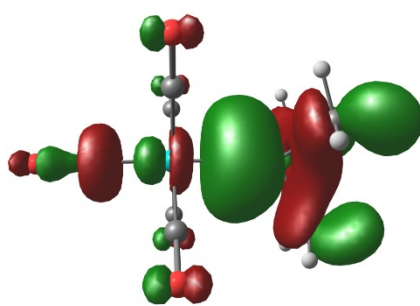
HOMO (e)



HOMO-1 (e)

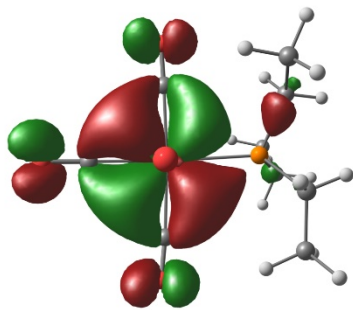


HOMO-2 (b₂)

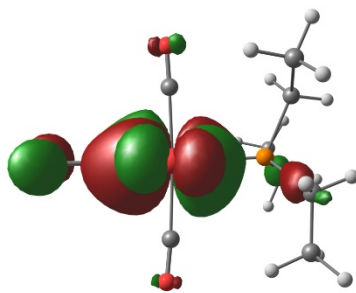


HOMO-3

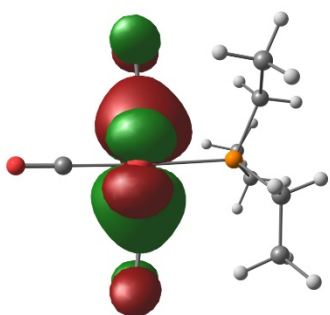
$L = \text{PEt}_3$



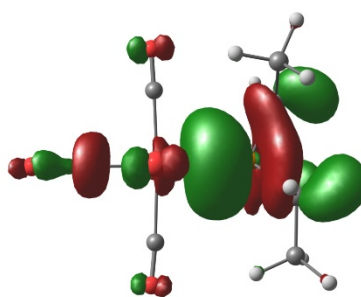
HOMO (e)



HOMO-1 (e)

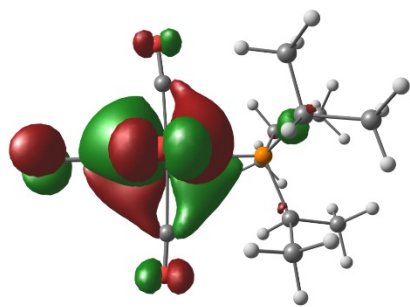


HOMO-2 (b2)

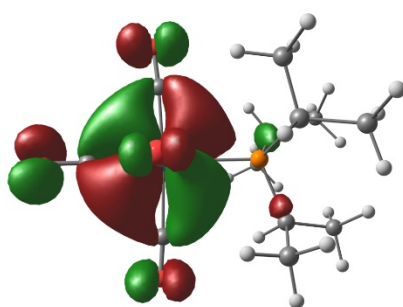


HOMO-3

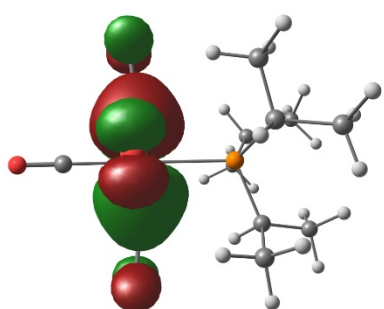
$L = \text{P}i\text{Pr}_3$



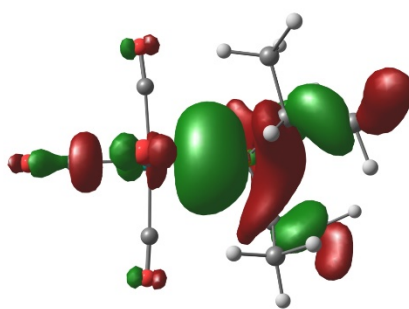
HOMO (e)



HOMO-1 (e)

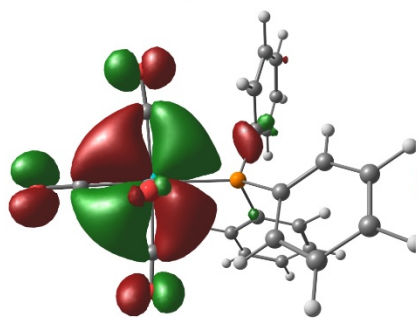


HOMO-2 (b₂)

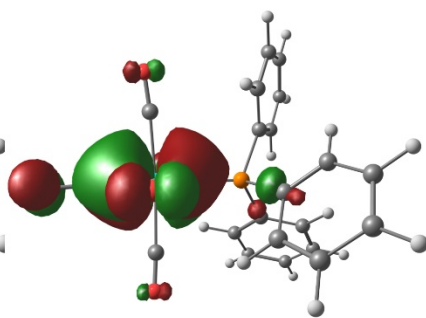


HOMO-3

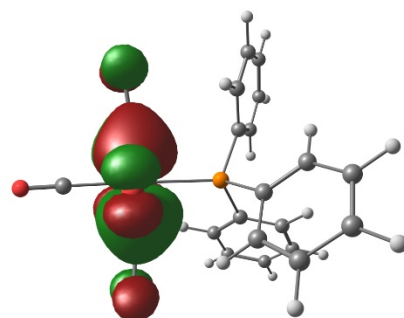
$L = PPh_3$



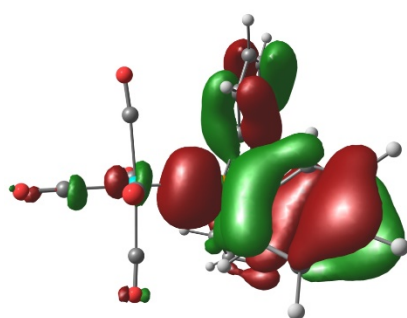
HOMO



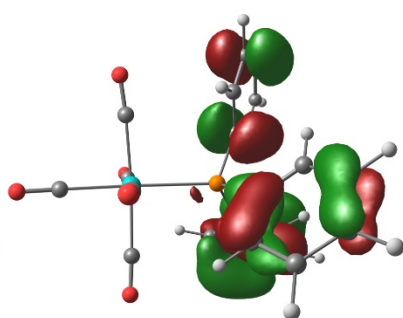
HOMO-1



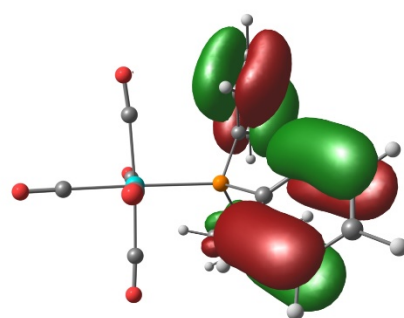
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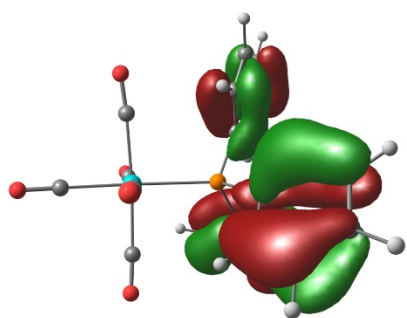
HOMO-3



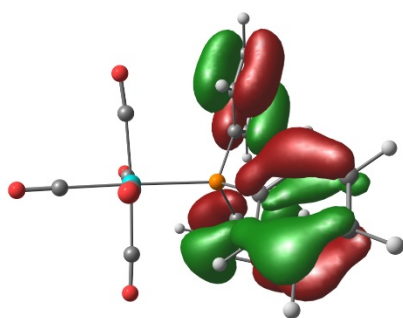
HOMO-4



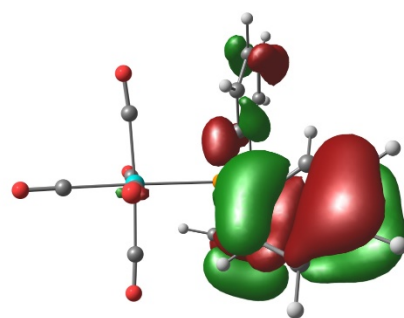
HOMO-5



HOMO-6

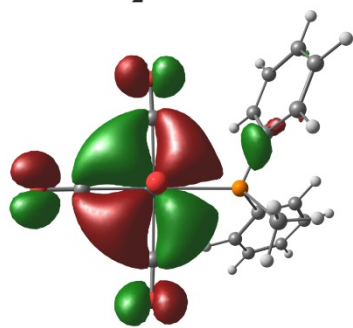


HOMO-7

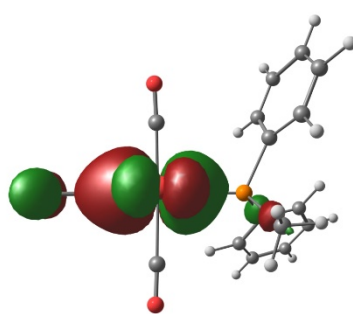


HOMO-8

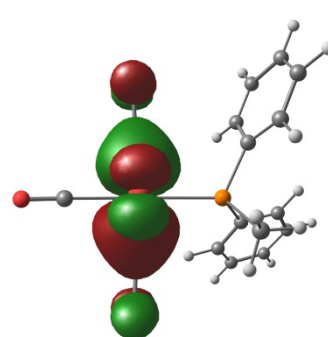
$L = PPh_2Me$



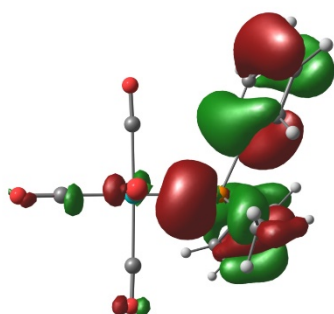
HOMO



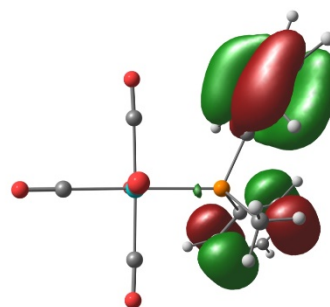
HOMO-1



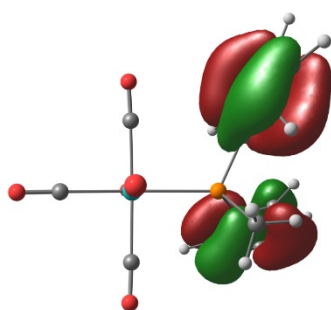
HOMO-2



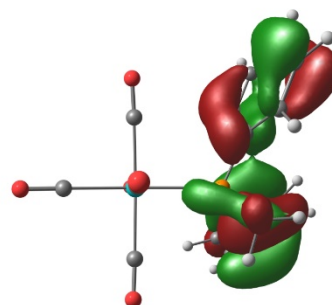
HOMO-3



HOMO-4

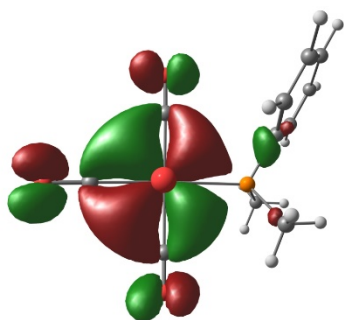


HOMO-5

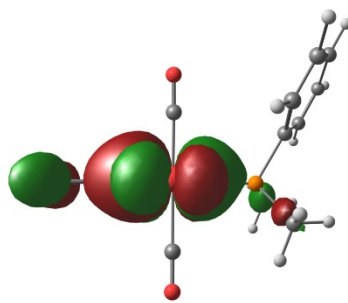


HOMO-6

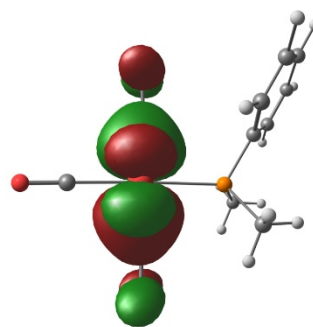
$L = PPhMe_2$



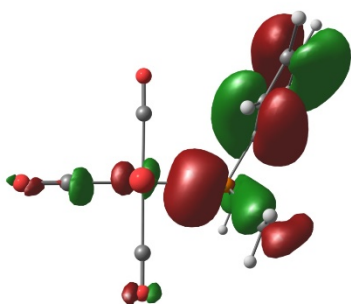
HOMO



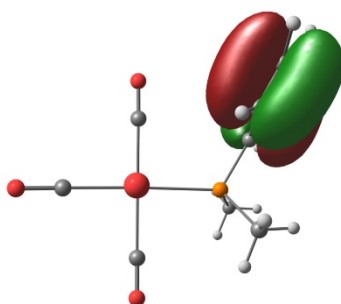
HOMO-1



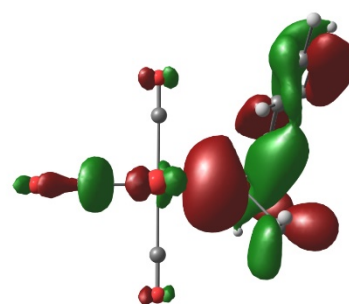
HOMO-2



HOMO-3

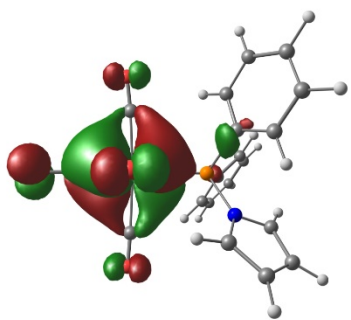


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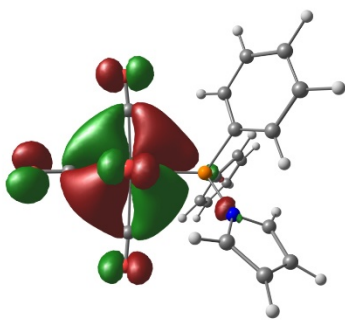


HOMO-5

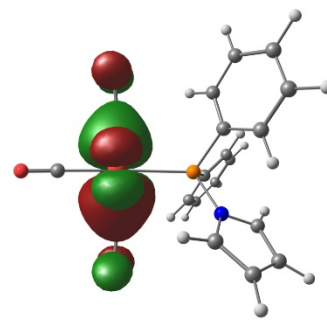
L = PPh₂Pyrl



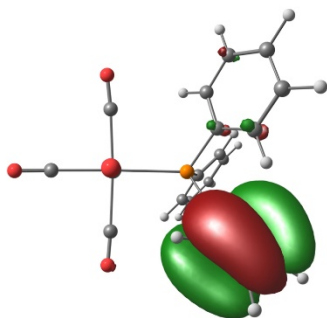
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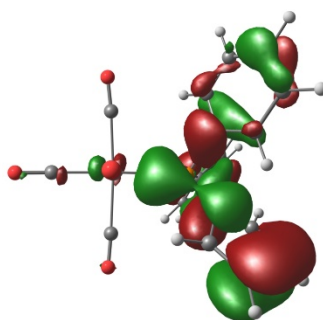
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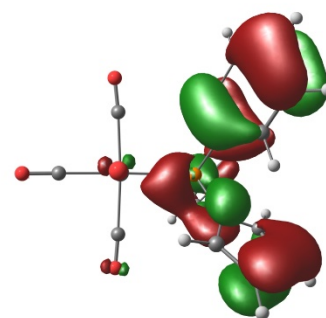
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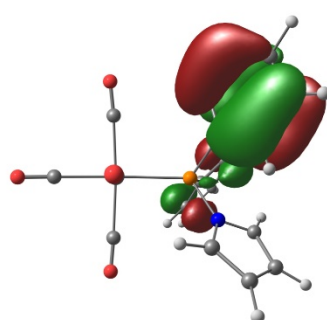
HOMO-3



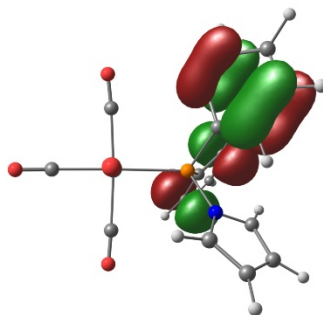
HOMO-4



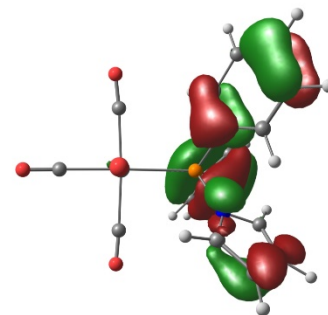
HOMO-5



HOMO-6

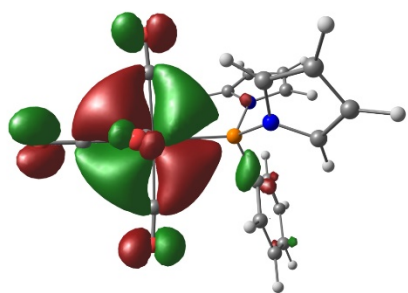


HOMO-7

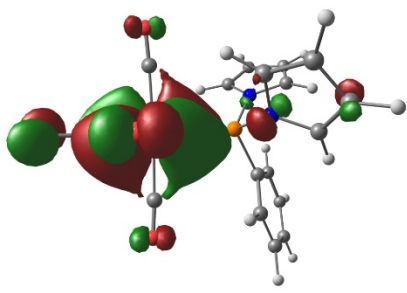


HOMO-8

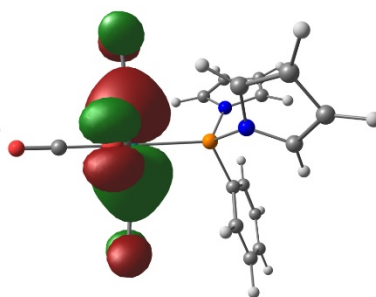
$L = \text{PPhPyrl}_2$



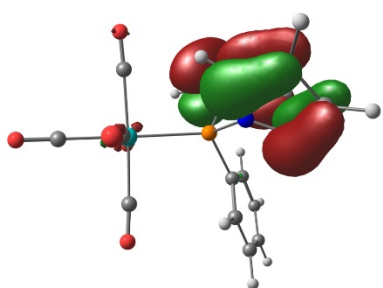
HOMO



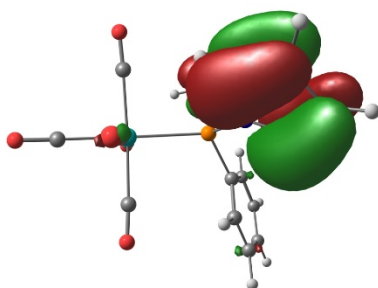
HOMO-1



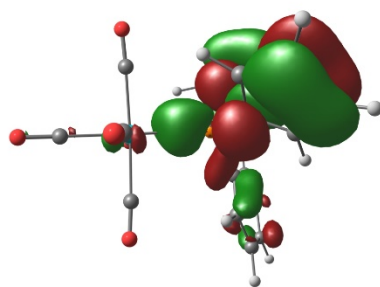
HOMO-2



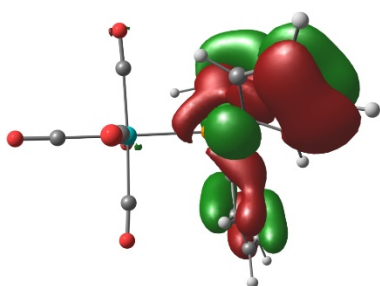
HOMO-3



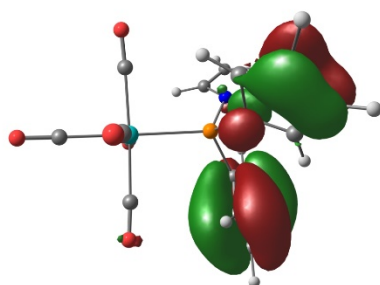
HOMO-4



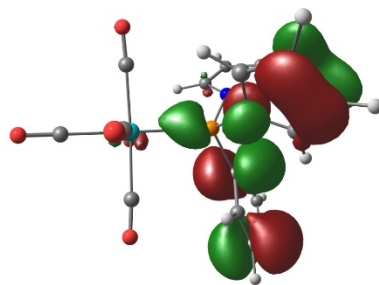
HOMO-5



HOMO-6



HOMO-7



HOMO-8

$L = \text{PPyrl}_3$

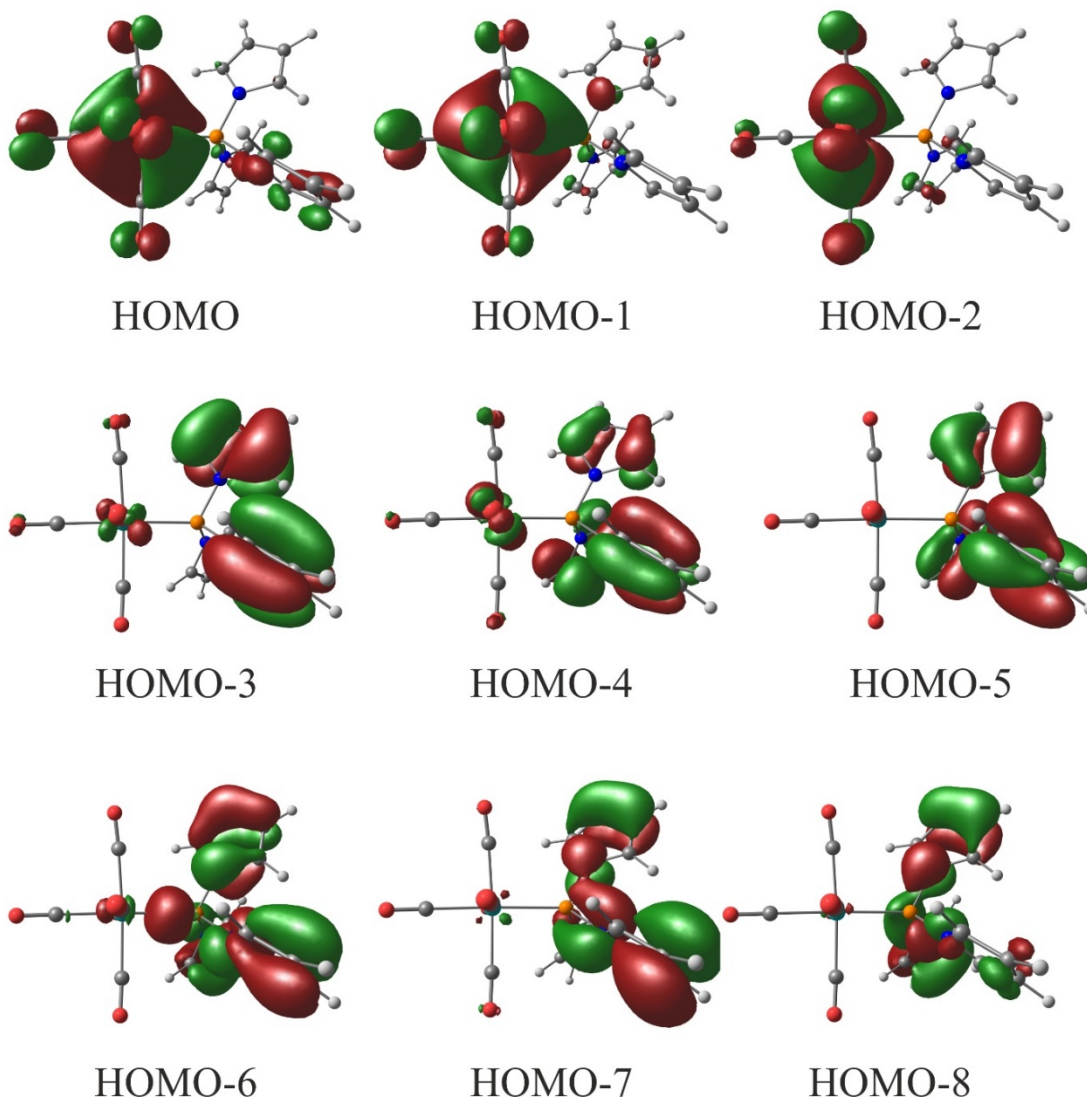
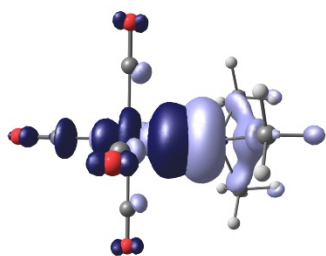


Figure S1. Kohn-Sham orbitals of all complexes studied in this work obtained at the LC- ω PBEh/Def2-TZVP level of theory. Isosurface value: 0.03 a.u.

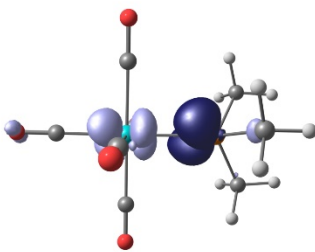
b. ETS-NOCV

a) PMe₃



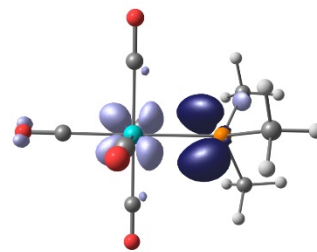
σ

$$\Delta E_{\text{orb},\sigma} = -32.8$$
$$v = 0.58$$



$\pi 1$

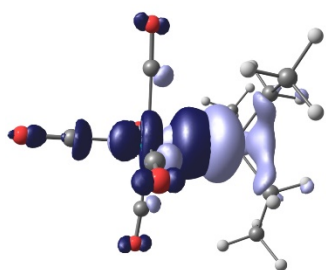
$$\Delta E_{\text{orb},\pi 1} = -5.9$$
$$v = 0.25$$



$\pi 2$

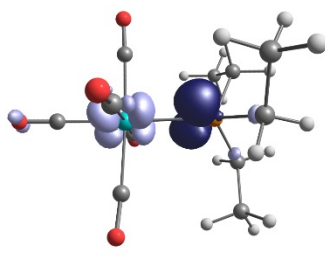
$$\Delta E_{\text{orb},\pi 2} = -5.9$$
$$v = 0.25$$

b) PEt₃



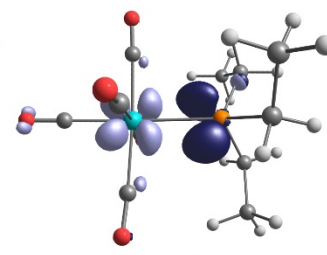
σ

$$\Delta E_{\text{orb},\sigma} = -31.3$$
$$v = 0.58$$



$\pi 1$

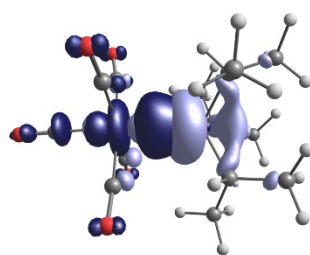
$$\Delta E_{\text{orb},\pi 1} = -5.5$$
$$v = 0.24$$



$\pi 2$

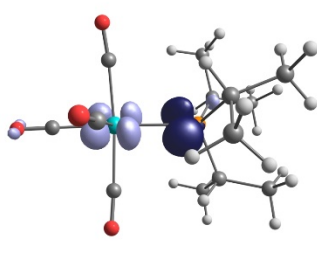
$$\Delta E_{\text{orb},\pi 2} = -5.9$$
$$v = 0.24$$

c) P*i*Pr₃



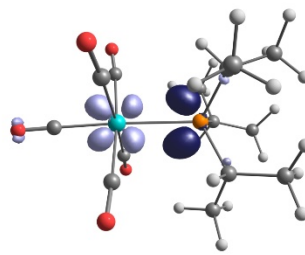
σ

$$\Delta E_{\text{orb},\sigma} = -30.1$$
$$v = 0.58$$



$\pi 1$

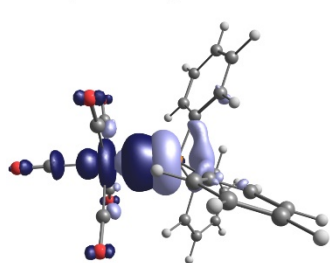
$$\Delta E_{\text{orb},\pi 1} = -5.5$$
$$v = 0.22$$



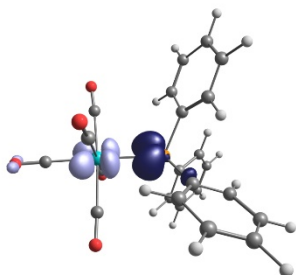
$\pi 2$

$$\Delta E_{\text{orb},\pi 2} = -5.9$$
$$v = 0.21$$

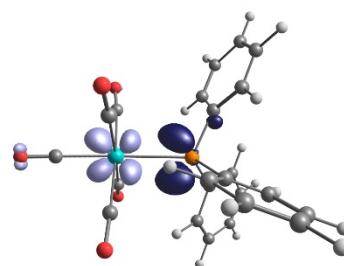
d) PPh₃



σ
 $\Delta E_{\text{orb},\sigma} = -28.6$
 $\nu = 0.56$

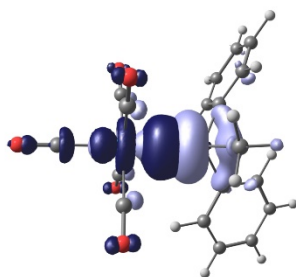


$\pi 1$
 $\Delta E_{\text{orb},\pi 1} = -6.0$
 $\nu = 0.26$

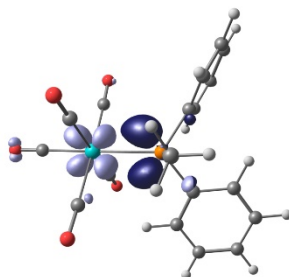


$\pi 2$
 $\Delta E_{\text{orb},\pi 2} = -5.6$
 $\nu = 0.26$

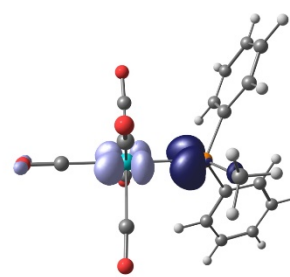
e) PPh₂Me



σ
 $\Delta E_{\text{orb},\sigma} = -30.4$
 $\nu = 0.57$

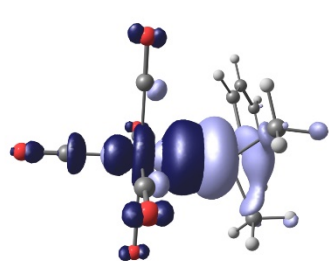


$\pi 1$
 $\Delta E_{\text{orb},\pi 1} = -6.3$
 $\nu = 0.27$

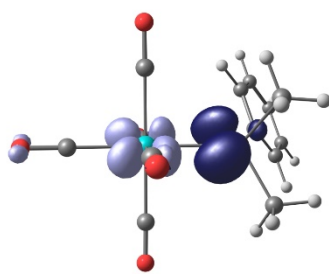


$\pi 2$
 $\Delta E_{\text{orb},\pi 2} = -5.7$
 $\nu = 0.25$

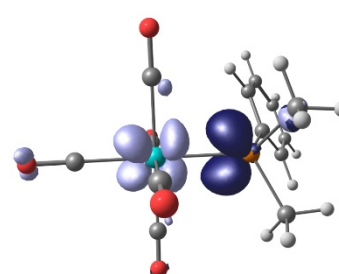
f) PPhMe₂



σ
 $\Delta E_{\text{orb},\sigma} = -31.9$
 $\nu = 0.59$

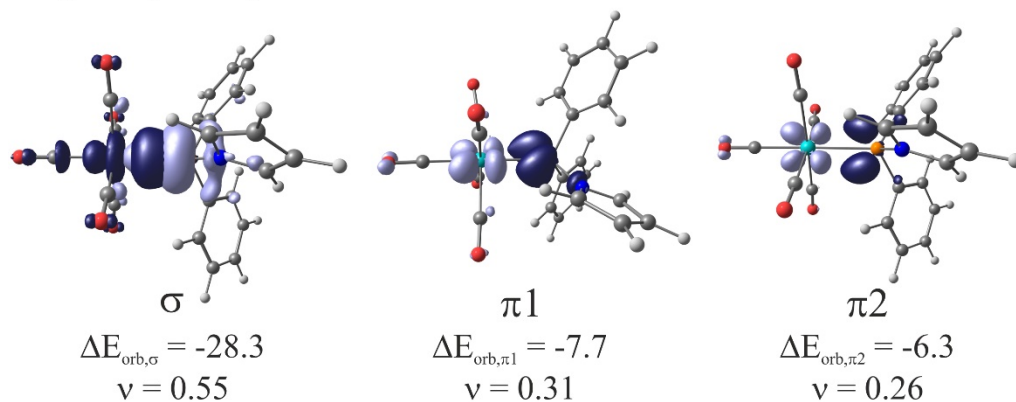


$\pi 1$
 $\Delta E_{\text{orb},\pi 1} = -6.2$
 $\nu = 0.26$

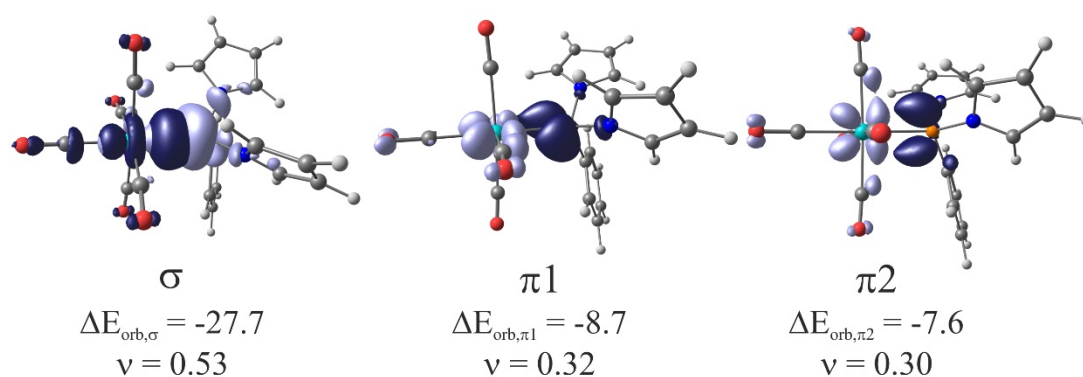


$\pi 2$
 $\Delta E_{\text{orb},\pi 2} = -5.8$
 $\nu = 0.25$

g) PPyrlPh₂



h) PPyrl₂Ph



i) PPyrl₃

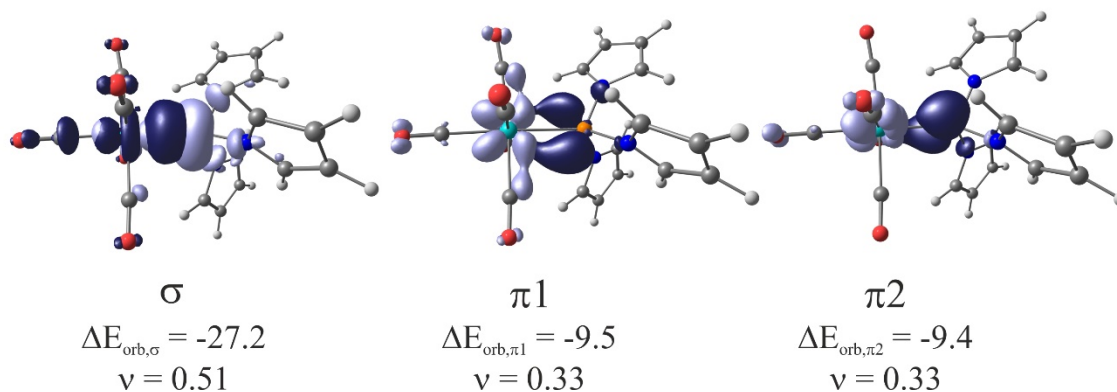


Figure S2. Contours of deformation density $\Delta\rho_{\sigma/\pi}$ connected with the pairs of interacting orbitals in all L-Mo(CO)₅ complex. Light purple surfaces represent a loss of electron density and dark blue surfaces, a gain of electron density. The associated orbital interaction energies ΔE_{orb} are given in kcal/mol. ν is the eigenvalue indicating the size of the charge flow. Isosurface value: 0.0025 a.u.

c. Average local ionization energies

The Multiwfn⁶ program was used to obtain the ALIE and VMD,⁷ for the visualization of the surfaces. For the three complexes presented in Fig. S3, the surfaces show ALIE values comprised between 0.45 and 0.55 a.u..

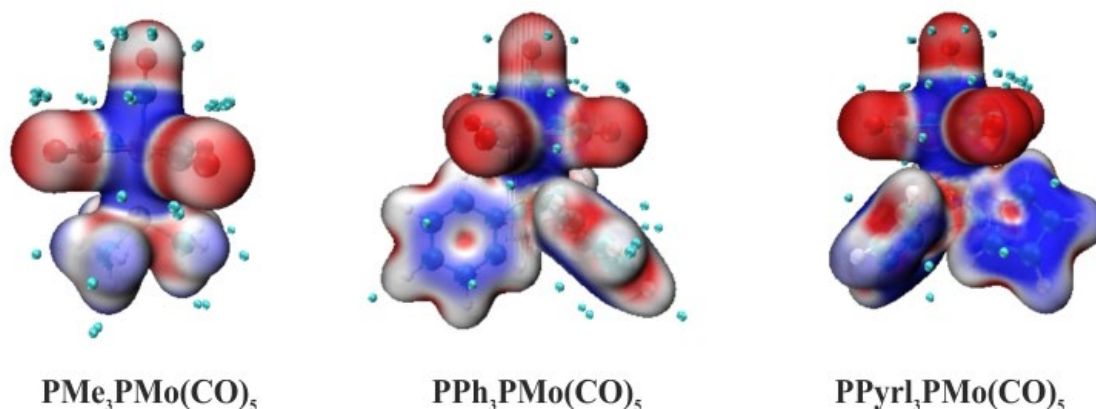


Figure S3 : ALIE mapped molecular surface ((iso 0.01 e.Bohr⁻³)). The blue color indicates the lower ALIE, white the intermediate and red the largest ALIE.

d. Cartesian coordinates

Table S4. Cartesian coordinates (x,y,z) of optimized geometries of compounds studied in this work obtained at the PBE0/Def2-TZVP level of theory.

	x	y	z
Mo(CO)₆			
O	-0.415211000000	3.151800000000	0.242505000000
C	0.266797000000	-2.028451000000	-0.156480000000
O	0.414665000000	-3.151889000000	-0.243051000000
C	-1.412450000000	-0.071883000000	-1.487175000000
O	-2.194596000000	-0.111499000000	-2.310680000000
C	1.463758000000	0.300509000000	-1.406441000000
O	2.274443000000	0.466965000000	-2.185253000000
C	-1.464237000000	-0.300566000000	1.405584000000
O	-2.274898000000	-0.467021000000	2.184422000000
C	-0.267304000000	2.028380000000	0.155769000000
Mo	-0.000239000000	-0.000027000000	-0.000428000000
C	1.412019000000	0.071859000000	1.486238000000

O	2.194243000000	0.111512000000	2.309670000000
Mo(CO)₆⁺			
O	-0.944779000000	2.602574000000	1.655393000000
C	0.613185000000	-1.691069000000	-1.088578000000
O	0.944578000000	-2.604277000000	-1.653943000000
C	-1.167019000000	-1.358213000000	1.103116000000
O	-1.797189000000	-2.091925000000	1.675786000000
C	-1.748735000000	0.312277000000	-1.123867000000
O	-2.693568000000	0.481247000000	-1.708793000000
C	1.748655000000	-0.313701000000	1.125073000000
O	2.693520000000	-0.482535000000	1.709992000000
C	-0.613331000000	1.689459000000	1.089914000000
Mo	-0.000040000000	-0.000765000000	0.000591000000
C	1.166921000000	1.356579000000	-1.102133000000
O	1.797030000000	2.090175000000	-1.675016000000
Mo(CO)₅PMe₃			
Mo	0.581563000000	0.003799000000	-0.007716000000
C	0.518505000000	1.426732000000	-1.465433000000
O	0.483969000000	2.221309000000	-2.284604000000
C	0.630283000000	-1.433352000000	1.437792000000
O	0.661480000000	-2.241030000000	2.243574000000
C	2.587027000000	0.075898000000	-0.009852000000
O	3.729159000000	0.121373000000	-0.009966000000
C	0.518657000000	1.449292000000	1.427202000000
O	0.481793000000	2.257525000000	2.232929000000
C	0.625980000000	-1.452642000000	-1.434473000000
O	0.654543000000	-2.270213000000	-2.230183000000
P	-1.935355000000	-0.032628000000	0.006774000000
C	-2.725703000000	-0.782198000000	1.470472000000
H	-2.412348000000	-1.823339000000	1.562919000000
H	-2.404889000000	-0.251666000000	2.368652000000
H	-3.815127000000	-0.739528000000	1.398031000000
C	-2.753566000000	-0.917225000000	-1.363311000000
H	-2.454096000000	-0.473261000000	-2.314228000000
H	-2.438979000000	-1.962136000000	-1.364010000000
H	-3.841419000000	-0.869307000000	-1.271763000000
C	-2.743945000000	1.601426000000	-0.064079000000
H	-2.426216000000	2.204947000000	0.787861000000
H	-2.442619000000	2.118355000000	-0.976722000000
H	-3.832280000000	1.505473000000	-0.049367000000
Mo(CO)₅PMe₃⁺			
Mo	0.616080000000	0.000627000000	0.087483000000
C	0.661143000000	-1.534527000000	1.499932000000
O	0.673005000000	-2.377607000000	2.249982000000
C	0.497290000000	1.554536000000	-1.266903000000
O	0.424267000000	2.425898000000	-1.983573000000

C	2.647159000000	0.005615000000	-0.340243000000
O	3.740654000000	0.008732000000	-0.617099000000
C	0.506268000000	-1.553858000000	-1.266802000000
O	0.439539000000	-2.426177000000	-1.982924000000
C	0.654578000000	1.534647000000	1.501639000000
O	0.663001000000	2.376694000000	2.252902000000
P	-1.946975000000	-0.002161000000	-0.055913000000
C	-2.579730000000	-0.033364000000	-1.756880000000
H	-2.233277000000	0.840846000000	-2.309886000000
H	-2.239488000000	-0.931880000000	-2.273517000000
H	-3.671822000000	-0.029400000000	-1.740542000000
C	-2.743172000000	1.446818000000	0.693334000000
H	-2.505351000000	1.500792000000	1.756828000000
H	-2.393391000000	2.360360000000	0.209847000000
H	-3.827336000000	1.378187000000	0.577994000000
C	-2.743149000000	-1.423479000000	0.745322000000
H	-2.391514000000	-2.354127000000	0.297092000000
H	-2.507351000000	-1.437145000000	1.810578000000
H	-3.827265000000	-1.360209000000	0.625315000000

Mo(CO)₅PEt₃

Mo	-0.931796000000	-0.009609000000	-0.005764000000
C	-1.119099000000	1.972080000000	0.432725000000
O	-1.296456000000	3.069567000000	0.694529000000
C	-0.866199000000	-2.013813000000	-0.380696000000
O	-0.861767000000	-3.138803000000	-0.575520000000
C	-2.924568000000	-0.107075000000	-0.122428000000
O	-4.064406000000	-0.168857000000	-0.197625000000
C	-0.861841000000	0.439124000000	-1.994076000000
O	-0.848034000000	0.710629000000	-3.103140000000
C	-1.065639000000	-0.379177000000	1.994590000000
O	-1.189029000000	-0.561601000000	3.115006000000
P	1.618652000000	0.037392000000	0.029453000000
C	2.443899000000	-1.391586000000	-0.787022000000
H	2.093999000000	-2.292117000000	-0.274873000000
H	3.518823000000	-1.308115000000	-0.588306000000
C	2.453419000000	0.049451000000	1.671923000000
H	2.002286000000	0.863510000000	2.246124000000
H	3.504193000000	0.316527000000	1.509656000000
C	2.448652000000	1.445756000000	-0.818418000000
H	2.039545000000	1.488407000000	-1.831656000000
H	3.508821000000	1.183178000000	-0.913708000000
C	2.185672000000	-1.512083000000	-2.280906000000
H	2.574372000000	-0.654138000000	-2.833304000000
H	2.672413000000	-2.405768000000	-2.677888000000

H	1.11924000000	-1.59404100000	-2.49847100000
C	2.29890500000	2.79829900000	-0.13986700000
H	2.72917500000	2.80005700000	0.86381800000
H	2.81592400000	3.56776900000	-0.71788700000
H	1.25384000000	3.09765200000	-0.05722400000
C	2.35577800000	-1.25615700000	2.44727100000
H	2.90660600000	-2.05981700000	1.95498200000
H	2.77850700000	-1.13402400000	3.44703100000
H	1.32155100000	-1.58278500000	2.56740600000

Mo(CO)₅PEt₃⁺

Mo	0.90491800000	-0.00259500000	-0.11114800000
C	1.23500200000	1.56744100000	-1.44595700000
O	1.47062300000	2.41470400000	-2.15407000000
C	0.67959700000	-1.62177200000	1.14312500000
O	0.58596500000	-2.53445900000	1.80501600000
C	2.86335900000	-0.08349600000	0.52142300000
O	3.92069200000	-0.12977700000	0.91504700000
C	0.73565300000	1.51549600000	1.27218500000
O	0.66564800000	2.38593500000	1.99130100000
C	1.10454300000	-1.44792800000	-1.60385200000
O	1.23865900000	-2.22673400000	-2.41002500000
P	-1.67976500000	0.04174200000	-0.00880300000
C	-2.41532200000	-0.63092300000	1.52607100000
H	-2.11380000000	-1.67817500000	1.60383100000
H	-3.49827900000	-0.63057400000	1.35932300000
C	-2.46023600000	-0.94471100000	-1.34577600000
H	-2.02159800000	-0.61356500000	-2.29081200000
H	-3.51319800000	-0.64071900000	-1.36750000000
C	-2.45475400000	1.69361500000	-0.16846200000
H	-2.02134700000	2.33738200000	0.60145600000
H	-3.50925100000	1.55763900000	0.09673000000
C	-2.07128800000	0.11885500000	2.80419800000
H	-2.36757000000	1.16820200000	2.76054800000
H	-2.59715700000	-0.33241600000	3.64688200000
H	-1.00398500000	0.07445900000	3.02917800000
C	-2.33446100000	2.34147900000	-1.53927500000
H	-2.82157100000	1.74936200000	-2.31541900000
H	-2.81575700000	3.32052100000	-1.52654600000
H	-1.29578300000	2.49735000000	-1.83391700000
C	-2.34703900000	-2.45367200000	-1.19497800000
H	-2.89214600000	-2.81727200000	-0.32331200000
H	-2.77274000000	-2.94327500000	-2.07226500000
H	-1.31160300000	-2.78868900000	-1.10931000000

Mo(CO)₅PiPr₃

Mo	1.355068000000	-0.021241000000	0.001210000000
C	1.280399000000	-0.761757000000	-1.898023000000
O	1.292956000000	-1.177851000000	-2.961498000000
C	1.628153000000	0.723558000000	1.876076000000
O	1.882476000000	1.142784000000	2.907821000000
C	3.336186000000	-0.117923000000	-0.134803000000
O	4.475716000000	-0.180305000000	-0.226199000000
C	1.478370000000	1.903587000000	-0.656449000000
O	1.623625000000	2.990332000000	-0.976984000000
C	1.387087000000	-1.892444000000	0.806782000000
O	1.464200000000	-2.923746000000	1.291097000000
P	-1.257473000000	0.023736000000	0.024137000000
C	-1.921573000000	1.361516000000	1.144202000000
C	-1.963053000000	-1.601417000000	0.611882000000
C	-1.953188000000	0.306127000000	-1.687253000000
C	-3.423359000000	-1.661325000000	1.050710000000
H	-3.640458000000	-2.671294000000	1.411990000000
H	-3.646841000000	-0.973973000000	1.865152000000
H	-4.115731000000	-1.453845000000	0.235639000000
C	-1.664456000000	-2.704483000000	-0.401473000000
H	-2.306947000000	-2.626259000000	-1.281052000000
H	-0.627918000000	-2.690179000000	-0.740742000000
H	-1.850570000000	-3.681031000000	0.052941000000
C	-1.692780000000	1.000423000000	2.610767000000
H	-2.438958000000	0.289015000000	2.968813000000
H	-0.708463000000	0.571050000000	2.792438000000
H	-1.779525000000	1.898689000000	3.227432000000
C	-3.350707000000	1.853820000000	0.939502000000
H	-3.511863000000	2.275023000000	-0.052135000000
H	-4.089486000000	1.067664000000	1.100370000000
H	-3.557308000000	2.646844000000	1.664912000000
C	-3.431588000000	0.019271000000	-1.936650000000
H	-3.690249000000	-1.022883000000	-1.756193000000
H	-4.094482000000	0.642036000000	-1.336788000000
H	-3.654414000000	0.225965000000	-2.987845000000
C	-1.577845000000	1.687220000000	-2.215821000000
H	-2.066174000000	2.489737000000	-1.658667000000
H	-0.503840000000	1.861150000000	-2.183966000000
H	-1.895768000000	1.775758000000	-3.258215000000
H	-1.348651000000	-1.798211000000	1.498291000000
H	-1.247737000000	2.191984000000	0.904061000000
H	-1.383914000000	-0.424921000000	-2.272967000000

Mo(CO)₅PiPr₃⁺

Mo	-1.725426000000	0.032775000000	-0.494755000000
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C	-1.647093000000	2.083027000000	-0.417109000000
O	-1.623002000000	3.214324000000	-0.363784000000
C	-1.772103000000	-2.019503000000	-0.486922000000
O	-1.822329000000	-3.151356000000	-0.470733000000
C	-3.594494000000	0.119742000000	-1.322413000000
O	-4.611035000000	0.172742000000	-1.816298000000
C	-1.170629000000	0.033391000000	-2.491412000000
O	-0.933288000000	0.032459000000	-3.597052000000
C	-2.675148000000	0.020964000000	1.379895000000
O	-3.252282000000	0.008758000000	2.348943000000
P	0.772628000000	0.000370000000	0.023318000000
C	1.795998000000	-1.415762000000	-0.452223000000
C	2.981788000000	-1.676048000000	0.238489000000
C	1.449349000000	-2.211115000000	-1.540116000000
C	3.795418000000	-2.724563000000	-0.151825000000
H	3.270973000000	-1.063455000000	1.084665000000
C	2.271544000000	-3.256708000000	-1.933169000000
H	0.536299000000	-2.021670000000	-2.090394000000
C	3.442178000000	-3.514669000000	-1.238666000000
H	4.711258000000	-2.924597000000	0.391531000000
H	1.993654000000	-3.869841000000	-2.781963000000
H	4.083780000000	-4.332983000000	-1.543404000000
C	0.504694000000	-0.106902000000	1.811170000000
C	0.268346000000	1.053610000000	2.562321000000
C	0.417176000000	-1.359726000000	2.432230000000
C	-0.028126000000	0.957529000000	3.909562000000
H	0.331274000000	2.028511000000	2.092238000000
C	0.117525000000	-1.444405000000	3.779834000000
H	0.599395000000	-2.263407000000	1.861858000000
C	-0.106592000000	-0.289089000000	4.519550000000
H	-0.197387000000	1.857699000000	4.488312000000
H	0.062374000000	-2.415121000000	4.257916000000
H	-0.341384000000	-0.360262000000	5.574995000000
C	1.770590000000	1.476384000000	-0.296217000000
C	1.607920000000	2.156116000000	-1.501584000000
C	2.756799000000	1.894555000000	0.598858000000
C	2.416134000000	3.238341000000	-1.809799000000
H	0.850602000000	1.844109000000	-2.211010000000
C	3.557451000000	2.981498000000	0.289428000000
H	2.897540000000	1.381736000000	1.543222000000
C	3.389542000000	3.652954000000	-0.913620000000
H	2.281506000000	3.760226000000	-2.749551000000
H	4.316667000000	3.305048000000	0.991590000000
H	4.018184000000	4.502885000000	-1.151326000000

Mo(CO)₅PPh₃

Mo	1.927450144631	-0.070390005114	0.05276600402
C	1.966600148625	1.138646085731	1.694470129189
O	2.046013153953	1.839429139996	2.592007195542
C	2.013427154516	-1.176433087885	-1.662079126277
O	2.121049159627	-1.769149136015	-2.629871198277
C	3.914356300705	-0.179450013944	0.153218011897
O	5.054522384583	-0.249443019173	0.218816016448
C	1.846604143188	-1.770805132715	1.180994087761
O	1.851603143073	-2.729827208377	1.799160137792
C	2.147290165095	1.603486123551	-1.091144082508
O	2.344666177413	2.528816192867	-1.728245131696
P	-0.637336046220	0.018966001429	-0.015911001215
C	-1.433250109471	-1.020226075977	-1.298986098956
C	-2.418698185676	-0.556850044059	-2.166068167945
C	-1.048227082642	-2.358902177851	-1.370305105423
C	-2.998326230493	-1.413957106030	-3.092272236989
H	-2.740765206862	0.476322036338	-2.121378159706
C	-1.634771124846	-3.214821247481	-2.286289174257
H	-0.283483021474	-2.736761208375	-0.700335052806
C	-2.609653198297	-2.742312208923	-3.154467243414
H	-3.760061285575	-1.037219079298	-3.765517288224
H	-1.324065099979	-4.252396325482	-2.327309179521
H	-3.063037231315	-3.409406262569	-3.878635296492
C	-1.320345100337	1.690023129968	-0.310958023836
C	-2.075848156668	2.361273177682	0.646063046907
C	-1.018360075286	2.340123180147	-1.508782112979
C	-2.520428193710	3.655061279648	0.409402031128
H	-2.319996177486	1.876893142940	1.583405122269
C	-1.474277110458	3.625004276494	-1.748441133778
H	-0.423818032265	1.837088139223	-2.263411174874
C	-2.224814171689	4.288162325636	-0.786664060813
H	-3.102464238431	4.166862316331	1.167351088641
H	-1.233346095723	4.113515312263	-2.685533204640
H	-2.573672198718	5.297923381754	-0.969998074366
C	-1.534117119371	-0.529363037840	1.487178113115
C	-0.905840069061	-0.517683039717	2.728674210528
C	-2.867037217430	-0.936058069101	1.412297108750
C	-1.592917120362	-0.895322067975	3.873681297840
H	0.130729010181	-0.216150016705	2.804918216734
C	-3.552010270572	-1.315876097926	2.554601195716
H	-3.371833259695	-0.963136074225	0.453678034901
C	-2.916853222802	-1.295130100762	3.788785291239
H	-1.086269084728	-0.881690065158	4.831722368843

H	-4.585828348859	-1.633453124239	2.479592188666
H	-3.452812264548	-1.596655122613	4.681563355464
Mo(CO)₅PPh₃⁺			
Mo	-1.725426000000	0.032775000000	-0.494755000000
C	-1.647093000000	2.083027000000	-0.417109000000
O	-1.623002000000	3.214324000000	-0.363784000000
C	-1.772103000000	-2.019503000000	-0.486922000000
O	-1.822329000000	-3.151356000000	-0.470733000000
C	-3.594494000000	0.119742000000	-1.322413000000
O	-4.611035000000	0.172742000000	-1.816298000000
C	-1.170629000000	0.033391000000	-2.491412000000
O	-0.933288000000	0.032459000000	-3.597052000000
C	-2.675148000000	0.020964000000	1.379895000000
O	-3.252282000000	0.008758000000	2.348943000000
P	0.772628000000	0.000370000000	0.023318000000
C	1.795998000000	-1.415762000000	-0.452223000000
C	2.981788000000	-1.676048000000	0.238489000000
C	1.449349000000	-2.211115000000	-1.540116000000
C	3.795418000000	-2.724563000000	-0.151825000000
H	3.270973000000	-1.063455000000	1.084665000000
C	2.271544000000	-3.256708000000	-1.933169000000
H	0.536299000000	-2.021670000000	-2.090394000000
C	3.442178000000	-3.514669000000	-1.238666000000
H	4.711258000000	-2.924597000000	0.391531000000
H	1.993654000000	-3.869841000000	-2.781963000000
H	4.083780000000	-4.332983000000	-1.543404000000
C	0.504694000000	-0.106902000000	1.811170000000
C	0.268346000000	1.053610000000	2.562321000000
C	0.417176000000	-1.359726000000	2.432230000000
C	-0.028126000000	0.957529000000	3.909562000000
H	0.331274000000	2.028511000000	2.092238000000
C	0.117525000000	-1.444405000000	3.779834000000
H	0.599395000000	-2.263407000000	1.861858000000
C	-0.106592000000	-0.289089000000	4.519550000000
H	-0.197387000000	1.857699000000	4.488312000000
H	0.062374000000	-2.415121000000	4.257916000000
H	-0.341384000000	-0.360262000000	5.574995000000
C	1.770590000000	1.476384000000	-0.296217000000
C	1.607920000000	2.156116000000	-1.501584000000
C	2.756799000000	1.894555000000	0.598858000000
C	2.416134000000	3.238341000000	-1.809799000000
H	0.850602000000	1.844109000000	-2.211010000000
C	3.557451000000	2.981498000000	0.289428000000
H	2.897540000000	1.381736000000	1.543222000000

C	3.389542000000	3.652954000000	-0.913620000000
H	2.281506000000	3.760226000000	-2.749551000000
H	4.316667000000	3.305048000000	0.991590000000
H	4.018184000000	4.502885000000	-1.151326000000

Mo(CO)₅PPh₂Me

Mo	1.693083000000	0.025838000000	-0.084917000000
C	1.253220000000	1.033505000000	-1.807103000000
O	1.040808000000	1.573959000000	-2.789019000000
C	2.168640000000	-1.041658000000	1.581869000000
O	2.449225000000	-1.650592000000	2.506023000000
C	3.615824000000	-0.009548000000	-0.631412000000
O	4.717756000000	-0.025365000000	-0.937023000000
C	2.048783000000	1.760000000000	0.922539000000
O	2.280587000000	2.723987000000	1.489484000000
C	1.403597000000	-1.733293000000	-1.086718000000
O	1.280384000000	-2.715763000000	-1.650071000000
P	-0.720330000000	0.043659000000	0.705957000000
C	-0.893489000000	0.088463000000	2.524911000000
H	-0.335823000000	-0.728752000000	2.983962000000
H	-0.463360000000	1.029028000000	2.872666000000
H	-1.940773000000	0.042790000000	2.828610000000
C	-1.819516000000	1.428054000000	0.227125000000
C	-1.280026000000	2.645951000000	-0.173900000000
C	-3.205942000000	1.302691000000	0.322996000000
C	-2.106197000000	3.720866000000	-0.470481000000
H	-0.205861000000	2.757357000000	-0.258563000000
C	-4.030534000000	2.374102000000	0.022645000000
H	-3.644975000000	0.357192000000	0.622299000000
C	-3.481811000000	3.586269000000	-0.374143000000
H	-1.670224000000	4.662448000000	-0.783678000000
H	-5.106348000000	2.261655000000	0.095711000000
H	-4.128365000000	4.423257000000	-0.612021000000
C	-1.691872000000	-1.419453000000	0.212386000000
C	-2.043399000000	-1.562482000000	-1.130422000000
C	-2.037789000000	-2.426125000000	1.108765000000
C	-2.734473000000	-2.680688000000	-1.562443000000
H	-1.775956000000	-0.789405000000	-1.843607000000
C	-2.724133000000	-3.552017000000	0.672295000000
H	-1.774590000000	-2.344786000000	2.156542000000
C	-3.075683000000	-3.680773000000	-0.661080000000
H	-3.003323000000	-2.775412000000	-2.608214000000
H	-2.984363000000	-4.329062000000	1.381976000000
H	-3.611869000000	-4.559373000000	-1.000637000000

Mo(CO)₅PPh₂Me⁺

Mo	1.693083000000	0.025838000000	-0.084917000000
C	1.253220000000	1.033505000000	-1.807103000000
O	1.040808000000	1.573959000000	-2.789019000000
C	2.168640000000	-1.041658000000	1.581869000000
O	2.449225000000	-1.650592000000	2.506023000000
C	3.615824000000	-0.009548000000	-0.631412000000
O	4.717756000000	-0.025365000000	-0.937023000000
C	2.048783000000	1.760000000000	0.922539000000
O	2.280587000000	2.723987000000	1.489484000000
C	1.403597000000	-1.733293000000	-1.086718000000
O	1.280384000000	-2.715763000000	-1.650071000000
P	-0.720330000000	0.043659000000	0.705957000000
C	-0.893489000000	0.088463000000	2.524911000000
H	-0.335823000000	-0.728752000000	2.983962000000
H	-0.463360000000	1.029028000000	2.872666000000
H	-1.940773000000	0.042790000000	2.828610000000
C	-1.819516000000	1.428054000000	0.227125000000
C	-1.280026000000	2.645951000000	-0.173900000000
C	-3.205942000000	1.302691000000	0.322996000000
C	-2.106197000000	3.720866000000	-0.470481000000
H	-0.205861000000	2.757357000000	-0.258563000000
C	-4.030534000000	2.374102000000	0.022645000000
H	-3.644975000000	0.357192000000	0.622299000000
C	-3.481811000000	3.586269000000	-0.374143000000
H	-1.670224000000	4.662448000000	-0.783678000000
H	-5.106348000000	2.261655000000	0.095711000000
H	-4.128365000000	4.423257000000	-0.612021000000
C	-1.691872000000	-1.419453000000	0.212386000000
C	-2.043399000000	-1.562482000000	-1.130422000000
C	-2.037789000000	-2.426125000000	1.108765000000
C	-2.734473000000	-2.680688000000	-1.562443000000
H	-1.775956000000	-0.789405000000	-1.843607000000
C	-2.724133000000	-3.552017000000	0.672295000000
H	-1.774590000000	-2.344786000000	2.156542000000
C	-3.075683000000	-3.680773000000	-0.661080000000
H	-3.003323000000	-2.775412000000	-2.608214000000
H	-2.984363000000	-4.329062000000	1.381976000000
H	-3.611869000000	-4.559373000000	-1.000637000000

Mo(CO)₅PPhMe₂

Mo	1.306916000000	-0.211139000000	-0.080725000000
C	1.101594000000	-1.069782000000	1.754197000000
O	0.990575000000	-1.558371000000	2.780786000000
C	1.510812000000	0.628391000000	-1.929278000000
O	1.632075000000	1.089814000000	-2.965952000000

C	2.992933000000	-1.253617000000	-0.375299000000
O	3.959057000000	-1.842762000000	-0.538414000000
C	0.214687000000	-1.726403000000	-0.915521000000
O	-0.378289000000	-2.577623000000	-1.386569000000
C	2.384076000000	1.308742000000	0.736377000000
O	2.987975000000	2.164263000000	1.192927000000
P	-0.772335000000	1.159973000000	0.333326000000
C	-0.909742000000	2.686960000000	-0.651898000000
H	-0.025880000000	3.294739000000	-0.449944000000
H	-0.918696000000	2.454175000000	-1.717263000000
H	-1.801924000000	3.260330000000	-0.392008000000
C	-0.935015000000	1.815234000000	2.032395000000
H	-0.971980000000	0.989729000000	2.743899000000
H	-0.060683000000	2.426461000000	2.264728000000
H	-1.840531000000	2.416433000000	2.134663000000
C	-2.378837000000	0.327645000000	0.094736000000
C	-2.654025000000	-0.812752000000	0.850233000000
C	-3.328636000000	0.768272000000	-0.822541000000
C	-3.856107000000	-1.483630000000	0.705110000000
H	-1.917521000000	-1.188270000000	1.553412000000
C	-4.529274000000	0.088362000000	-0.976003000000
H	-3.141496000000	1.644681000000	-1.430809000000
C	-4.797751000000	-1.034667000000	-0.210987000000
H	-4.054436000000	-2.366108000000	1.302406000000
H	-5.256217000000	0.441545000000	-1.698536000000
H	-5.735529000000	-1.564577000000	-0.331313000000

Mo(CO)₅PPhMe₂⁺

Mo	1.116950000000	-0.302014000000	-0.076647000000
C	1.352797000000	-0.246026000000	1.958532000000
O	1.471562000000	-0.229663000000	3.085182000000
C	0.817452000000	-0.371108000000	-2.122617000000
O	0.659317000000	-0.393303000000	-3.242726000000
C	2.943610000000	-1.253351000000	-0.138162000000
O	3.964803000000	-1.735889000000	-0.149032000000
C	0.044179000000	-2.085274000000	0.241154000000
O	-0.501465000000	-3.055978000000	0.416013000000
C	2.227034000000	1.395964000000	-0.464392000000
O	2.830062000000	2.322225000000	-0.703162000000
P	-0.722341000000	1.415028000000	0.289919000000
C	-0.815898000000	2.781921000000	-0.898449000000
H	0.029404000000	3.453009000000	-0.734368000000
H	-0.765426000000	2.416632000000	-1.923825000000
H	-1.743961000000	3.339256000000	-0.757681000000
C	-0.826642000000	2.242529000000	1.898118000000

H	-0.836713000000	1.524600000000	2.717170000000
H	0.047211000000	2.885630000000	2.020676000000
H	-1.729785000000	2.854206000000	1.942027000000
C	-2.233384000000	0.444352000000	0.087655000000
C	-2.827843000000	-0.172469000000	1.192575000000
C	-2.775982000000	0.244454000000	-1.185705000000
C	-3.957611000000	-0.953973000000	1.026253000000
H	-2.421944000000	-0.036267000000	2.188218000000
C	-3.905824000000	-0.539470000000	-1.343615000000
H	-2.330504000000	0.709392000000	-2.057681000000
C	-4.496994000000	-1.139942000000	-0.240182000000
H	-4.422600000000	-1.415982000000	1.888889000000
H	-4.328843000000	-0.678869000000	-2.331229000000
H	-5.381262000000	-1.753095000000	-0.366671000000

Mo(CO)₅PPh₂Pyrl

Mo	1.852423000000	-0.027183000000	-0.102655000000
C	1.821223000000	1.643780000000	-1.276318000000
O	1.855431000000	2.557320000000	-1.956748000000
C	1.983620000000	-1.765468000000	0.959882000000
O	2.104833000000	-2.751627000000	1.519515000000
C	3.843556000000	-0.043758000000	-0.281060000000
O	4.982562000000	-0.049121000000	-0.374082000000
C	1.769188000000	-1.155089000000	-1.798608000000
O	1.797138000000	-1.779865000000	-2.752329000000
C	2.083110000000	1.128873000000	1.569372000000
O	2.261885000000	1.788289000000	2.481430000000
P	-0.667481000000	0.026942000000	0.171179000000
C	-1.530434000000	1.490535000000	-0.498663000000
C	-2.642540000000	1.406694000000	-1.331269000000
C	-1.049640000000	2.747760000000	-0.132252000000
C	-3.256201000000	2.561764000000	-1.796618000000
H	-3.038156000000	0.439647000000	-1.616293000000
C	-1.671134000000	3.897596000000	-0.586782000000
H	-0.185460000000	2.827811000000	0.518316000000
C	-2.773854000000	3.806428000000	-1.425508000000
H	-4.118751000000	2.483883000000	-2.448534000000
H	-1.289298000000	4.867692000000	-0.290843000000
H	-3.255242000000	4.706931000000	-1.789273000000
C	-1.569294000000	-1.393153000000	-0.531925000000
C	-1.487946000000	-1.644322000000	-1.901707000000
C	-2.283721000000	-2.270154000000	0.279405000000
C	-2.123296000000	-2.744636000000	-2.452315000000
H	-0.928359000000	-0.975628000000	-2.546643000000
C	-2.908814000000	-3.378597000000	-0.274870000000

H	-2.353890000000	-2.092569000000	1.346169000000
C	-2.833066000000	-3.616565000000	-1.637913000000
H	-2.055601000000	-2.925864000000	-3.518728000000
H	-3.458453000000	-4.057661000000	0.366754000000
H	-3.322992000000	-4.483016000000	-2.067077000000
N	-1.250450000000	0.063428000000	1.796887000000
C	-2.512547000000	0.460761000000	2.192741000000
C	-0.623773000000	-0.514095000000	2.882050000000
C	-2.670421000000	0.152228000000	3.512417000000
H	-3.181410000000	0.942121000000	1.499096000000
C	-1.471469000000	-0.469658000000	3.950130000000
H	0.376595000000	-0.901401000000	2.799961000000
H	-3.546069000000	0.364827000000	4.106291000000
H	-1.249344000000	-0.828736000000	4.942985000000

Mo(CO)₅PPh₂PyrI⁺

Mo	-1.738787000000	0.042899000000	-0.360538000000
C	-1.905214000000	-1.863098000000	0.375654000000
O	-2.039277000000	-2.903981000000	0.804865000000
C	-1.611972000000	1.999705000000	-0.975607000000
O	-1.580259000000	3.083144000000	-1.303973000000
C	-3.596373000000	-0.159918000000	-1.187314000000
O	-4.607997000000	-0.297474000000	-1.675092000000
C	-1.142575000000	-0.572012000000	-2.247685000000
O	-0.873985000000	-0.884777000000	-3.300422000000
C	-2.754551000000	0.718248000000	1.346292000000
O	-3.414405000000	1.083063000000	2.186682000000
P	0.764193000000	-0.018211000000	0.171940000000
C	1.812737000000	-1.375908000000	-0.387936000000
C	3.202065000000	-1.229715000000	-0.365687000000
C	1.255133000000	-2.576279000000	-0.827795000000
C	4.014373000000	-2.277643000000	-0.763376000000
H	3.649148000000	-0.295863000000	-0.046692000000
C	2.073342000000	-3.620217000000	-1.227435000000
H	0.181152000000	-2.705502000000	-0.862056000000
C	3.452000000000	-3.471848000000	-1.193407000000
H	5.091018000000	-2.158410000000	-0.744392000000
H	1.632333000000	-4.548557000000	-1.569790000000
H	4.091386000000	-4.287339000000	-1.510443000000
C	1.714230000000	1.488608000000	-0.123299000000
C	1.672172000000	2.043482000000	-1.402635000000
C	2.513574000000	2.072756000000	0.858992000000
C	2.424009000000	3.167077000000	-1.697686000000
H	1.058460000000	1.596211000000	-2.177941000000
C	3.254649000000	3.205929000000	0.559156000000

H	2.563659000000	1.646210000000	1.853545000000
C	3.211454000000	3.752120000000	-0.714825000000
H	2.391184000000	3.590832000000	-2.694109000000
H	3.870445000000	3.660678000000	1.325973000000
H	3.792329000000	4.637686000000	-0.943855000000
N	0.769135000000	-0.159688000000	1.889673000000
C	1.029861000000	-1.272125000000	2.634570000000
C	0.052718000000	0.741364000000	2.681762000000
C	0.521614000000	-1.078397000000	3.899504000000
H	1.554691000000	-2.114045000000	2.213194000000
C	-0.096771000000	0.192302000000	3.924132000000
H	-0.190037000000	1.724604000000	2.310729000000
H	0.614613000000	-1.769834000000	4.722620000000
H	-0.569630000000	0.666186000000	4.770248000000

Mo(CO)₅PPhPyrl₂

Mo	-1.774807000000	0.159816000000	0.033919000000
C	-2.089961000000	-1.726625000000	0.767352000000
O	-2.305831000000	-2.772667000000	1.162395000000
C	-1.560947000000	2.047583000000	-0.707685000000
O	-1.500896000000	3.108452000000	-1.119315000000
C	-3.755478000000	0.464049000000	0.097129000000
O	-4.884475000000	0.627755000000	0.138905000000
C	-2.027574000000	-0.493573000000	-1.889158000000
O	-2.230248000000	-0.806343000000	-2.964868000000
C	-1.672250000000	0.980165000000	1.898954000000
O	-1.672246000000	1.484421000000	2.921707000000
P	0.699294000000	-0.251062000000	-0.026035000000
C	1.757935000000	1.223753000000	-0.095929000000
C	1.701575000000	2.057140000000	-1.213225000000
C	2.550596000000	1.583383000000	0.990180000000
C	2.444691000000	3.224244000000	-1.249470000000
H	1.082564000000	1.789163000000	-2.062570000000
C	3.284624000000	2.760461000000	0.952999000000
H	2.600275000000	0.945123000000	1.864754000000
C	3.235511000000	3.578790000000	-0.164393000000
H	2.400961000000	3.862024000000	-2.124530000000
H	3.899368000000	3.034368000000	1.802501000000
H	3.811574000000	4.496594000000	-0.191203000000
N	1.374938000000	-1.138360000000	1.284502000000
C	2.615957000000	-1.747857000000	1.294098000000
C	0.851876000000	-1.209972000000	2.561600000000
C	2.862710000000	-2.203680000000	2.555141000000
H	3.200776000000	-1.824976000000	0.392137000000
C	1.745139000000	-1.858919000000	3.361124000000

H	-0.117131000000	-0.801531000000	2.787493000000
H	3.743367000000	-2.745548000000	2.863992000000
H	1.604709000000	-2.079383000000	4.407829000000
N	1.301443000000	-1.156883000000	-1.354726000000
C	2.518640000000	-1.024238000000	-2.001232000000
C	0.702937000000	-2.318161000000	-1.805211000000
C	2.668102000000	-2.075094000000	-2.856383000000
H	3.160699000000	-0.182975000000	-1.803921000000
C	1.518002000000	-2.899483000000	-2.728461000000
H	-0.250131000000	-2.633959000000	-1.414139000000
H	3.508129000000	-2.231052000000	-3.515581000000
H	1.309706000000	-3.812254000000	-3.264456000000

Mo(CO)₅PPhPyrI₂⁺

Mo	-1.646638000000	0.372036000000	-0.164172000000
C	-2.180802000000	-1.611618000000	-0.186809000000
O	-2.506232000000	-2.696716000000	-0.173035000000
C	-1.140482000000	2.356293000000	-0.017276000000
O	-0.895171000000	3.457197000000	0.084728000000
C	-3.571488000000	0.867526000000	-0.671126000000
O	-4.624658000000	1.131830000000	-0.985495000000
C	-1.364513000000	0.425026000000	-2.223237000000
O	-1.269488000000	0.493235000000	-3.346672000000
C	-2.330291000000	0.506614000000	1.809495000000
O	-2.809099000000	0.635937000000	2.824156000000
P	0.808970000000	-0.246893000000	-0.022487000000
C	2.053208000000	1.040216000000	0.138307000000
C	2.080338000000	2.046527000000	-0.829255000000
C	2.986382000000	1.045819000000	1.174713000000
C	3.037022000000	3.043399000000	-0.763328000000
H	1.364829000000	2.048357000000	-1.645112000000
C	3.933540000000	2.056025000000	1.240269000000
H	2.984022000000	0.263544000000	1.923665000000
C	3.959870000000	3.051261000000	0.274929000000
H	3.060874000000	3.817915000000	-1.520227000000
H	4.656376000000	2.060847000000	2.047230000000
H	4.702943000000	3.838025000000	0.329744000000
N	0.956605000000	-1.140954000000	1.444134000000
C	1.112690000000	-2.487864000000	1.568486000000
C	0.444022000000	-0.642750000000	2.644841000000
C	0.741467000000	-2.852217000000	2.847345000000
H	1.472515000000	-3.087595000000	0.747031000000
C	0.316490000000	-1.687431000000	3.520028000000
H	0.327347000000	0.418826000000	2.795891000000
H	0.803238000000	-3.849934000000	3.253671000000

H	-0.012137000000	-1.613924000000	4.544991000000
N	1.453096000000	-1.289467000000	-1.178809000000
C	2.810443000000	-1.515069000000	-1.393887000000
C	0.741021000000	-2.234435000000	-1.913219000000
C	2.937065000000	-2.562674000000	-2.249631000000
H	3.553635000000	-0.890040000000	-0.927892000000
C	1.628949000000	-3.018074000000	-2.578005000000
H	-0.334172000000	-2.260488000000	-1.894487000000
H	3.869877000000	-2.958181000000	-2.620551000000
H	1.374588000000	-3.827830000000	-3.244008000000

Mo(CO)₅PPyrl₃

Mo	1.716892000000	-0.027195000000	-0.000938000000
C	1.873607000000	1.945915000000	-0.527566000000
O	2.034079000000	3.025126000000	-0.850368000000
C	1.725380000000	-2.029317000000	0.392358000000
O	1.783836000000	-3.151087000000	0.584447000000
C	3.720569000000	-0.057649000000	0.163287000000
O	4.855555000000	-0.077714000000	0.271283000000
C	1.945258000000	-0.475678000000	-1.977861000000
O	2.148001000000	-0.711037000000	-3.074245000000
C	1.636903000000	0.461265000000	1.987816000000
O	1.637299000000	0.747790000000	3.088917000000
P	-0.767428000000	-0.004423000000	-0.035066000000
N	-1.548827000000	-0.444183000000	1.422515000000
C	-2.736813000000	0.076643000000	1.909950000000
C	-1.175161000000	-1.500996000000	2.234291000000
C	-3.093520000000	-0.636067000000	3.014293000000
H	-3.209603000000	0.918015000000	1.430606000000
C	-2.106800000000	-1.639322000000	3.217591000000
H	-0.283299000000	-2.069666000000	2.035176000000
H	-3.962963000000	-0.448525000000	3.625157000000
H	-2.079054000000	-2.373324000000	4.007803000000
N	-1.554902000000	1.483763000000	-0.343508000000
C	-2.709638000000	1.686713000000	-1.079736000000
C	-1.224720000000	2.670873000000	0.283292000000
C	-3.086997000000	2.987342000000	-0.927627000000
H	-3.146355000000	0.887651000000	-1.655570000000
C	-2.149723000000	3.610358000000	-0.059138000000
H	-0.368920000000	2.733861000000	0.935081000000
H	-3.938589000000	3.450437000000	-1.401523000000
H	-2.151035000000	4.638076000000	0.269034000000
N	-1.594238000000	-1.013978000000	-1.141471000000
C	-2.724585000000	-1.775311000000	-0.893812000000
C	-1.309112000000	-1.087862000000	-2.492640000000

C	-3.133341000000	-2.325068000000	-2.071370000000
H	-3.123046000000	-1.867342000000	0.102841000000
C	-2.240586000000	-1.885021000000	-3.086200000000
H	-0.479797000000	-0.549178000000	-2.917829000000
H	-3.976913000000	-2.986895000000	-2.191936000000
H	-2.274652000000	-2.134466000000	-4.135283000000

Mo(CO)₅PPyrl₃⁺

Mo	-1.681931000000	-0.048918000000	0.000000000000
C	-3.727676000000	0.018456000000	-0.000001000000
C	-1.750975000000	-0.002433000000	2.049175000000
C	-1.750974000000	-0.002440000000	-2.049176000000
C	-1.792122000000	-2.093859000000	0.000003000000
C	-1.683389000000	2.006402000000	-0.000004000000
O	-4.859003000000	0.055289000000	-0.000001000000
O	-1.695906000000	3.140431000000	-0.000005000000
O	-1.811595000000	0.045133000000	-3.182408000000
O	-1.869736000000	-3.228334000000	0.000006000000
O	-1.811597000000	0.045144000000	3.182408000000
P	0.717536000000	0.000323000000	0.000000000000
N	1.611181000000	-0.671185000000	1.322229000000
C	1.147336000000	-1.694187000000	2.109715000000
C	2.957061000000	-0.502980000000	1.602496000000
C	2.180440000000	-2.156870000000	2.902893000000
H	0.122126000000	-2.020730000000	2.049472000000
C	3.316305000000	-1.403423000000	2.586471000000
H	3.545752000000	0.257301000000	1.120961000000
H	2.100676000000	-2.947388000000	3.632537000000
H	4.298610000000	-1.487050000000	3.025358000000
N	1.611181000000	-0.671192000000	-1.322226000000
C	1.147336000000	-1.694197000000	-2.109707000000
C	2.957062000000	-0.502990000000	-1.602492000000
C	2.180440000000	-2.156885000000	-2.902882000000
H	0.122126000000	-2.020739000000	-2.049464000000
C	3.316305000000	-1.403437000000	-2.586463000000
H	3.545753000000	0.257294000000	-1.120961000000
H	2.100676000000	-2.947406000000	-3.632522000000
H	4.298611000000	-1.487067000000	-3.025349000000
N	1.501669000000	1.536215000000	-0.000004000000
C	1.741134000000	2.308258000000	1.116460000000
C	1.741135000000	2.308252000000	-1.116472000000
C	2.178421000000	3.547960000000	0.701901000000
H	1.561182000000	1.929833000000	2.109884000000
C	2.178422000000	3.547957000000	-0.701919000000
H	1.561185000000	1.929822000000	-2.109894000000

H	2.457637000000	4.360717000000	1.354001000000
H	2.457638000000	4.360710000000	-1.354022000000

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